Data Classification: model based approaches, discriminant analysis

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Florent Chatelain * Olivier Michel *

*Univ. Grenoble Alpes, GIPSA-lab

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Classification problem

Variable terminology

- observed data referred to as *input* variables, *predictors* or *features* $\leftarrow$ usually denoted as X
- data to predict referred to as *output* variables, or *responses* $\leftarrow$ usually denoted as Y

Classification task

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

- $\texttt{email} \in \{\texttt{spam}, \texttt{ham}\}$,
- $\texttt{handwritten digits} \in \{0, \ldots, 9\}$

Given a feature vector $X \in \mathbb{R}^p$, 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 $\mathcal{E}[f] \equiv \Pr(f(X) \neq Y)$

Bayes rule for classification

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

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

Bayes rule :

$$p(Y = k|X = x) = \frac{p(Y = k)p(x|Y = k)}{p(x)} = \frac{p(Y = k)p(x|Y = k)}{\sum_{j=1}^{K} p(x|Y = j)p(Y = j)},$$

$$= \frac{\pi_k\, p_k(x)}{\sum_{j=1}^{K} \pi_j\, p_j(x)}$$

- $p_k(x) \equiv p(x|Y = k)$ 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

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

Theorem

The Bayes classification rule f^* is optimal in the misclassification rate sense where $\mathcal{E}[f] = p(f(X) \neq Y)$:

$$\text{for any rule } f, \ \mathcal{E}[f] \geq \mathcal{E}[f^*],$$

Remarks

- In real-word applications, the distribution of (X, Y) is unknown $\Rightarrow$ no analytical expression of $f^*(X)$. But useful reference on academic examples.

Estimation of $f^*(X)$

Two kinds of approaches based on a model :

1. **Discriminative approaches** : direct learning of $p(Y|X)$,
   e.g. logistic regression
2. **Generative models** : learning of the joint distribution $p(X, Y)$

$$p(X, Y) = \underbrace{p(X|Y)}_{\text{likelihood}} \underbrace{\Pr(Y)}_{\text{prior}},$$

   e.g. linear/quadratic discriminant analysis, Naïve Bayes

Generative models : Estimation problem

Assumptions

- classification problem with K classes : $Y \in \mathcal{Y} = \{1, \ldots, K\}$,
- input variables : $X \in \mathbb{R}^p$

Bayes rule :

$$p(Y = k|X = x) = \frac{p(x|Y = k)p(Y = k)}{\sum_{j=1}^{K} p(x|Y = j)p(Y = j)}.$$

In practice, the following quantities are unknown :

- densities of each class $p_k(x) \equiv p(x|Y = k)$
- weights, or prior probabilities, of each class $\pi_k \equiv p(Y = k)$

Estimation problem

These quantities must be learned on a training set :

learning problem $\Leftrightarrow$ estimation problem in a parametric/non-parametric way

Discriminant Analysis

Two kinds of Discriminant Analysis :

- Linear Discriminant Analysis
- Quadratic Discriminant Analysis

In both cases, the key assumption is that, within each class, the input variables X_i are assumed to be normally distributed.

Supplementary materials

- short (12mn) Sidney Univ. online video
  https://www.youtube.com/watch?time_continue=719&v=D4C7YbfFQSk&feature=emb_logo
- 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

Quadratic Discriminant Analysis (QDA)

Supervised classification assumptions

- $X \in \mathbb{R}^p$, $Y \in \mathcal{Y} = \{1, \ldots, K\}$,
- sized n training set $(X_1, Y_1), \ldots (X_n, Y_n)$

QDA Assumptions

The input variables X, given a class $Y = k$, are distributed according to a parametric and Gaussian distribution :

