Data Science for Geosciences

Data classification

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Outline

Model based approaches for classification

Model based approaches for classification

Bayes Classifier

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

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

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

Model based approaches for classification

Linear/Quadratic Discriminant Analysis

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:

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

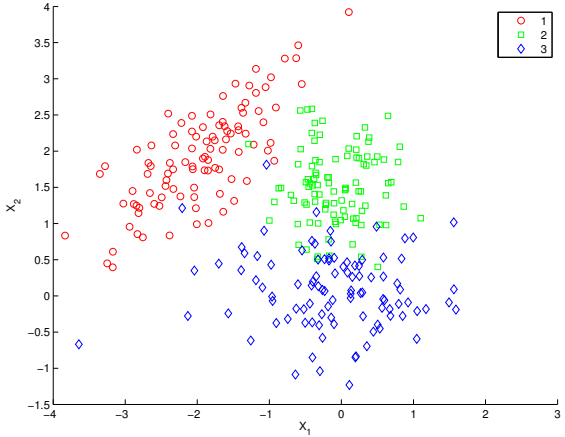
The Gaussian parameters are, for each class $k = 1, \ldots, K$

- 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 $k = 1, \ldots, K$.

Mixture of $K = 3$ Gaussians

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



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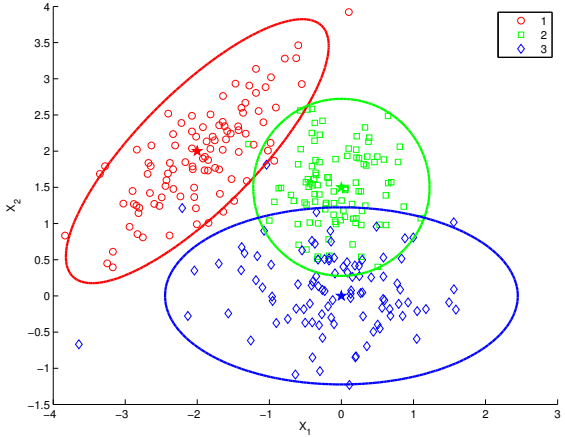


QDA parameter estimation

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)

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

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

For model based approaches, Bayes classifier is defined as

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

- equivalent to consider a set of functions $\delta_k(x)$, for $k \in \mathcal{Y}$, derived from a monotone transformation of posterior probability $p(Y = k|X = x)$
- decision boundary between classes k and l is then defined as the set $\{x \in \mathcal{X} \ : \ \delta_k(x) = \delta_l(x)\}$

Definition

$\delta_k(x)$ are called the discriminant functions of each class k

☞ x is predicted in the k_0 class such that $k_0 = \arg\max_{k \in \mathcal{Y}} \delta_k(x)$

The classification rule becomes

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

where

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

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... only if the Gaussian model is correct!

