

“Generative” models: Discriminant Analysis, Naïve Bayes

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Reminder on classification problem

Variable terminology

- ▶ observed data referred to as *input* variables, *predictors* or *features* ← usually denoted as x
- ▶ data to predict referred to as *output* variables, or *responses* ← usually denoted as y

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Classification task

y are *categorical* data (discrete qualitative variables) that take values in a discrete set \mathcal{Y} , e.g.

- ▶ $\text{email} \in \{\text{spam}, \text{ham}\},$
- ▶ $\text{handwritten digits} \in \{0, \dots, 9\}$

Given a feature vector $x \in \mathbb{R}^d$, build a function $f(x)$ that takes as input the feature vector x and predicts its value for $y \in \mathcal{Y}$

- 🔗 Try to minimize the **misclassification rate** $\mathcal{R}(f) = \mathbb{P}(f(x) \neq y)$ (aka expected risk for the 0 – 1 loss)

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Bayes rule for classification

Classification problem with K classes : $y \in \mathcal{Y} = \{1, \dots, K\}$.

Probability of class $y = k$ given $X = x$

Bayes rule :

$$\begin{aligned}\mathbb{P}(Y = k|X = x) &= \frac{\mathbb{P}(Y = k)p(x|Y = k)}{p(x)} = \frac{\mathbb{P}(Y = k)p(x|Y = k)}{\sum_{j=1}^K p(x|Y = j)\mathbb{P}(Y = j)}, \\ &= \frac{\pi_k p_k(x)}{\sum_{j=1}^K \pi_j p_j(x)}\end{aligned}$$

- ▶ $p_k(x) \equiv p(x|Y = k)$ is the *density* for X in class k
- ▶ $\pi_k \equiv p(Y = k)$ is the *weight*, or *prior* probability of class k

Bayes classifier

Definition

The Bayes classification rule f^* is defined as

$$f^*(x) = \arg \max_{k \in \mathcal{Y}} \mathbb{P}(Y = k | X = x) = \arg \max_{k \in \mathcal{Y}} \mathbb{P}(Y = k) p(x | Y = k).$$

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Theorem

The Bayes classification rule f^* is optimal in the misclassification rate sense where $\mathcal{R}(f) = \mathbb{P}(f(X) \neq Y)$:

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Remarks

- In practice, the distribution of (x, y) is unknown \Rightarrow no analytical expression of $f^*(x)$. But useful reference on academic examples.

Estimation of $f^*(X)$

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1. Discriminative approaches : direct learning of $\mathbb{P}(Y|X)$

- ▶ e.g. logistic regression : $\mathbb{P}(Y = k | x) \approx \text{sigmoid}_k(f(x)) = \frac{e^{f(x)_k}}{\sum_{\ell} e^{f(x)_{\ell}}}$ where f is a linear function, a neural net...
- ▶ Very powerful, but not very interpretable

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2. Generative models : learning of the joint distribution $p(X, Y)$

$$\mathbb{P}(X = x, Y = k) = p(x | Y = k) \mathbb{P}(Y = k),$$

- ▶ $p_k(x) = p(x | Y = k)$ is the data distribution of class k
- ▶ $\pi_k = \mathbb{P}(Y = k)$ is the weight (proportion) of class k
- ▶ linear/quadratic discriminant analysis, Naïve Bayes
- ▶ Interpretable, but requires good generative models (difficult)
- ▶ Can generate new data !

Maximum likelihood estimation (MLE)

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$$\mathcal{L}(\theta) = p_\theta((x_1, y_1), \dots, (x_n, y_n))$$

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- ▶ Products are complicated, hence one always work with the **log-likelihood** :

$$\ell(\theta) = \log \mathcal{L}(\theta) = \sum_i \log p_\theta(x_i, y_i) = \sum_i (\log \pi_{y_i} + \log p_{y_i}(x_i))$$

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- ▶ MLE is a classic, interpretable source of loss functions ! The log-likelihood is directly the empirical risk ! (up to $1/n$)

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Discriminant Analysis

Two kinds of Discriminant Analysis : **Linear** and **Quadratic**. In both cases, the key assumption is that, within each class, the input variables X_i are assumed to be **normally distributed**.