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

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

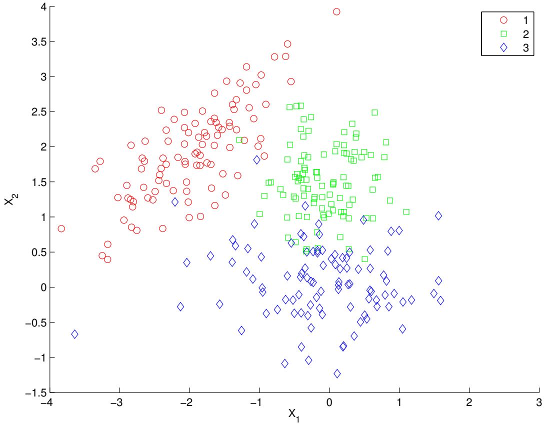
- mean vectors $\mu_k \in \mathbb{R}^p$,
- covariance matrices $\Sigma_k \in \mathbb{R}^{p \times p}$,

☞ set of parameters $\theta_k \equiv \{\mu_k, \Sigma_k\}$, plus the weights π_k, for $k = 1, \ldots, K$.

Example

Mixture of $K = 3$ Gaussians

- $Y \in \{1, 2, 3\}$
- $X \in \mathbb{R}^2$



Example

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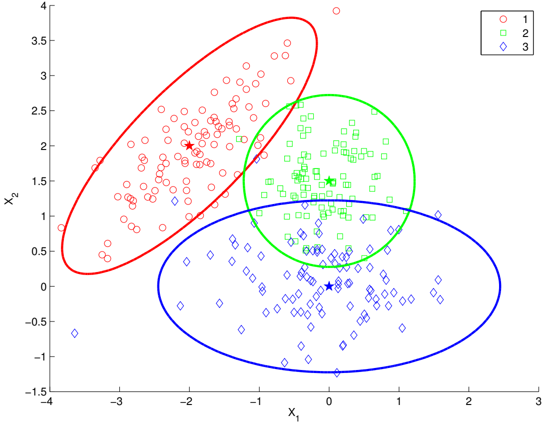


True mean μ_k and covariance Σ_k parameters, for $k = 1, 2, 3$

QDA parameter estimation

Log-likelihood

For the training set,

$$\begin{aligned}
\ell(\theta_1, \ldots, \theta_K, \pi_1, \ldots, \pi_{K-1}) &= \log p((x_1, y_1), \ldots, (x_n, y_n)), \\
&= \sum_{i=1}^{n} \log p((x_i, y_i)), \quad \leftarrow \text{ i.i.d. training set}, \\
&= \sum_{i=1}^{n} \log [p(x_i | y_i) \Pr(y_i)], \\
&= \sum_{i=1}^{n} \log [\pi_{y_i} \; p_{y_i}(x_i; \theta_{y_i})].
\end{aligned}$$

Rk : $\pi_K = 1 - \sum_{j=1}^{K-1} \pi_j$ is not a parameter

QDA parameter estimation (Cont'd)

Notations

- $n_k = \#\{y_i = k\}$ is the number of training samples in class k,
- $\sum_{y_i=k}$ is the sum over all the indices i of the training samples in class k

(Unbiased) Maximum likelihood estimators (MLE)

- $\widehat{\pi}_k = \dfrac{n_k}{n}$, $\leftarrow$ sample proportion
- $\widehat{\mu}_k = \dfrac{\sum_{y_i=k} x_i}{n_k}$, $\leftarrow$ sample mean
- $\widehat{\Sigma}_k = \frac{1}{n_k-1} \sum_{y_i=k} (x_i - \widehat{\mu}_k)(x_i - \widehat{\mu}_k)^T$, $\leftarrow$ sample covariance

Rk : $\frac{1}{n_k-1}$ is a bias correction factor for the covariance MLE (otherwise $\frac{1}{n_k}$)

QDA decision rule

The classification rule becomes

$$
\begin{aligned}
f(x) &= \arg\max_{k \in \mathcal{Y}} \Pr(Y = k | X = x, , \widehat{\theta}, \widehat{\pi}), \\
&= \arg\max_{k \in \mathcal{Y}} \underbrace{\log \Pr(Y = k | X = x, \widehat{\theta}, \widehat{\pi})}_{\delta_k(x)},
\end{aligned}
$$

where

$$
\delta_k(x) = -\frac{1}{2} \log \left| \widehat{\Sigma}_k \right| - \frac{1}{2} (x - \widehat{\mu}_k)^T \widehat{\Sigma}_k^{-1} (x - \widehat{\mu}_k) + \log \widehat{\pi}_k + \cancel{\mathrm{Cst}},
$$

is the discriminant function

Remarks

1. different rule than the Bayes classifier as θ replaced by $\widehat{\theta}$ (and π replaced by $\widehat{\pi}$)
2. when $n \gg p$, $\widehat{\theta} \to \theta$ (and $\widehat{\pi} \to \pi$) : convergence to the optimal classifier if the Gaussian model is correct...