QDA decision boundary

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

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

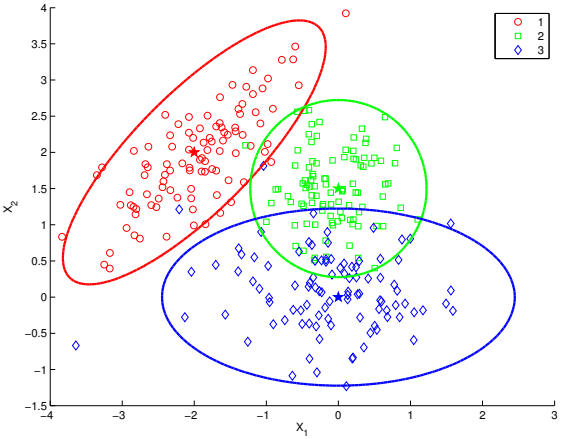
where

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

☞ Quadratic discriminant analysis

Mixture of $K = 3$ Gaussians

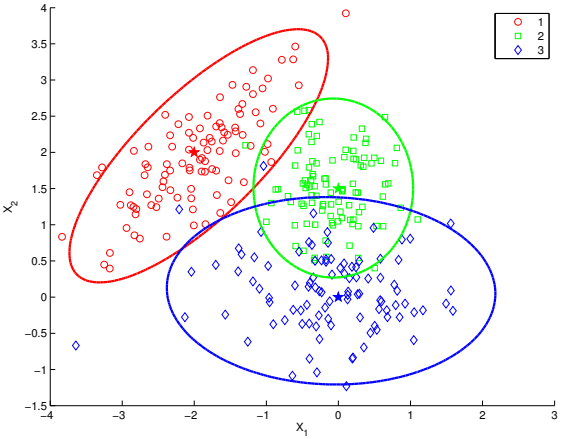
- Estimation of the parameters $\hat{\mu}_k$, $\hat{\Sigma}_k$ and $\hat{\pi}_k$, for $k = 1, 2, 3$



95% true confidence regions

Mixture of $K = 3$ Gaussians

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

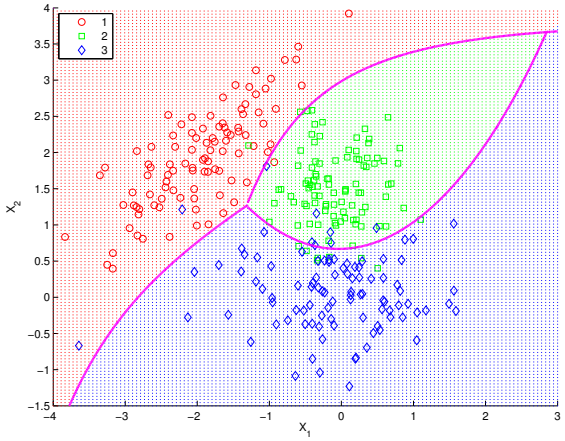


95% estimated confidence regions

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

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

LDA discriminant function

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

LDA decision boundary

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

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

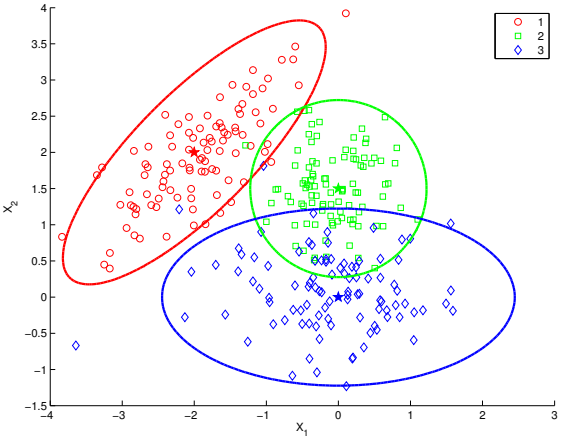
where

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

☞ Linear discriminant analysis

Mixture of $K = 3$ Gaussians

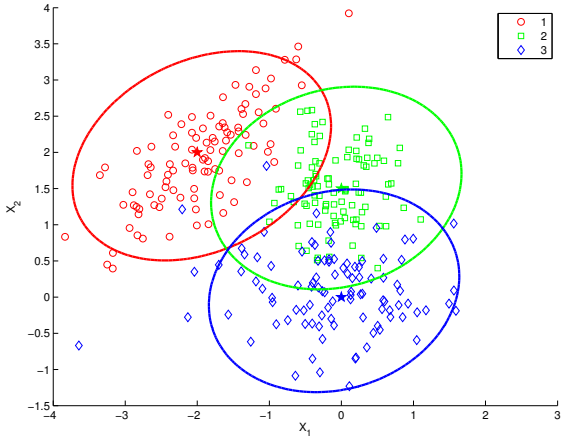
- Estimation of the parameters $\hat{\mu}_k$, $\hat{\pi}_k$, for $k = 1, 2, 3$, and $\hat{\Sigma}$