Supplementary materials

- ▶ Wikipedia page (quite complete and detailed)
https://en.wikipedia.org/wiki/Linear_discriminant_analysis
- ▶ short and simple Scikit-learn documentation (with examples)
https://scikit-learn.org/stable/modules/lda_qda.html

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Supervised classification assumptions

- ▶ $x \in \mathbb{R}^d$, $y \in \mathcal{Y} = \{1, \dots, K\}$,
- ▶ sized n training set $(x_1, y_1), \dots (x_n, y_n)$

QDA Assumptions

The input variables x , given a class $y = k$, are distributed according to a Gaussian distribution :

$$X|Y = k \sim \mathcal{N}(\mu_k, \Sigma_k) \Leftrightarrow p_k(x) = \frac{1}{(2\pi)^{p/2} |\Sigma_k|^{1/2}} e^{-\frac{1}{2}(x-\mu_k)^T \Sigma_k^{-1} (x-\mu_k)}$$

Quadratic Discriminant Analysis (QDA)

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The Gaussian parameters are, for each class $k = 1, \dots, K$

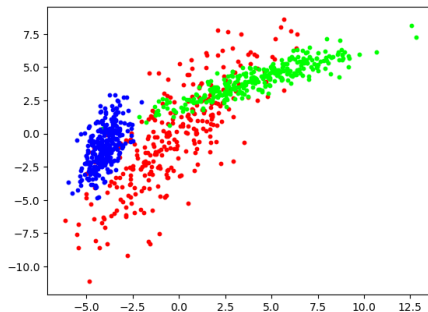
- ▶ mean vectors $\mu_k \in \mathbb{R}^d$,
- ▶ covariance matrices $\Sigma_k \in \mathbb{R}^{d \times d}$,
- ▶ set of parameters $\theta_k = \{\mu_k, \Sigma_k\}$, plus the weights π_k , for $k = 1, \dots, K$.

Example

Mixture of $K = 3$ Gaussians

► $\mathcal{Y} = \{1, 2, 3\}$

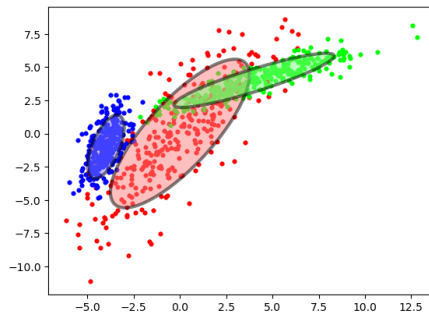
► $d = 2$



Example

Mixture of $K = 3$ Gaussians

- ▶ $\mathcal{Y} = \{1, 2, 3\}$
- ▶ $d = 2$



True mean μ_k and covariance Σ_k parameters, for $k = 1, 2, 3$

QDA parameter estimation

Log-likelihood

The log-likelihood with Gaussians is :

$$\begin{aligned}\ell(\theta) &= \sum_{i=1}^n \log \pi_{y_i} + \log p(x_i, \theta_{y_i}) \\ &= \sum_{i=1}^n \log \pi_{y_i} - \frac{1}{2} \log |\Sigma_{y_i}| - \frac{1}{2} (x_i - \mu_{y_i})^T \Sigma_{y_i}^{-1} (x_i - \mu_{y_i})\end{aligned}$$

Remark : $\pi_K = 1 - \sum_{j=1}^{K-1} \pi_j$ so there is one less parameter.

QDA parameter estimation (Cont'd)

Maximizing $\ell(\theta)$ by setting its gradient to 0, we obtain

- $\hat{\pi}_k = \frac{n_k}{n}$ where $n_k = \#\{y_i = k\}$. Sample proportion, valid for any model p_k .

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- ▶ $\hat{\pi}_k = \frac{n_k}{n}$ where $n_k = \#\{y_i = k\}$. Sample proportion, valid for any model p_k .
- ▶ $\hat{\mu}_k = \frac{\sum_{y_i=k} x_i}{n_k}$: empirical mean, a classic quantity. Easy derivation.

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► $\hat{\mu}_k = \frac{\sum_{y_i=k} x_i}{n_k}$: empirical mean, a classic quantity. Easy derivation.

► $\hat{\Sigma}_k = \frac{1}{n_k} \sum_{y_i=k} (x_i - \hat{\mu}_k)(x_i - \hat{\mu}_k)^T$. Empirical covariance, again classic.

Zeroing the gradient is a bit harder! hint : derive wrt Σ^{-1} and not Σ , use the chain rule.