QDA decision boundary

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

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

where

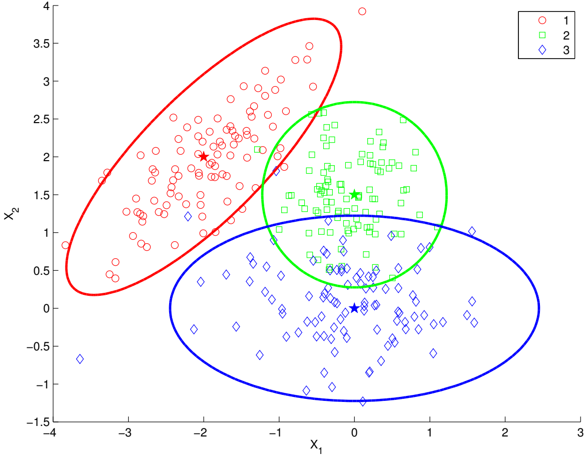
- $C_{k,l} = -\frac{1}{2} \log \frac{|\widehat{\Sigma}_k|}{|\widehat{\Sigma}_l|} + \log \frac{\widehat{\pi}_k}{\widehat{\pi}_l} - \frac{1}{2} \widehat{\mu}_k^T \widehat{\Sigma}_k^{-1} \widehat{\mu}_k + \frac{1}{2} \widehat{\mu}_l^T \widehat{\Sigma}_l^{-1} \widehat{\mu}_l, \quad \leftarrow \text{scalar}$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

☞ 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 $k = 1, 2, 3$

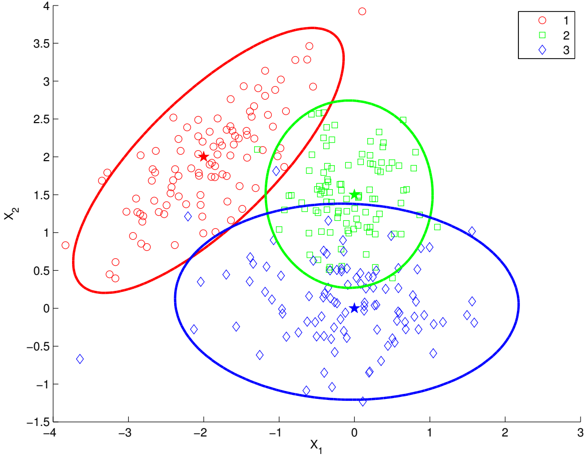


true parameters

QDA example

Mixture of $K = 3$ Gaussians

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

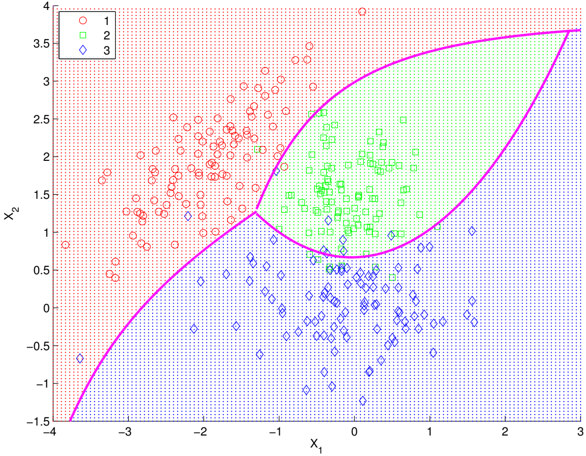


estimated parameters

QDA example (Cont'd)

Mixture of $K = 3$ Gaussians

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



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 $k = 1, \ldots, K$

(Unbiased) Maximum likelihood estimators (MLE)