95% true confidence regions

Mixture of $K = 3$ Gaussians

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

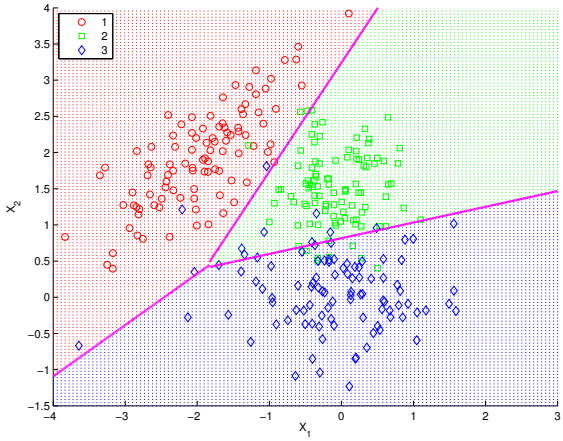


95% estimated confidence regions

LDA example (Cont'd)

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 $z_k = \Sigma^{-1}\widehat{\mu}_k \leftarrow$ dimension reduction from p to $K-1$!

Conclusions on discriminant analysis

Generative models

- learning/estimation of $p(X, Y) = p(X|Y)p(Y)$,
- derivation of $p(Y|X)$ 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

Notebook

Perspectives

Model free approaches: direct learning of the prediction rule f

Model free approaches for classification

Model free approaches for classification

K Nearest Neighbors (K-NN)

Binary classification problem

For a binary classification problem $Y \in \{-1, +1\}$, the classification rule can be derived, for $X = x$, as

$$f(x) = \begin{cases} +1 \text{ if } \widehat{Y}(x) > 0, \\ -1 \text{ otherwise} \end{cases}$$

where $\widehat{Y}(x) = \frac{1}{k} \sum_{X_i \in N_k(x)} Y_i$ is the average of the binary labels of the k nearest neighbors of the testing point $X = x$.

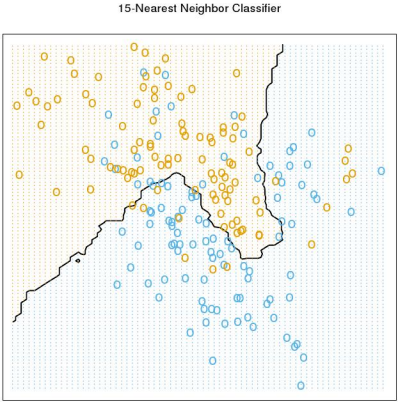
Multiclass problem with k-NN

The binary classification problem can be directly extended for an arbitray number of class K:

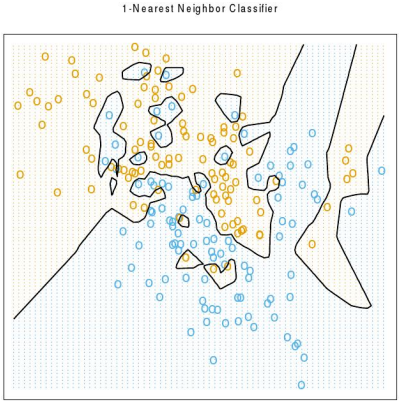
$$\begin{aligned} f(x) &\equiv \text{majority vote among the } k \text{ closest neighbors of the testing point } x, \\ &\equiv \text{assignement to the most common class among the } k \text{ nearest neighbors} \end{aligned}$$

k-NN: complexity parameter k

The effective number of parameters expresses as $N_{\text{eff}} = \frac{n}{k}$, where n is the size of the training sample