► Unlike $\hat{\mu}$, $\hat{\Sigma}$ is **biased**. An unbiased version is

$$\frac{n_k}{n_k-1} \hat{\Sigma}_k = \frac{1}{n_k-1} \sum_{y_i=k} (x_i - \hat{\mu}_k)(x_i - \hat{\mu}_k)^T$$

see <https://people.eecs.berkeley.edu/~jordan/courses/260-spring10/other-readings/chapter13.pdf>

QDA decision rule

Since we have estimated $p(x, y)$, we can derive a classification rule. Starting from the expression of the Bayes estimator :

$$\begin{aligned} f(x) &= \arg \max_{k \in \mathcal{Y}} \mathbb{P}(Y = k) p(x|Y = k) \\ &\approx \arg \max_{k \in \mathcal{Y}} \hat{\pi}_k p(x|\hat{\theta}_k) = \arg \max_{k \in \mathcal{Y}} \hat{\pi}_k p(x|\hat{\theta}_k) \end{aligned}$$

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Taking the logarithm, which does not change the argmax : $f(x) = \arg \max_k \delta_k(x)$ where

$$\delta_k(x) = -\frac{1}{2} \log |\hat{\Sigma}_k| - \frac{1}{2} (x - \hat{\mu}_k)^T \hat{\Sigma}_k^{-1} (x - \hat{\mu}_k) + \log \hat{\pi}_k + \text{const},$$

is the **discriminant function**

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Remarks

If the Gaussian model is correct :

1. this is an estimation of the Bayes classifier with θ replaced by $\hat{\theta}$ (and π replaced by $\hat{\pi}$)
2. when $n \gg d$, $\hat{\theta} \rightarrow \theta$ (and $\hat{\pi} \rightarrow \pi$) : convergence to the Bayes classifier

QDA decision boundary

The boundary between two classes k and l is described by the equation

$$\delta_k(x) = \delta_l(x) \Leftrightarrow C_{k,l} + L_{k,l}^T x + x^T Q_{k,l}^T x = 0,$$

where

- ▶ $C_{k,l} = -\frac{1}{2} \log \frac{|\hat{\Sigma}_k|}{|\hat{\Sigma}_l|} + \log \frac{\hat{\pi}_k}{\hat{\pi}_l} - \frac{1}{2} \hat{\mu}_k^T \hat{\Sigma}_k^{-1} \hat{\mu}_k + \frac{1}{2} \hat{\mu}_l^T \hat{\Sigma}_l^{-1} \hat{\mu}_l, \quad \leftarrow \text{scalar}$
- ▶ $L_{k,l} = \hat{\Sigma}_k^{-1} \hat{\mu}_k - \hat{\Sigma}_l^{-1} \hat{\mu}_l, \quad \leftarrow \text{vector in } \mathbb{R}^d$
- ▶ $Q_{k,l} = \frac{1}{2} \left(-\hat{\Sigma}_k^{-1} + \hat{\Sigma}_l^{-1} \right), \quad \leftarrow \text{matrix in } \mathbb{R}^{d \times d}$

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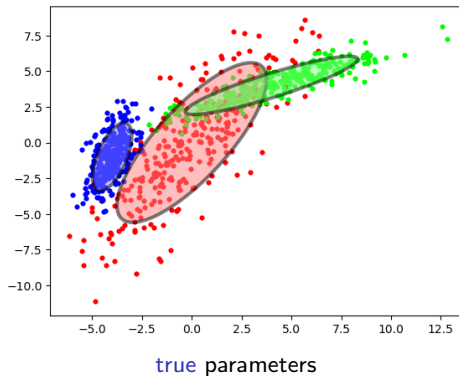
► This is a **quadratic equation**, which defines an ellipsoid

👉 hence **Quadratic discriminant analysis**

QDA example

Mixture of $K = 3$ Gaussians

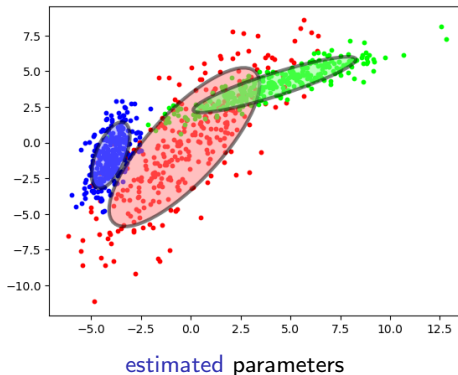
- Estimation of the parameters $\hat{\mu}_k$, $\hat{\Sigma}_k$ and $\hat{\pi}_k$, for $k = 1, 2, 3$