- $\widehat{\pi}_k$ and $\widehat{\mu}_k$ are unchanged,
- $\widehat{\Sigma} = \frac{1}{n-K} \sum_{k=1}^{K} \sum_{y_i=k} (x_i - \widehat{\mu}_k)(x_i - \widehat{\mu}_k)^T$, $\leftarrow$ pooled covariance

Rk : $\frac{1}{n-K}$ is a bias correction factor for the covariance MLE (otherwise $\frac{1}{n}$)

LDA discriminant function

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

LDA decision boundary

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

$$\delta_k(x) = \delta_l(x) \Leftrightarrow C_{k,l} + L_{k,l}^T x = 0, \quad \leftarrow \text{linear equation}$$

where

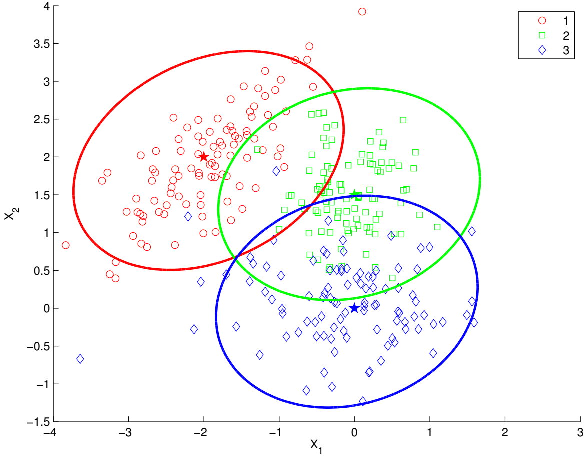
- $C_{k,l} = \log \frac{\widehat{\pi}_k}{\widehat{\pi}_l} - \frac{1}{2}\widehat{\mu}_k^T \widehat{\Sigma}^{-1}\widehat{\mu}_k + \frac{1}{2}\widehat{\mu}_l^T \widehat{\Sigma}^{-1}\widehat{\mu}_l, \quad \leftarrow \text{scalar}$
- $L_{k,l} = \widehat{\Sigma}^{-1}\left(\widehat{\mu}_k - \widehat{\mu}_l\right), \quad \leftarrow \text{vector in } \mathbb{R}^p$
- $Q_{k,l} = 0,$

☞ 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 $\hat{\Sigma}$

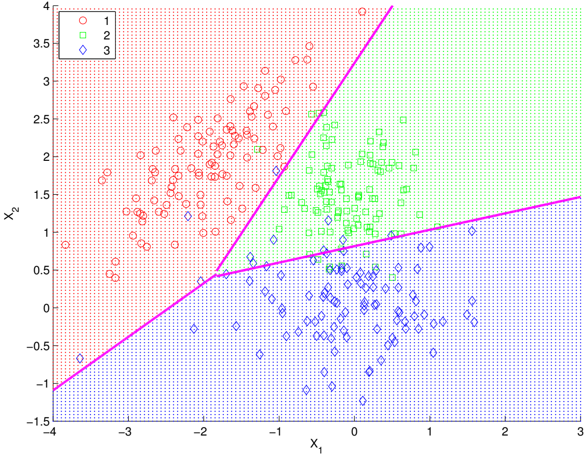


estimated parameters

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 : $(K-1)\times(p+1) = O(Kp)$
- QDA : $(K-1)\times\left(\frac{p(p+3)}{2}+1\right) = O(Kp^2)$

Remarks

- in high dimension, i.e. $p \approx n$ or $p > n$, 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-word 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 $z_k = \widehat{\Sigma}^{-1}\widehat{\mu}_k \leftarrow$ dimension reduction from p to $K-1$!

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.