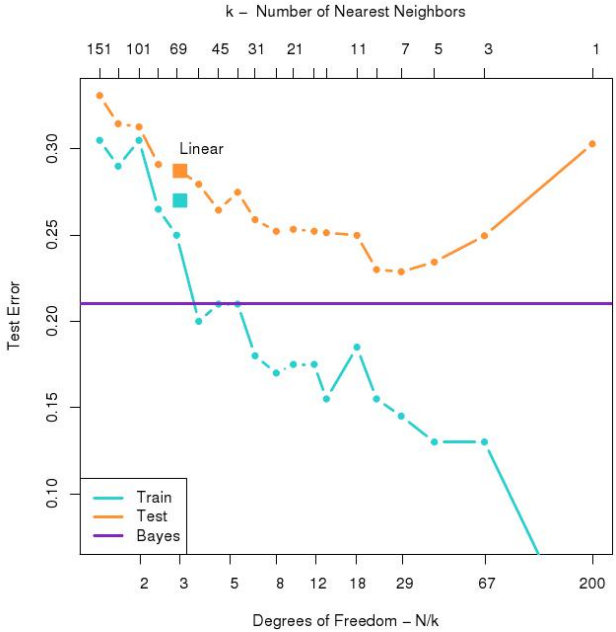
$k = 15,\ N_{\text{eff}} \approx 13$



$k = 1,\ N_{\text{eff}} \approx 200$

- $k = 1 \rightarrow$ training error is always 0 !

Model Selection



Model free approaches for classification

Support Vector Machine (SVM)

Support Vector Machine (SVM)

Theory elaborated in the early 1990's (Vapnik *et al*) based on the idea of 'maximum margin'

- geometrical criterion optimized on the training set ← supervised classification

☞ general, i.e. model free, linear classification rule

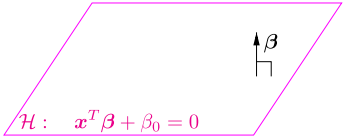
☞ classification rule is linear in a transformed space of higher (possible infinite) dimension than the original input space

Binary classification problem

- $X \in \mathbb{R}^p$
- $Y \in \{-1, 1\} \leftarrow$ 2 classes
- Training set (x_i, y_i), for $i = 1, \ldots, n$

Defining a linear discriminant function $h(x) \Leftrightarrow$ defining a separating hyperplane $\mathcal{H}$ with equation

$$x^T \boldsymbol{\beta} + \beta_0 = 0,$$



- $\boldsymbol{\beta} \in \mathbb{R}^p$ is the normal vector (vector normal to the hyperplane $\mathcal{H}$),
- $\beta_0 \in \mathbb{R}$ is the intercept/offset (regression or geometrical interpretation)

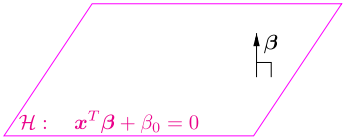
☞ $\mathcal{H}$ is an *affine subspace* of dimension $p - 1$

☞ $h(x) \equiv x^T \boldsymbol{\beta} + \beta_0$ is the associated (linear) discriminant function

Separating hyperplane and prediction rule

For a given separating hyperplane $\mathcal{H}$ with equation

$$\boldsymbol{x}^T\boldsymbol{\beta} + \beta_0 = 0,$$



the prediction rule can be expressed as

- $\widehat{y} = +1$, if $h(\boldsymbol{x}) = \boldsymbol{x}^T\boldsymbol{\beta} + \beta_0 \geq 0$,
- $\widehat{y} = -1$, otherwise,

or in an equivalent way:

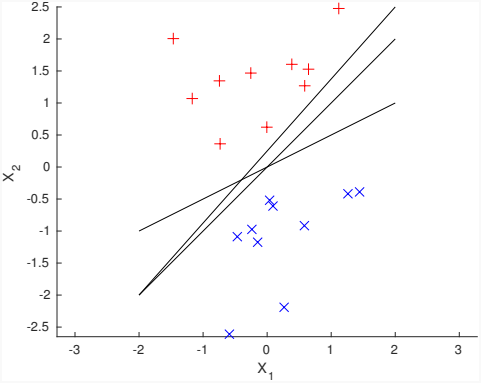
$$\widehat{y} \equiv G(\boldsymbol{x}) = \text{sign}\left[\boldsymbol{x}^T\boldsymbol{\beta} + \beta_0\right]$$