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QDA example

Mixture of $K = 3$ Gaussians

- ▶ Classification rule : $\arg \max_{k=1,2,3} \delta_k(x)$
- ▶ Quadratic boundaries $\{x; \delta_k(x) = \delta_l(x)\}$

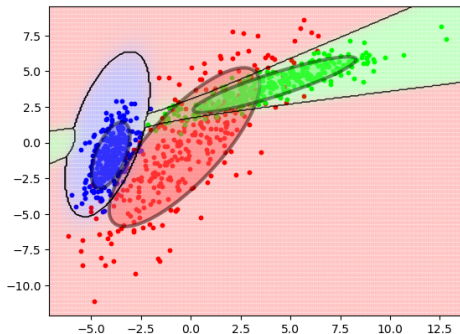


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LDA principle

LDA Assumptions

Additional simplifying assumption w.r.t. QDA : all the class covariance matrices are identical ("homoscedasticity"), i.e. $\Sigma_k = \Sigma$, for $k = 1, \dots, K$

Maximum likelihood estimators (MLE)

- ▶ $\hat{\pi}_k$ and $\hat{\mu}_k$ are unchanged,
- ▶ $\hat{\Sigma} = \frac{1}{n} \sum_{k=1}^K \sum_{y_i=k} (x_i - \hat{\mu}_k)(x_i - \hat{\mu}_k)^T$ pooled covariance
 - ▶ Again, this is a biased estimator. The unbiased version is $\frac{n}{n-K} \hat{\Sigma}$.

LDA discriminant function

$$\delta_k(x) = -\frac{1}{2} \log |\hat{\Sigma}| - \frac{1}{2} (x - \hat{\mu}_k)^T \hat{\Sigma}^{-1} (x - \hat{\mu}_k) + \log \hat{\pi}_k + \text{Cst},$$

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The boundary between two classes k and l reduces to the equation

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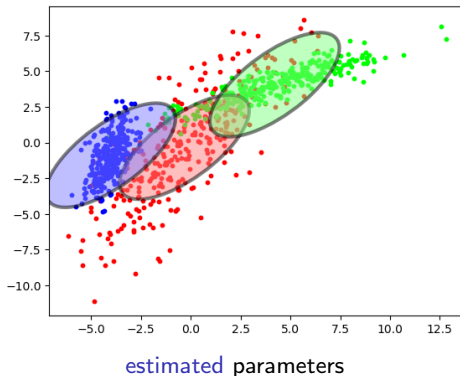
▶ This is a linear equation

🔗 Linear discriminant analysis

Linear Discriminant Analysis (LDA)

Mixture of $K = 3$ Gaussians

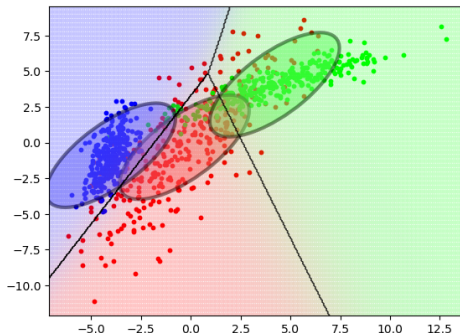
- Estimation of the parameters $\hat{\mu}_k$, $\hat{\pi}_k$, for $k = 1, 2, 3$, and $\hat{\Sigma}$



Linear Discriminant Analysis (LDA)

Mixture of $K = 3$ Gaussians

- ▶ Classification rule : $\arg \max_{k=1,2,3} \delta_k(x)$
- ▶ linear boundaries $\{x; \delta_k(x) = \delta_l(x)\}$



Complexity of discriminant analysis methods

Effective number of parameters

- ▶ LDA : $K - 1 + Kd + \frac{d(d+1)}{2} = O(Kd + d^2)$
- ▶ QDA : $K - 1 + Kd + K\frac{d(d+1)}{2} = O(Kd^2)$

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Remarks

- ▶ in high dimension, i.e. $d \approx n$ or $d > n$, LDA is more stable than QDA which is more prone to overfitting,
- ▶ both methods appear however to be robust on a large number of real-world datasets
- ▶ LDA can be viewed in some cases as a least squares regression method
- ▶ LDA performs a dimension reduction to a subspace of dimension $\leq K - 1$ generated by the vectors $z_k = \hat{\Sigma}^{-1} \hat{\mu}_k \leftarrow$ dimension reduction from p to $K - 1$! (same for QDA, but more rarely used)

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Non-parametric modelling

Non-parametric estimation of $p_k(x) = p(x|Y = k)$: **density estimation**. Then $f(\hat{x}) = \arg \max_k \hat{\pi}_k \hat{p}_k(x)$ as usual.