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)

General assumptions

- $X = (X_1, \ldots, X_p) \in \mathbb{R}^p$, $Y \in \mathcal{Y} = \{1, \ldots, K\}$,

NB Assumption

Simplifying assumption : given Y, the components $X_1, \ldots, X_p$ are assumed to be independent :

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

Remarks

- independence reduces one estimation problem in p dimensions to p much simpler 1D estimation problems $\leftarrow$ 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, for $k = 1, \dots, K$
- NB + LDA : $X|Y = k \sim \mathcal{N}(\mu_k, \Sigma)$, where Σ is diagonal,

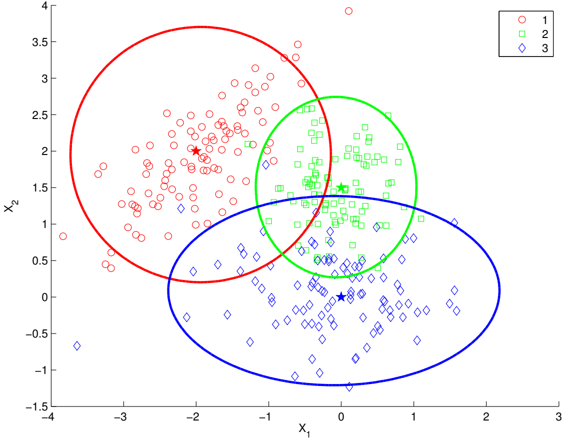
Other classical parametric models

- Bernoulli NB for binary events models (e.g., word occurence 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 $\Sigma_k = \begin{pmatrix} \sigma^2_{1\,k} & 0 \\ 0 & \sigma^2_{2\,k} \end{pmatrix}$

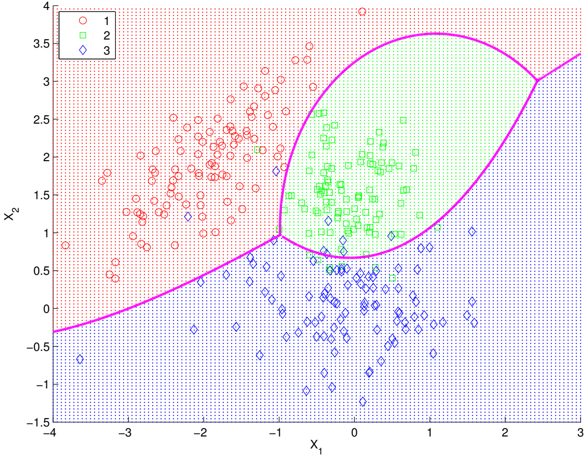


estimated parameters

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 jth component of x

Empirical approach

$$\hat{p}_{k,j}(x_j) = \frac{\#\{x_{j,i} \in V(x_j) \,|\, y_i = k\}}{n_k \lambda}$$

where $V_\lambda(x_j)$ is a neighborhood of x_j with volume λ (and $n_k = \#\{y_i = k\}$)

Parzen kernel approach

$$\hat{p}_{k,j}(x_j) = \frac{1}{n_k \lambda} \sum_{i \text{ st } y_i = k} K_\lambda(x_j, x_{j,i})$$

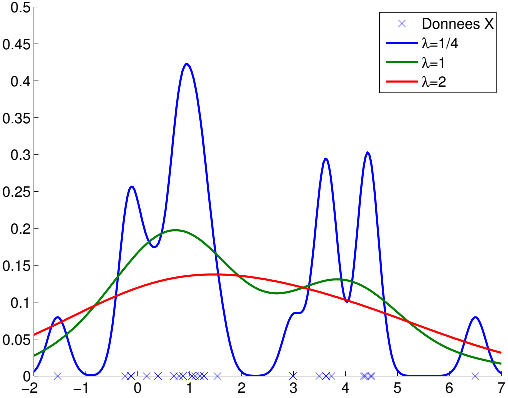
where K_λ is a given kernel, e.g. :

- 0-1 kernel : $K_\lambda(x, x_i) = 1$ if $x_i \in V_\lambda(x)$, 0 otherwise $\leftarrow$ empirical approach,
- 1D Gaussian kernel : $K_\lambda(x, x_0) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2\lambda^2}(x - x_0)^2}$,

$$\Rightarrow \quad \hat{p}_{k,j}(x_j) = \frac{1}{n_k \lambda \sqrt{2\pi}} \sum_{i, y_i = k} e^{-\frac{1}{2\lambda^2}(x_j - x_{j,i})^2}$$

Kernel density estimation

1D estimation : $X \in \mathbb{R}$



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

Conclusions

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
- NB : independence of the feature X components given Y
  - useful when p is very large (high dimension)

Perspectives

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