San José State University

Math 251: Statistical and Machine Learning Classification

Bayes classifiers

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Outline

- A probabilistic model for classification
- Bayes classification rule
- Examples of Bayes classifiers
  - Discriminant Analysis: LDA, QDA
  - Naive Bayes: Gaussian, Bernoulli, Multinomial, Multivariate multinomial
- Assignment 3

Recall the statistical perspective of classifcation

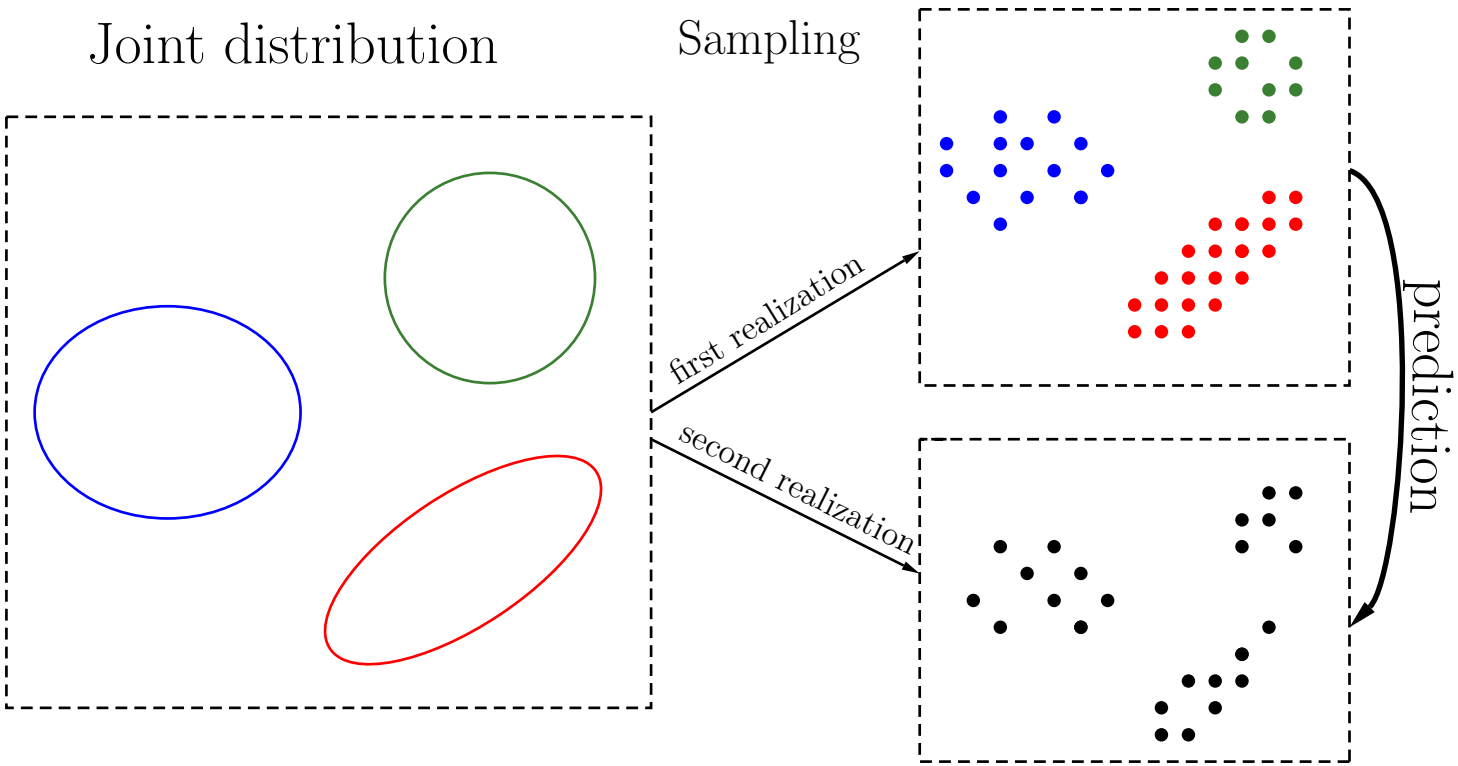
Let $\vec{X} \in \mathbb{R}^d, Y \in \mathbb{R}$ be two random variables representing the location and label of a data point to be observed. Suppose they have a joint distribution $f_{\vec{X},Y}$, and marginal distributions $f_{\vec{X}}$ (continuous) and f_Y (discrete).

The training data can be modeled by a random sample from the joint distribution:

$$(\vec{X}_1, Y_1), \ldots, (\vec{X}_n, Y_n) \overset{iid}{\sim} f_{\vec{X},Y}$$

The test data (without labels) is an independent sample from the marginal distribution of $\vec{X}$:

$$\vec{X}_{n+1}, \ldots, \vec{X}_{n+m} \overset{iid}{\sim} f_{\vec{X}}$$



The problem of classification is thus to predict the value of the label Y for each of the test point locations $\vec{X}_{n+j},\ 1 \leq j \leq m$.

How to classify a new sample naively

Let the range of Y be $\{1, 2, \ldots, c\}$, with probabilities

$$P(Y = j) = \pi_j, \quad 1 \leq j \leq c.$$

We call π_j a prior probability, i.e., the probability that a new point belongs to class j before it is seen (i.e., the value of $\vec{X}$ has not been observed).

A naive way would be to assign any new data point to the class with the largest prior probability

$$\hat{j} = \text{argmax}_j \ \pi_j$$

This method makes a constant prediction (i.e., the most frequent value of Y) with test error rate $1 - \pi_{\hat{j}}$.

We don't know the true values of π_j, so we'll estimate them using a random sample from the joint distribution:

$$(\vec{X}_1, Y_1), \ldots, (\vec{X}_n, Y_n) \overset{iid}{\sim} f_{\vec{X},Y}.$$

Let the count of the observations in the above sample that come from class j be

$$N_j = \sum_{i=1}^{n} I(Y_i = j), \quad 1 \le j \le c$$

Then

$$\mathrm{E}(N_j) = \sum_{i=1}^{n} \mathrm{E}[I(Y_i = j)] = \sum_{i=1}^{n} (1 \cdot \pi_j + 0 \cdot (1 - \pi_j)) = n\,\pi_j$$

This shows that N_j/n is an unbiased estimator of π_j.

When given a specific training data set:

$$(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n),$$

a point estimate of π_j is thus

$$\hat{\pi}_j = \frac{n_j}{n}, \quad \forall\, j = 1, \ldots, c$$

where n_j is the actual number of training points from C_j:

$$n_j = \sum_{i=1}^{n} I(y_i = j), \quad 1 \leq j \leq c$$

Bayes classification rule

Given a new data point $\mathbf{x}$, a better way is to assign the label based on the largest posterior probability:

$$\hat{j} = \text{argmax}_j \; P(Y = j \mid \vec{X} = \mathbf{x}) \longleftarrow \text{generic Bayes classifier}$$