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Parzen kernel approach

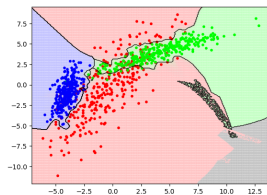
To locally estimate the density, take a **weighted average** of the number of points in the neighborhood of the desired location :

$$\hat{p}_k(x) = \frac{1}{n_k} \sum_{y_i=k} k_\lambda(x, x_i)$$

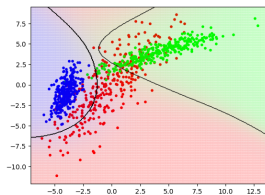
for a **kernel function** k_λ . Usually λ is a **bandwidth**, and $k_\lambda(x, x') = \frac{1}{\lambda^d} k(\frac{x-x'}{\lambda})$, with $\int k = 1$. Classic choice includes :

- ▶ **0-1 kernel** : $k(x, x') = 1/V_d$ if $\|x - x'\| \leq 1$, 0 otherwise, where V_d is the volume of the d -sphere. **True unweighted average** of the number of points in a fixed-radius neighborhood.
- ▶ **Gaussian kernel** : $k(x, x') = \frac{1}{(2\pi)^{d/2}} e^{-\frac{1}{2}\|x-x'\|^2}$. Classic choice.
- ▶ Same problem than k -NN : in high-dimension, the space is mostly empty !

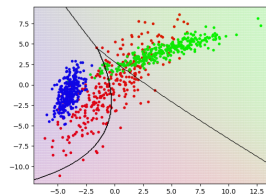
KDE example



$\lambda = 0.25$



$\lambda = 2$



$\lambda = 5$

Complexity parameter λ (kernel bandwidth)

- ▶ large λ w.r.t. to the dispersion of $X \rightarrow$ under-fitting
- ▶ small λ w.r.t. to the dispersion of $X \rightarrow$ over-fitting

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Naïve Bayes (NB)

NB classifiers

Family of "probabilistic classifiers" based on applying Bayes' theorem on a generative model, with **strong (naïve) independence assumptions between the features**. Particularly useful for **high-dimensional data** (avoids quadratic cost d^2).

Naïve Bayes (NB)

NB classifiers

Family of "probabilistic classifiers" based on applying Bayes' theorem on a generative model, with **strong (naïve) independence assumptions between the features**. Particularly useful for high-dimensional data (avoids quadratic cost d^2).

Can be coupled with

- ▶ parametric models (Gaussian, Bernoulli, Multinomial,...) with maximum likelihood estimation
- ▶ or non-parametric models with kernel density estimation

Supplementary materials

- ▶ Wikipedia page (quite detailed)
https://en.wikipedia.org/wiki/Naive_Bayes_classifier
- ▶ short and simple Scikit-learn documentation
https://scikit-learn.org/stable/modules/naive_bayes.html

Naïve Bayes (NB)

► $x = (x^1, \dots, x^d) \in \mathbb{R}^d$, $y \in \mathcal{Y} = \{1, \dots, K\}$

Naive Bayes Assumption

Simplifying assumption : given Y , the components x^1, \dots, x^d are assumed to be independent :

$$p(x|Y = k) = p_k(x) = \prod_{j=1}^d p_{k,j}(x^j).$$

Naïve Bayes (NB)

► $x = (x^1, \dots, x^d) \in \mathbb{R}^d$, $y \in \mathcal{Y} = \{1, \dots, K\}$

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Remarks

- independence reduces one estimation problem in d dimensions to d much simpler 1D estimation problems ← prevent from curse of dimensionality
- independence assumption is naïve, i.e. not realistic in practice... but yields efficient/stable/robust approaches especially in high dimension !