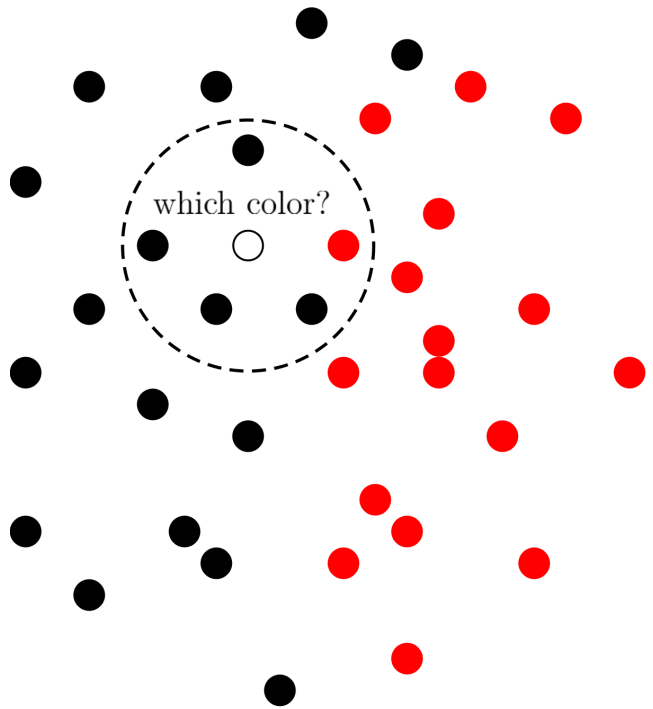
The Bayes classifier is optimal with **Bayes error rate**

$$1 - E_{\vec{X}} \left(\max_{1 \le j \le c} P(Y = j \mid \vec{X}) \right)$$

This is the lowest possible test error rate that may be achieved by a classifier.

Remark. Recall that kNN is also a Bayes classifier (but it is nonparametric):

$$P(Y = j \mid \vec{X} = \mathbf{x}) \approx \frac{\#\text{nearest neighbors from class } j}{\#\text{all nearest neighbors examined}}$$



Model-based Bayes classification

Suppose that for each $j = 1, \ldots, c$,

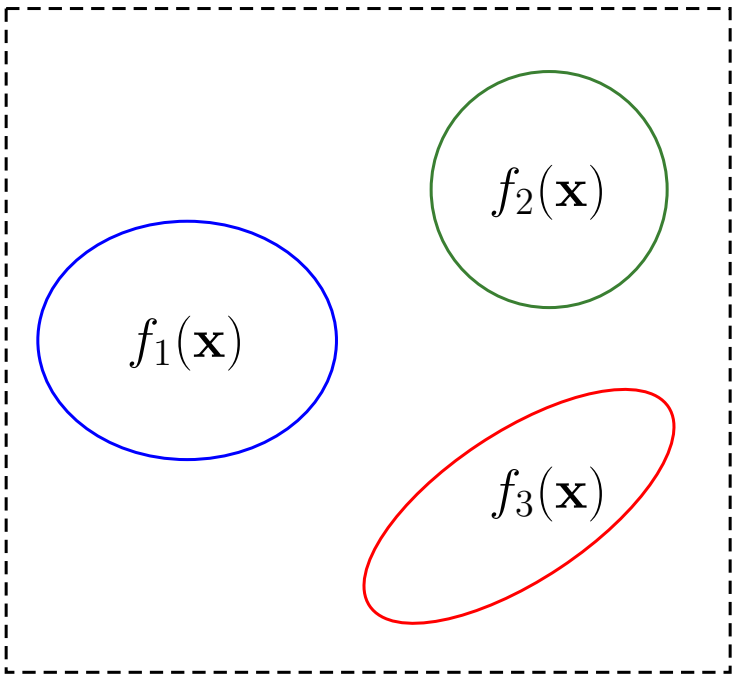
$$f(\mathbf{x} \mid Y = j) = f_j(\mathbf{x}).$$

The joint distribution of $\vec{X}$ and Y is

$$\begin{aligned} f_{\vec{X},Y}(\mathbf{x}, Y = j) &= f(\mathbf{x} \mid Y = j)\, P(Y = j) \\ &= f_j(\mathbf{x})\, \pi_j \end{aligned}$$

and the marginal density of $\vec{X}$ is

$$f_{\vec{X}}(\mathbf{x}) = \sum_j f_{\vec{X},Y}(\mathbf{x}, Y = j) = \sum_j \pi_j f_j(\mathbf{x})$$

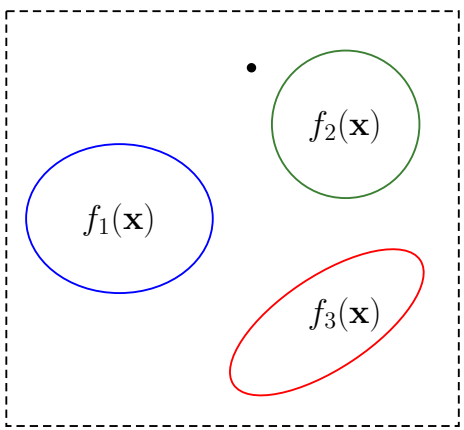


According to Bayes' rule, the posterior probabilities are given by

$$P(Y = j \mid \vec{X} = \mathbf{x}) = \frac{f(\mathbf{x} \mid Y = j) \cdot P(Y = j)}{f(\mathbf{x})} \propto f_j(\mathbf{x})\, \pi_j$$

Therefore, the Bayes classification rule can be stated as

$$\hat{j} = \text{argmax}_j \underbrace{f_j(\mathbf{x})}_{\text{likelihood}} \cdot \underbrace{\pi_j}_{\text{prior prob}} \longleftarrow \text{model-based Bayes classifier}$$



Estimating class-conditional probabilities $f_j(\mathbf{x})$

We need to select a template (i.e., model) for each component first.

Different kinds of $f_j(\mathbf{x})$ lead to different Bayes classifiers:

- **LDA/QDA** - multivariate Gaussian distributions

$$f_j(\mathbf{x}) = \frac{1}{(2\pi)^{d/2}|\mathbf{\Sigma}_j|^{1/2}} e^{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_j)^T \mathbf{\Sigma}_j^{-1}(\mathbf{x}-\boldsymbol{\mu}_j)}, \quad j = 1, \ldots, c$$

- **Naive Bayes** - by assuming independent features in $\mathbf{x} = (x_1, \ldots, x_d)$:

$$f_j(\mathbf{x}) = \prod_{k=1}^{d} f_{jk}(x_k) \longleftarrow \text{1D distributions to be specified}$$

What are multivariate Gaussians?

Briefly speaking, they are generalizations of the 1D Gaussian distribution

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

to higher dimensions:

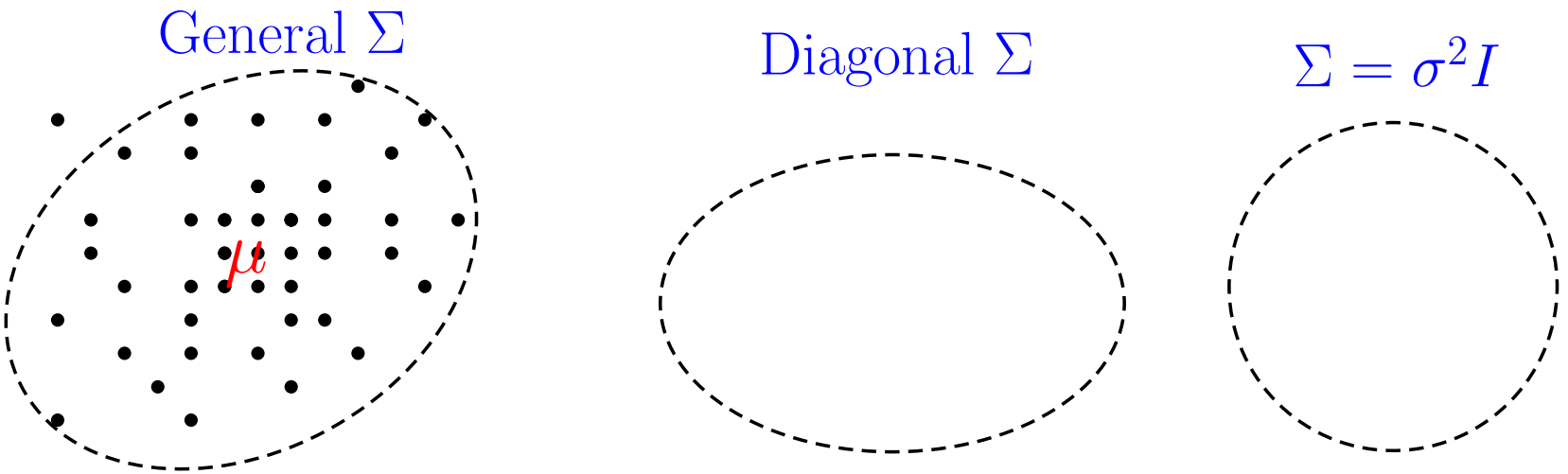
$$f(\mathbf{x}) = \frac{1}{(2\pi)^{d/2}|\mathbf{\Sigma}|^{1/2}} e^{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \mathbf{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})}, \quad \forall\ \mathbf{x} \in \mathbb{R}^d$$

Remark. If $\mathbf{\Sigma} = \sigma^2\mathbf{I}$ (i.e., constant diagonal), then the above formula reduces to

$$f(\mathbf{x}) = \frac{1}{(2\pi\sigma^2)^{d/2}} e^{-\frac{\|\mathbf{x}-\boldsymbol{\mu}\|^2}{2\sigma^2}}, \quad \forall\ \mathbf{x} \in \mathbb{R}^d$$

In the pdf of a multivariate Gaussian,

- $\boldsymbol{\mu} \in \mathbb{R}^d$: center of the distribution
- $\boldsymbol{\Sigma} \in \mathbb{R}^{d \times d}$: covariance matrix



The Bivariate normal ($d = 2$)

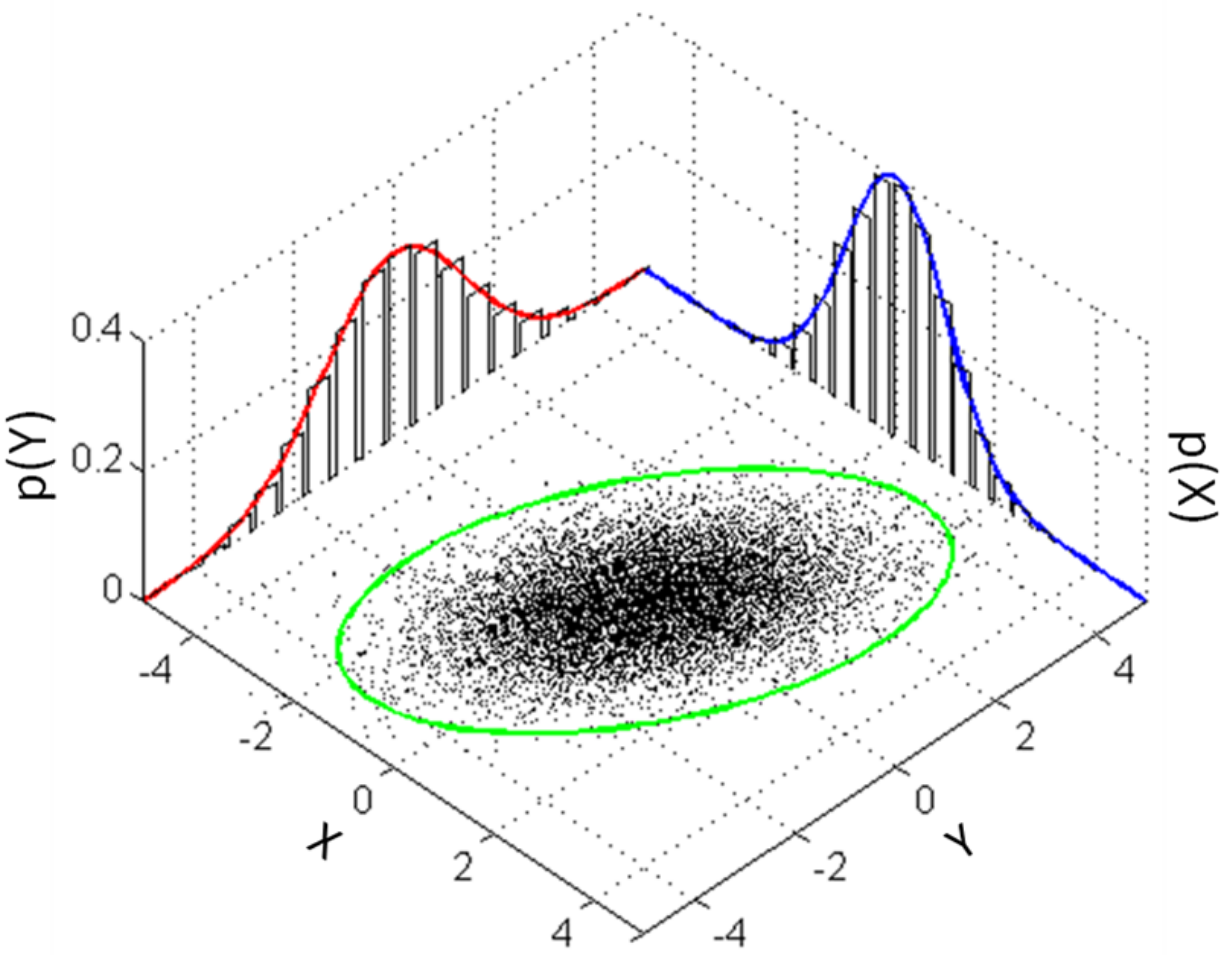
Write

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \quad \boldsymbol{\mu} = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \quad \boldsymbol{\Sigma} = \begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix}$$

The joint density is

$$f(x_1, x_2) = \frac{1}{2\pi\sigma_1\sigma_2\sqrt{1-\rho^2}} \cdot \exp\left(-\frac{1}{2(1-\rho^2)}\left[\frac{(x_1-\mu_1)^2}{\sigma_1^2} + \frac{(x_2-\mu_2)^2}{\sigma_2^2} - \frac{2\rho(x_1-\mu_1)(x_2-\mu_2)}{\sigma_1\sigma_2}\right]\right)$$

Marginals of the bivariate normal are 1D normal distributions: $\mathrm{N}(\mu_i, \sigma_i^2)$



Bayes classification with multivariate Gaussians

Under such a mixture of Gaussians model,

$$f_j(\mathbf{x}) = \frac{1}{(2\pi)^{d/2}|\mathbf{\Sigma}_j|^{1/2}} e^{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_j)^T \mathbf{\Sigma}_j^{-1}(\mathbf{x}-\boldsymbol{\mu}_j)}, \quad \forall\ j = 1, \ldots, c$$