Naïve Bayes for parametric estimation

Gaussian model

- ▶ NB + QDA : $X|Y = k \sim \mathcal{N}(\mu_k, \Sigma_k)$, where the Σ_k are diagonal
 - ▶ $\hat{\mu}_k$ don't change
 - ▶ $(\hat{\Sigma}_k)_{jj} = \frac{1}{n_k - 1} \sum_{y_i=k} (x_i^j - \mu_k^j)^2$
- ▶ NB + LDA : $X|Y = k \sim \mathcal{N}(\mu_k, \Sigma)$, where Σ is diagonal.
 - ▶ $\hat{\Sigma}_{jj} = \frac{1}{n - K} \sum_k \sum_{y_i=k} (x_i^j - \mu_k^j)^2$

Naïve Bayes for parametric estimation

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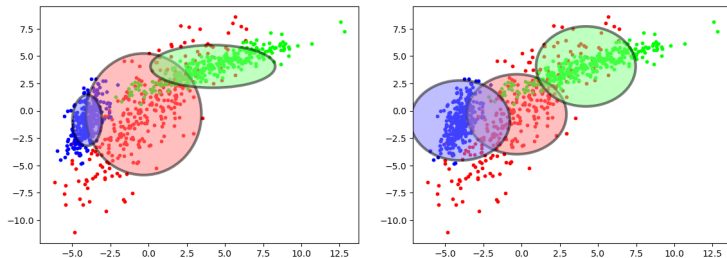
Other classical parametric models

- ▶ Bernoulli NB for binary events models (e.g., word occurrence vectors in text processing)
- ▶ Multinomial NB for multiple events models (e.g., word count vectors in text processing)
- ▶ Mixed models (e.g. Gaussian and Multinomial) for mixed quantitative/qualitative features
- ▶ ...

NB + QDA example

Mixture of $K = 3$ Gaussians

- Gaussian model : $X|Y = k \sim \mathcal{N}(\mu_k, \Sigma_k)$ with $\hat{\Sigma}_k = \begin{pmatrix} (\hat{\Sigma}_k)_{11} & 0 \\ 0 & (\hat{\Sigma}_k)_{22} \end{pmatrix}$

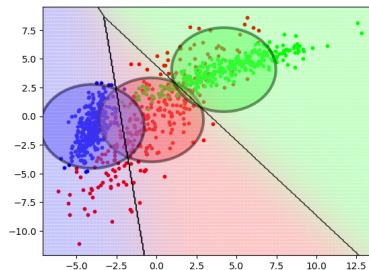
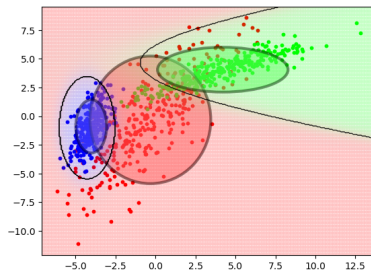


Naive Bayes QDA (left), LDA (right). The Gaussians are “axis-aligned”

Naïve Bayes (NB)

Mixture of $K = 3$ Gaussians

- Classification rule : $\arg \max_{k=1,2,3} \delta_k(x)$
- quadratic boundaries $\{x; \delta_k(x) = \delta_l(x)\}$



Naïve Bayes for non-parametric estimation

Non-parametric estimation of $p_{k,j}(x^j) = p(x^j | Y = k)$, where x^j is the j th component of x : **univariate** density estimation. Then $\hat{p}_k(x) = \prod_j p_{k,j}(x^j)$, and $\hat{f}(x) = \arg \max_k \hat{\pi}_k$.

Parzen kernel approach

Apply Parzen window to each component, with a univariate kernel (not necessarily the same for each component) :

$$\hat{p}_{k,j}(x^j) = \frac{1}{n_k \lambda} \sum_{y_i=k} k^j \left(\frac{x_j - x_{j,i}}{\lambda} \right)$$

- ▶ Avoids the curse of dimensionality, to the price of simplification
- ▶ Note : when $n \rightarrow \infty$, regular KDE with classic Gaussian kernel is already **Naïve Bayes** ! Since $\frac{1}{(2\pi)^{d/2}} e^{-\|x-x_i\|^2} = \prod_j \frac{1}{\sqrt{2\pi}} e^{-(x^j-x_i^j)^2}$. The only difference is how we compute their empirical versions.

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Generative models

- ▶ learning/estimation of $p(X, Y) = p(X|Y) \Pr(Y)$,
- ▶ derivation of $\Pr(Y|X)$ from Bayes rule,

Different assumptions on the class densities $p_k(x) = p(X = x|Y = k)$

- ▶ QDA/LDA : Gaussian parametric model
 - ▶ performs well on many real-word datasets
 - ▶ LDA is especially useful when n is small
- ▶ Parzen window (aka KDE) : non-parametric
 - ▶ more flexible, necessitates a lot of data, poor performance in high-dimension
- ▶ Naive Bayes : independence of the feature X components given Y
 - ▶ useful when d is very large (high dimension)

Incoming...

Discriminative approaches : direct learning of $\Pr(Y|X)$