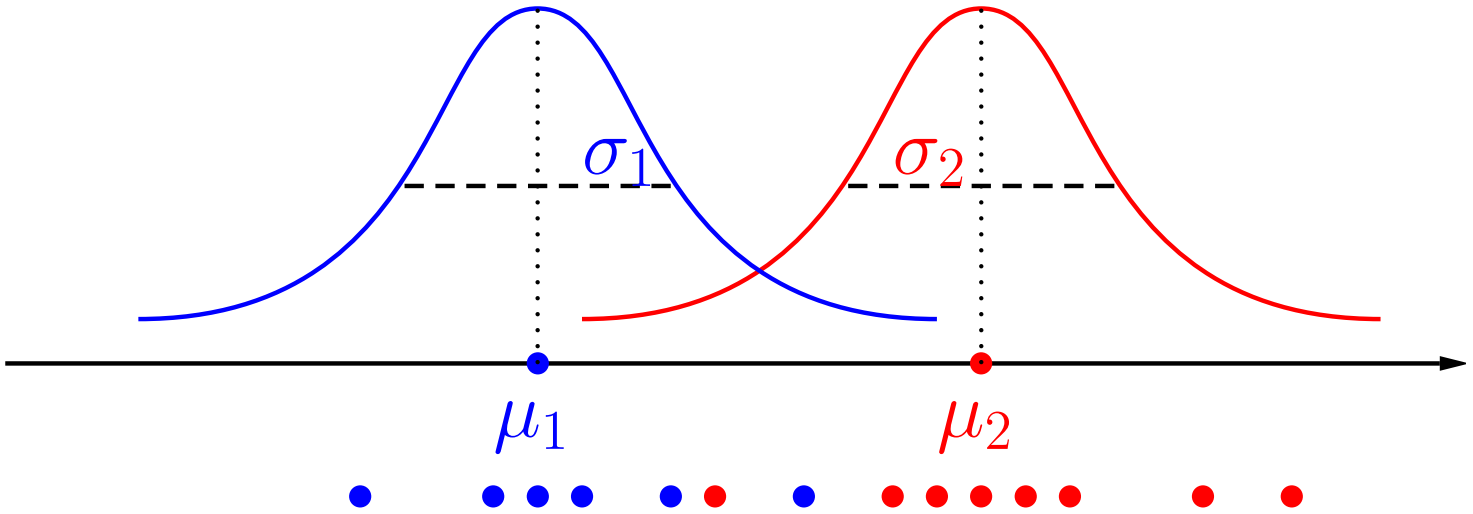
the Bayes classification rule (for a new data point $\mathbf{x}$)

$$\hat{j} = \text{argmax}_j\ f_j(\mathbf{x})\pi_j$$

becomes the following:

$$\begin{aligned}\hat{j} &= \text{argmax}_j\ \frac{1}{(2\pi)^{d/2}|\mathbf{\Sigma}_j|^{1/2}} e^{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_j)^T \mathbf{\Sigma}_j^{-1}(\mathbf{x}-\boldsymbol{\mu}_j)} \cdot \pi_j \\ &= \text{argmax}_j\ \log \pi_j - \frac{1}{2}\log|\mathbf{\Sigma}_j| - \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_j)^T \mathbf{\Sigma}_j^{-1}(\mathbf{x}-\boldsymbol{\mu}_j)\end{aligned}$$

Example 0.1. Let's consider the special case of two 1D Gaussians:



Suppose we know the true values of $\mu_1, \mu_2, \sigma_1, \sigma_2$. The corresponding Bayes decision rule is

$$\hat{j} = \text{argmax}_j \ \log \pi_j - \frac{1}{2}\log(\sigma_j^2) - \frac{(x-\mu_j)^2}{2\sigma_j^2}$$

Remark.

- If $\pi_1 = \pi_2$ and $\sigma_1 = \sigma_2$, then the rule will assign x to the closer mean μ_j (larger π_j will favor the class further).
- The boundary point can be found by solving the following (quadratic) equation

$$\log \pi_1 - \frac{1}{2}\log(\sigma_1^2) - \frac{(x-\mu_1)^2}{2\sigma_1^2} = \log \pi_2 - \frac{1}{2}\log(\sigma_2^2) - \frac{(x-\mu_2)^2}{2\sigma_2^2}$$

To simplify the math, we assume that the two components have equal variance (i.e., $\sigma_1 = \sigma_2 = \sigma$), in which case we obtain

$$x = \frac{\mu_1 + \mu_2}{2} + \frac{\sigma^2 \log(\pi_1/\pi_2)}{\mu_2 - \mu_1}$$

Quadratic Discriminant Analysis (QDA)

The decision boundary of a classifier consists of points that have a tie.

For the Bayes classification rule based on a mixture of Gaussians model, the decision boundaries are given by

$$\begin{aligned} &\log \pi_j - \frac{1}{2}\log|\mathbf{\Sigma}_j| - \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_j)^T\mathbf{\Sigma}_j^{-1}(\mathbf{x}-\boldsymbol{\mu}_j) \\ =&\log \pi_\ell - \frac{1}{2}\log|\mathbf{\Sigma}_\ell| - \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_\ell)^T\mathbf{\Sigma}_\ell^{-1}(\mathbf{x}-\boldsymbol{\mu}_\ell) \end{aligned}$$

This shows that such a Bayes classifier has quadratic boundaries (between each pair of training classes), and is thus called *Quadratic Discriminant Analysis (QDA)*.

Parameter estimation for QDA

The QDA classifier

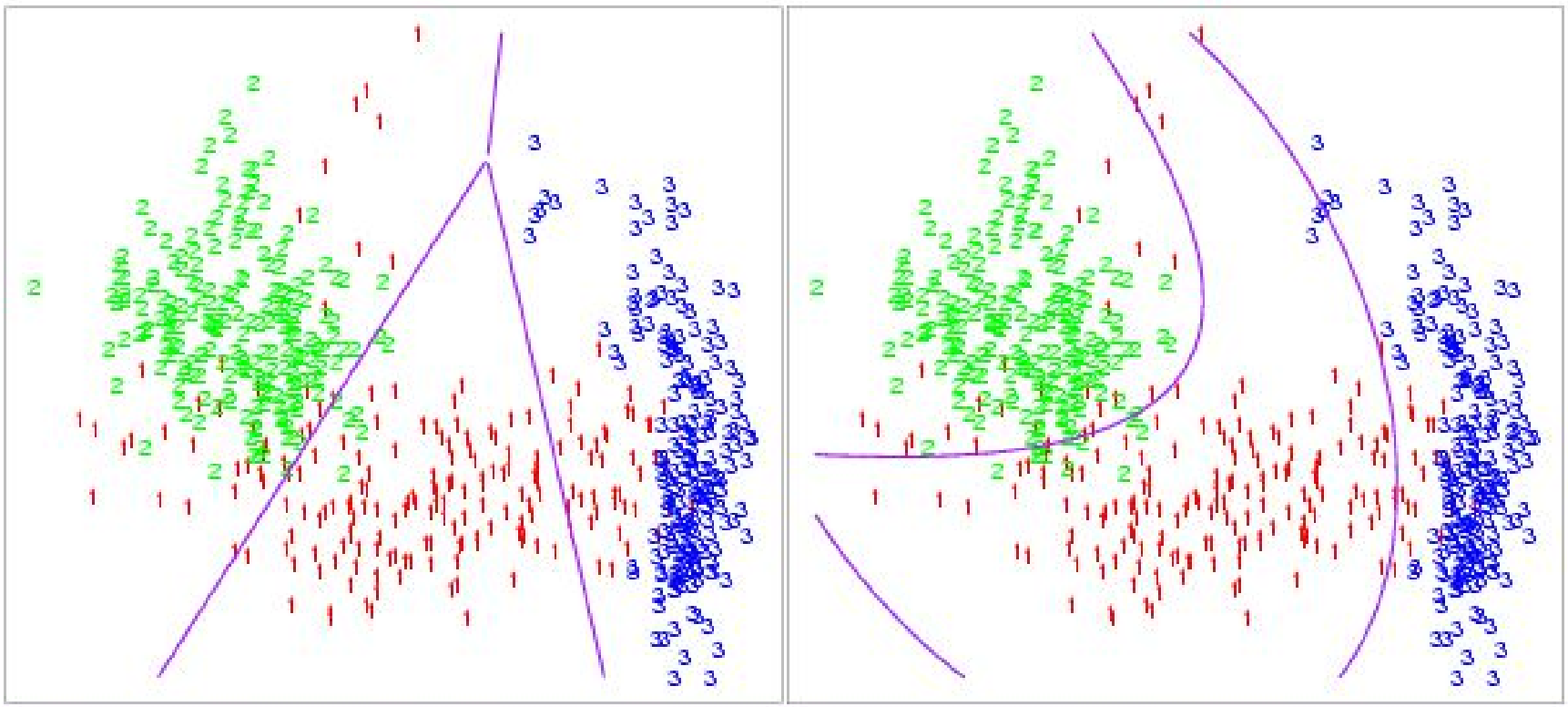
$$\hat{j} = \text{argmax}_j \ \log \pi_j - \frac{1}{2} \log |\boldsymbol{\Sigma}_j| - \frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_j)^T \boldsymbol{\Sigma}_j^{-1} (\mathbf{x} - \boldsymbol{\mu}_j)$$

depends on the model parameters $\pi_j, \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j$ but their true values are typically unknown.

Given training data, we estimate them as follows:

$$\hat{\pi}_j = \frac{n_j}{n}, \quad \hat{\boldsymbol{\mu}}_j = \frac{1}{n_j} \sum_{\mathbf{x} \in C_j} \mathbf{x}, \quad \hat{\boldsymbol{\Sigma}}_j = \frac{1}{n_j - 1} \sum_{\mathbf{x} \in C_j} (\mathbf{x} - \hat{\boldsymbol{\mu}}_j)(\mathbf{x} - \hat{\boldsymbol{\mu}}_j)^T$$

LDA (left) and QDA (right)



Linear Discriminant Analysis (LDA)

In QDA we assume that the component distributions are all multivariate Gaussians but allow them to have separate means $\boldsymbol{\mu}_j$ and covariances $\boldsymbol{\Sigma}_j$.

However, these are a lot of parameters to be estimated from the training data (especially when the dimension is large).

There is also a risk of overfitting the data.

To ease the computational burden, we assume that all the components have the same covariance

$$\boldsymbol{\Sigma}_1 = \cdots = \boldsymbol{\Sigma}_c = \boldsymbol{\Sigma}$$

In this special setting, the Bayes classification rule becomes

$$\begin{aligned}\hat{j} &= \text{argmax}_j \ \log \pi_j - \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_j)^T\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_j) \\ &= \text{argmax}_j \ \mathbf{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_j - \frac{1}{2}\boldsymbol{\mu}_j^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_j + \log \pi_j.\end{aligned}$$

The corresponding decision boundary is

$$\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_j - \frac{1}{2}\boldsymbol{\mu}_j^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_j + \log \pi_j = \mathbf{x}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_\ell - \frac{1}{2}\boldsymbol{\mu}_\ell^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_\ell + \log \pi_\ell$$

which simplifies to

$$\mathbf{x}^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_j - \boldsymbol{\mu}_\ell) = \frac{1}{2}\left(\boldsymbol{\mu}_j^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_j - \boldsymbol{\mu}_\ell^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_\ell\right) + \log\frac{\pi_\ell}{\pi_j}$$

This is a hyperplane with normal vector $\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_j - \boldsymbol{\mu}_\ell)$.

Parameter estimation for LDA

Similarly, we can use the training data to estimate the parameters $\pi_j, \boldsymbol{\mu}_j$ as follows:

$$\hat{\pi}_j = \frac{n_j}{n}, \quad \hat{\boldsymbol{\mu}}_j = \frac{1}{n_j} \sum_{\mathbf{x} \in C_j} \mathbf{x}$$

For the shared covariance matrix $\boldsymbol{\Sigma}$, we use the following pooled estimator:

$$\hat{\boldsymbol{\Sigma}} = \frac{1}{n-c} \sum_{j=1}^{c} \sum_{\mathbf{x} \in C_j} (\mathbf{x} - \hat{\boldsymbol{\mu}}_j)(\mathbf{x} - \hat{\boldsymbol{\mu}}_j)^T$$

This leads to the following practical LDA classifier:

$$\hat{j} = \text{argmax}_j \ \mathbf{x}^T \hat{\boldsymbol{\Sigma}}^{-1} \hat{\boldsymbol{\mu}}_j - \frac{1}{2} \hat{\boldsymbol{\mu}}_j^T \hat{\boldsymbol{\Sigma}}^{-1} \hat{\boldsymbol{\mu}}_j + \log \hat{\pi}_j.$$

When statistics meets optimization

We have introduced LDA both as a supervised dimensionality reduction method and as a Bayes classifier. This is not a conflict in name.

In the two-class setting,

- As a classifier, the LDA decision boundary is a hyperplane with normal vector $\hat{\boldsymbol{\Sigma}}^{-1}(\hat{\boldsymbol{\mu}}_1 - \hat{\boldsymbol{\mu}}_2)$.
- As a dimensionality reduction technique, LDA projects the data onto the following direction

$$\mathbf{v} = \mathbf{S}_w^{-1}(\mathbf{m}_1 - \mathbf{m}_2)$$

It turns out that the two vectors are the same:

$$\mathbf{S}_w = \sum_{j=1}^{2} \sum_{\mathbf{x} \in C_j} (\mathbf{x} - \mathbf{m}_j)(\mathbf{x} - \mathbf{m}_j)^T = (n-2)\hat{\mathbf{\Sigma}}$$

$$\mathbf{m}_1 = \hat{\boldsymbol{\mu}}_1$$

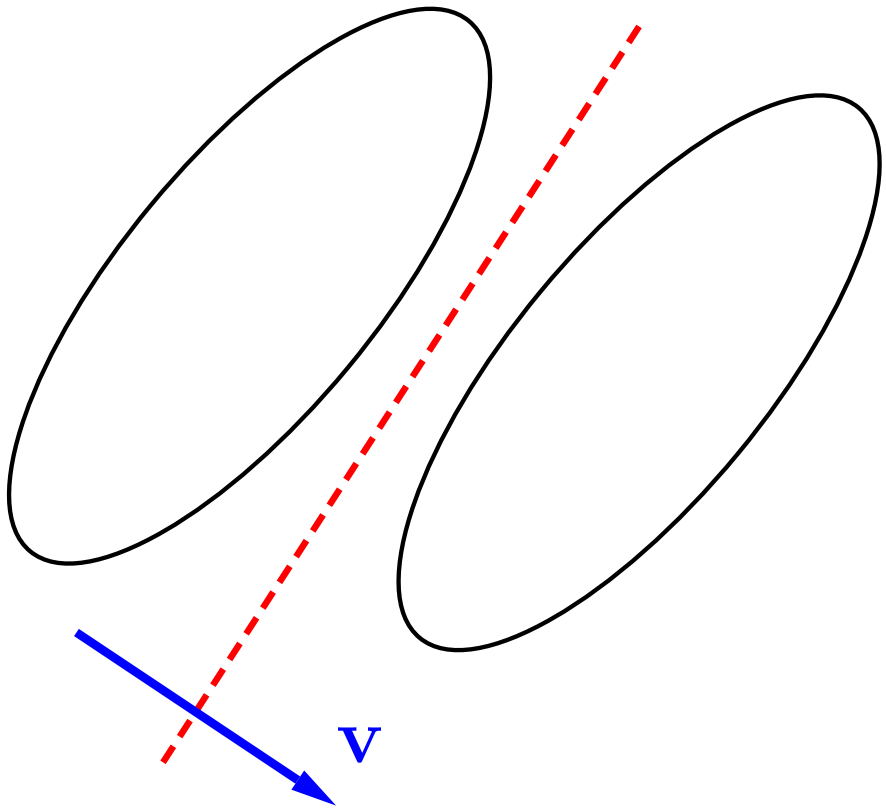
$$\mathbf{m}_2 = \hat{\boldsymbol{\mu}}_2$$

This shows that the two LDAs are indeed the same thing.

Therefore, we can combine both perspectives to fully understand LDA (see next slide).

Remark. LDA

- is a linear classifier (which classifies data using a hyperplane)
- uses a mixture of Gaussians model (with equal covariance)
- is a Bayes classifier
- projects data onto the most discriminative direction
- is also applicable to data from other distributions



MATLAB implementation of LDA/QDA

% fit a discriminant analysis classifier

mdl = fitcdiscr(trainData, trainLabels, 'DiscrimType', type)

% where **type** is one of the following:

- **'Linear'** (default): LDA
- **'Quadratic'**: QDA

% classify new data

pred = predict(mdl, testData)

Python scripts for LDA/QDA

```
from sklearn.discriminant_analysis import LinearDiscriminantAnalysis

#from sklearn.discriminant_analysis import QuadraticDiscriminant-
Analysis

lda = LinearDiscriminantAnalysis()

pred = lda.fit(trainData,trainLabels).predict(testData)

print("Number of mislabeled points: %d" %(testLabels != pred).sum())
```

The singularity issue in LDA/QDA

Both LDA and QDA require inverting covariance matrices, which may be (nearly) singular in the case of high dimensional data.

Common fixes:

- Apply PCA to reduce dimensionality first, or
- Regularize the covariance matrices, or
- Use psuedoinverse: 'pseudoLinear', 'pseudoQuadratic':

$$(\mathbf{S}_w)^\dagger = (\mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^T)^\dagger = \mathbf{Q}\mathbf{\Lambda}^\dagger\mathbf{Q}^T, \quad \mathbf{\Lambda}^\dagger_{ii} = \begin{cases} \frac{1}{\lambda} i, & \lambda_i > 0 \\ 0, & \lambda_i = 0 \end{cases}$$

LDA/QDA on the MNIST

See poster at

`https://www.sjsu.edu/faculty/guangliang.chen/Math285S16/poster-DA.pdf`

Naive Bayes

The naive Bayes classifier is also based on the Bayes decision rule:

$$\hat{j} = \text{argmax}_j \ f_j(\mathbf{x})\pi_j$$

Unlike Discriminant Analysis (LDA/QDA) which assumes that $\vec{X}$, when conditioned on $Y = j$, follows a multivariate Gaussian distribution $f_j(\mathbf{x})$, Naive Bayes assumes that the individual components of $\vec{X} = (X_1, \ldots X_d)$ are conditionally independent given a class $Y = j$:

$$f_j(\mathbf{x}) = f_{\vec{X}}(\mathbf{x} \mid Y = j) = \prod_{s=1}^{d} f_{X_s}(x_s \mid Y = j) = \prod_{s=1}^{d} f_{sj}(x_s).$$

This thus reduces the high dimensional density estimation problem ($\{f_j(\mathbf{x})\}_j$) to a union of simple 1D problems ($\{f_{sj}(x_s)\}_{j,s}$).

Depending on the data types and the corresponding models used for the component density functions $\{f_{sj}(x_s)\}_{j,s}$, the naive Bayes classifier has different versions:

- Continuous data: Gaussian naive Bayes
- Binary/Boolean data: Bernoulli naive Bayes
- Frequency/count data: Multinomial naive Bayes
- Categorical/discrete data: multivariate multinomial naive Bayes

Gaussian naive Bayes

For continuous features (e.g., image data), the standard choice for modeling $\{f_{sj}(x_s)\}_{j,s}$ is the 1D normal distribution:

$$f_{sj}(x_s) = \frac{1}{\sqrt{2\pi}\sigma_{sj}} e^{-(x_s-\mu_{sj})^2/2\sigma_{sj}^2}$$

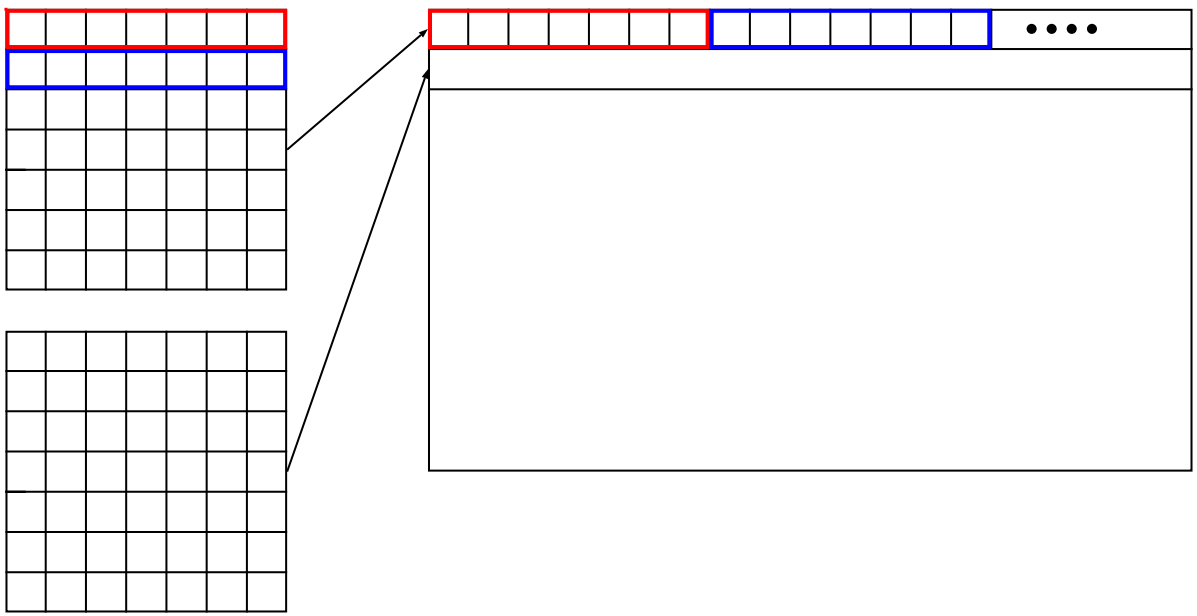
where μ_{sj}, σ_{sj} can be estimated similarly using the training data (in every class j and in every dimension s).

The resulting classification rule for a new data point $\mathbf{x} = (x_1, \ldots, x_d)'$ is

$$\hat{j} = \text{argmax}_j \ \log \hat{\pi}_j - \sum_{s=1}^{d} \left[\log \hat{\sigma}_{sj} + (x_s - \hat{\mu}_{sj})^2/2\hat{\sigma}_{sj}^2\right]$$

Gaussian naive Bayes can be used to classify digital images (such as the MNIST handwritten digits).

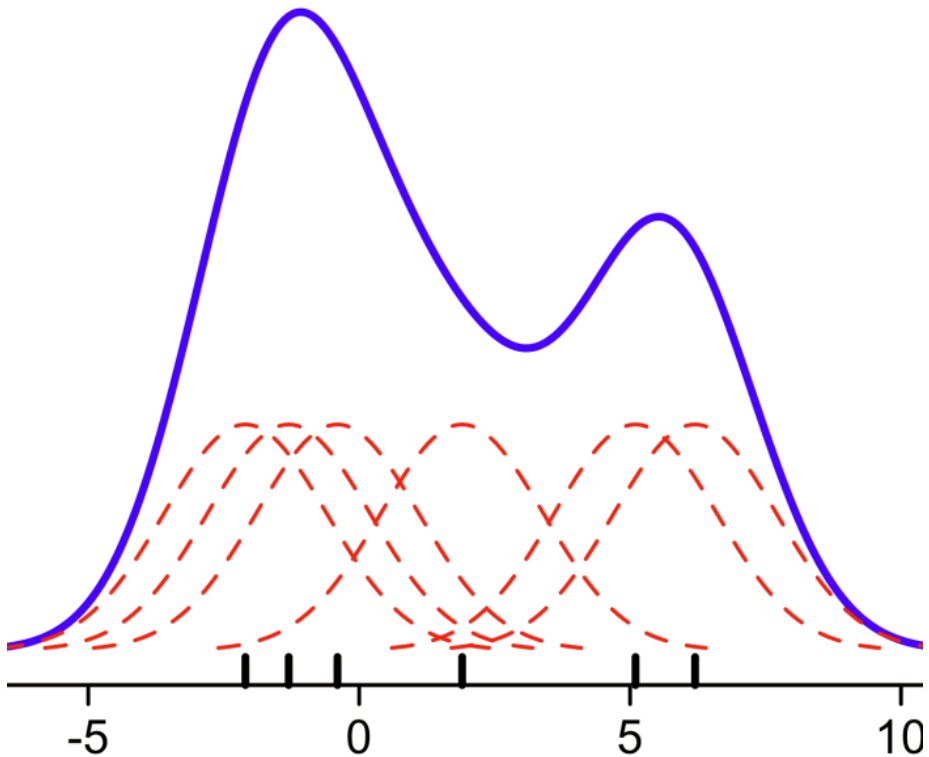
In this case, each pixel is a feature, and their intensities are assumed to be independent random variables.



Improving Gaussain naive Bayes

1. **Independence assumption**: Apply PCA to obtain uncorrelated features (closer to being independent) and meanwhile get rid of low-variance dimensions

2. **Choice of distribution**: Use kernel smoothing instead of Gaussian to better model feature distributions However, this will be at the expense of speed.



Bernoulli naive Bayes

For binary features (i.e., 0/1 valued), we can use the Bernoulli distribution to modeling them:

$$f_{sj}(x_s) = p_{sj}^{x_s}(1-p_{sj})^{1-x_s}, \quad x_s = 0, 1$$

where p_{sj} is the probability of X_s taking the value of 1 within class j. Similarly, it can be estimated using the training data.

The resulting classification rule for a new data point $\mathbf{x} = (x_1, \ldots, x_d)'$ is

$$\hat{j} = \text{argmax}_j \ \log \hat{\pi}_j + \sum_{s=1}^{d} [x_s \log \hat{p}_{sj} + (1-x_s)\log(1-\hat{p}_{sj})]$$

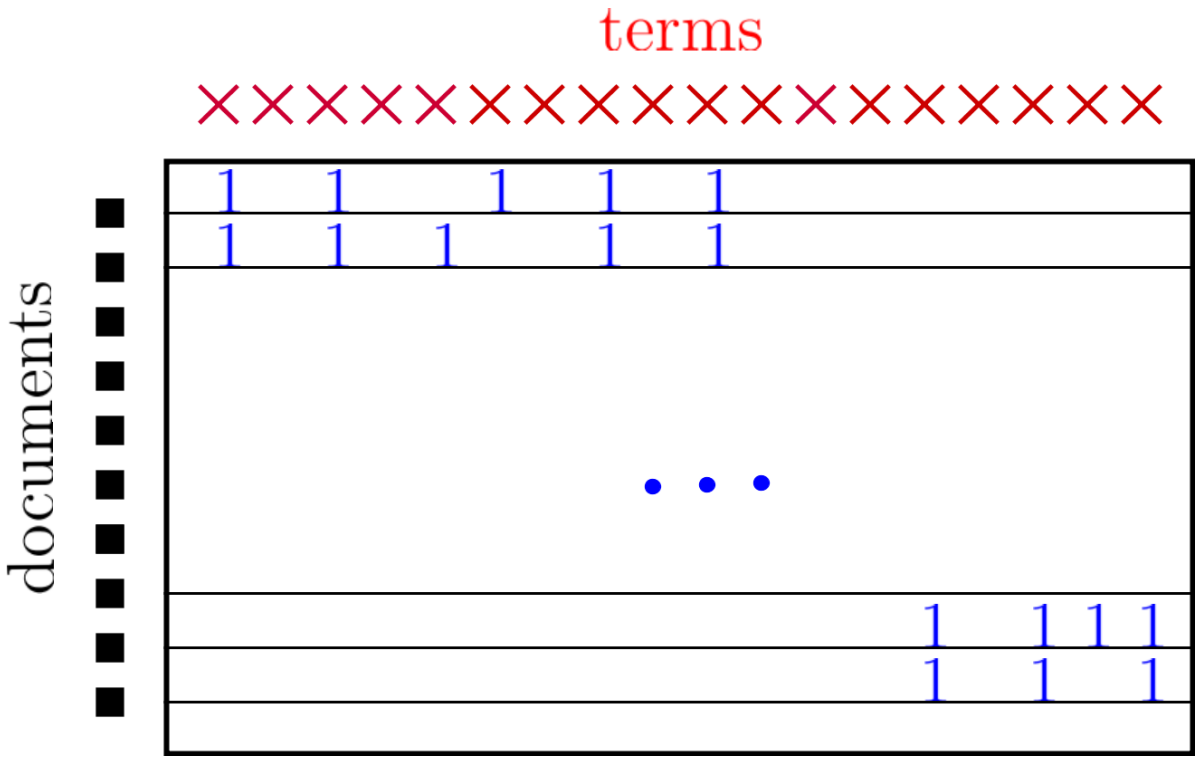
Remark. Bernoulli naive Bayes is a linear classifier, because for each j,

$$\begin{aligned}
&\log \hat{\pi}_j + \sum_{s=1}^{d} [x_s \log \hat{p}_{sj} + (1 - x_s) \log(1 - \hat{p}_{sj})] \\
=&\log \hat{\pi}_j + \sum_{s=1}^{d} \left[x_s \log \frac{\hat{p}_{sj}}{1 - \hat{p}_{sj}} + \log(1 - \hat{p}_{sj}) \right] \\
=&\mathbf{w}_j^T \cdot \mathbf{x} + b_j
\end{aligned}$$

where

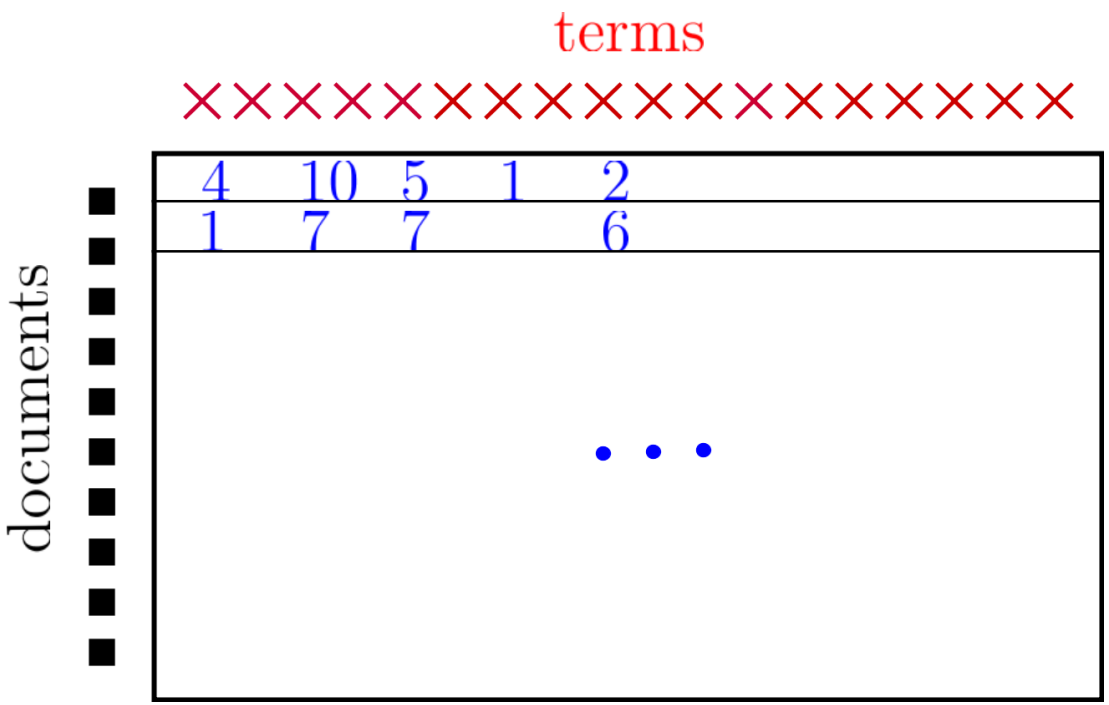
$$\mathbf{w}_j = \left(\log \frac{\hat{p}_{1j}}{1 - \hat{p}_{1j}}, \ldots, \log \frac{\hat{p}_{dj}}{1 - \hat{p}_{dj}} \right)^T, \quad b_j = \log \hat{\pi}_j + \sum_{s=1}^{d} \log(1 - \hat{p}_{sj})$$

Remark. Bernoulli naive Bayes is popular for document classification tasks where binary term occurrence features are used (1 if the term occurs in the document, 0 otherwise).



Multinomial naive Bayes

This Bayes classifier is very useful for modeling count data, such as the bag-of-words model for text documents.



To classify text documents, multinomial naive Bayes assumes that each document is a collection of frequency counts

$$\vec{X} = (X_1, X_2, \ldots, X_d)$$

of terms that are randomly and independently selected from a vocabulary of size d according to a multinomial distribution at the class level:

$$f_j(\mathbf{x}) = f_{\vec{X}|Y}(\mathbf{x} \mid Y = j) = \frac{(\sum x_s)!}{\prod x_s!} \prod_{s=1}^{d} p_{sj}^{x_s}, \quad \text{for all } x_1, \ldots, x_s \geq 0$$

where j is fixed and

$$p_{sj} \geq 0, \text{ for each } 1 \leq s \leq d, \qquad \text{and} \quad \sum p_{sj} = 1$$

are the probabilities of generating terms from a fixed topic.

It can be shown that the MLE of p_{sj} based on the jth training class is

$$\hat{p}_{sj} = \frac{\sum_{i=1}^{n_j} x_s^{(i)}}{\sum_{s=1}^{d}\sum_{i=1}^{n_j} x_s^{(i)}} \xrightarrow[\text{smoothing}]{\text{Laplace}} \frac{1+\sum_{i=1}^{n_j} x_s^{(i)}}{d+\sum_{s=1}^{d}\sum_{i=1}^{n_j} x_s^{(i)}}$$

where $x_s^{(i)}$ is the (observed) frequency of word s in the ith document of class j and

- $\sum_{i=1}^{n_j} x_s^{(i)}$: word count of sth term over all documents in class j
- $\sum_{s=1}^{d}\sum_{i=1}^{n_j} x_s^{(i)}$: total word count of class j

The resulting classification rule for a new data point $\mathbf{x} = (x_1, \ldots, x_d)'$ is

$$\begin{aligned}
\hat{j} &= \text{argmax}_j \ \hat{\pi}_j f_j(\mathbf{x}) \\
&= \text{argmax}_j \ \log \hat{\pi}_j + \sum_{s=1}^{d} x_s \log \hat{p}_{sj} \\
&= \text{argmax}_j \ \mathbf{w}_j^T \cdot \mathbf{x} + b_j
\end{aligned}$$

where

$$\mathbf{w}_j = (\log \hat{p}_{1j}, \ldots, \log \hat{p}_{dj})^T, \quad b_j = \log \hat{\pi}_j.$$

This shows that like Bernoulli naive Bayes, multinomial naive Bayes is also a linear classifier.

Comments on multinomial naive Bayes[1]

Overall, naive Bayes is not naive!

- Very fast, low storage requirements
- Robust to irrelevant features
- Very good in domains with many equally important features
- Optimal Bayes classifier if the independence assumptions hold
- A good dependable baseline for text classification

[1] https://web.stanford.edu/~jurafsky/slp3/slides/7_NB.pdf

Multivariate multinomial naive Bayes

For categorical features $\vec{X} = (X_1, \ldots, X_d)$, they are assumed to be independent. We then fit a joint model for them within each class.

Suppose X_s has L distinct levels, which occur in class j with probabilities

$$P(X_s = \ell \mid Y = j) = p_{sj}^{(\ell)}, \quad \ell = 1, \ldots, L$$

It can be shown that the MLE of $p_{sj}^{(\ell)}$ is the observed fraction of level ℓ of X_s in class j. Then for a data point $\mathbf{x} = (x_1, \ldots, x_d)'$, the decision rule is

$$\hat{j} = \text{argmax}_j \ \hat{\pi}_j \prod_{s=1}^{d} P(X_s = x_s \mid Y = j) = \text{argmax}_j \ \hat{\pi}_j \prod_{s=1}^{d} \hat{p}_{sj}^{(x_s)}$$

MATLAB function for naive Bayes

% fit a Gaussian naive Bayes classifier

mdl = fitcnb(trainData, trainLabels, 'DistributionNames', 'normal')

% fit a naive Bayes classifier with kernel smoothing

mdl = fitcnb(trainData, trainLabels, 'DistributionNames', 'kernel')

% fit a multinomial naive Bayes classifier

mdl = fitcnb(trainData, trainLabels, 'DistributionNames', 'mn')

% fit a multivaraite multinomial naive Bayes classifier

mdl = fitcnb(trainData, trainLabels, 'DistributionNames', 'mvmn')

% classify new data

pred = predict(mdl, testData)

Python scripts for naive Bayes

See

`https://scikit-learn.org/stable/modules/classes.html\#module-sklearn.naive_bayes`

Summary

- **Bayes decision rule**

$$\hat{j} = \text{argmax}_j \; P(Y = j \mid \mathbf{x})$$

- Examples of Bayes classifiers
  - **QDA**: multivariate Gaussians
  - **LDA**: multivariate Gaussians with equal covariance
  - **Naive Bayes**: independent features $x_1, \ldots, x_d$

Assignment 3

1. Use PCA with each value of $s = s_{\min}\ (80\%)\ :\ s_{\max}\ (95\%)$ to project the Fashion-MNIST data set (both training and test) into an s-dimensional space and then apply each of the following classifiers to classify the test data. Plot the test accurate rates for all the four methods as functions of s in one figure and discuss your results.
    - LDA
    - QDA
    - Gaussian Naive Bayes
    - Naive Bayes with kernel smoothing

2. Apply the multinomial naive Bayes classifier to the 20newsgroups data (bydate version) available at `http://qwone.com/~jason/20Newsgroups/`. Discuss your results.