Rk: $\boldsymbol{x}$ is in class $y \in \{-1, 1\}$: prediction $G(\boldsymbol{x})$ is correct iff $y\left(\boldsymbol{x}^T\boldsymbol{\beta} + \beta_0\right) \geq 0$

Linear separability assumption: $\exists \boldsymbol{\beta} \in \mathbb{R}^p$ and $\beta_0 \in \mathbb{R}$ s.t. the hyperplane $\boldsymbol{x}^T\boldsymbol{\beta} + \beta_0 = 0$ perfectly separates the two classes on the training set:

$$y_k \left(x_k^T \boldsymbol{\beta} + \beta_0 \right) \geq 0, \qquad \text{for } k = 1, \ldots, n,$$

Separable case ($p = 2$ example)

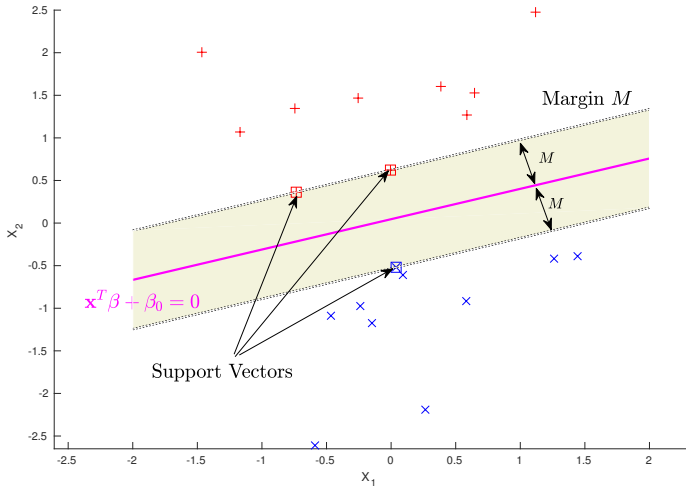


Pb: infinitely many possible perfect separating hyperplanes $\boldsymbol{x}^T\boldsymbol{\beta} + \beta_0 = 0$

☞ Find the 'optimal' separating hyperplane

Maximum margin principle

We are interested in the 'optimal' perfect separating hyperplane maximizing the distance $M > 0$, called the margin, between the separating hyperplane and the training data, i.e. with the biggest gap



Find $\boldsymbol{\beta} \in \mathbb{R}^p$ and $\beta_0 \in \mathbb{R}$ s.t. the margin

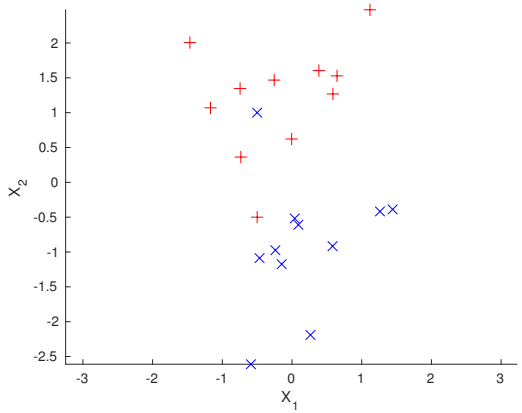
$$M = \min_{1 \leq k \leq n} \{d(x_k, \mathcal{H})\}$$

is maximized. Subject to

$$y_k \left(x_k^T \boldsymbol{\beta} + \beta_0 \right) \geq 0, \quad \text{for } k = 1, \ldots, n,$$

Nonseparable case

- in general, overlap of the 2 classes (unless $n < p$)
- no hyperplane that perfectly separates the training data



☞ we can soften what we mean by "separates"

Solution for the nonseparable case

Considering a *soft-margin* that allows wrong classifications

- introduction of *slack variables* $\xi_i \geq 0$ s.t.

$$y_i(\boldsymbol{x_i}^T\boldsymbol{\beta} + \beta_0) \geq (1 - \xi_i)$$

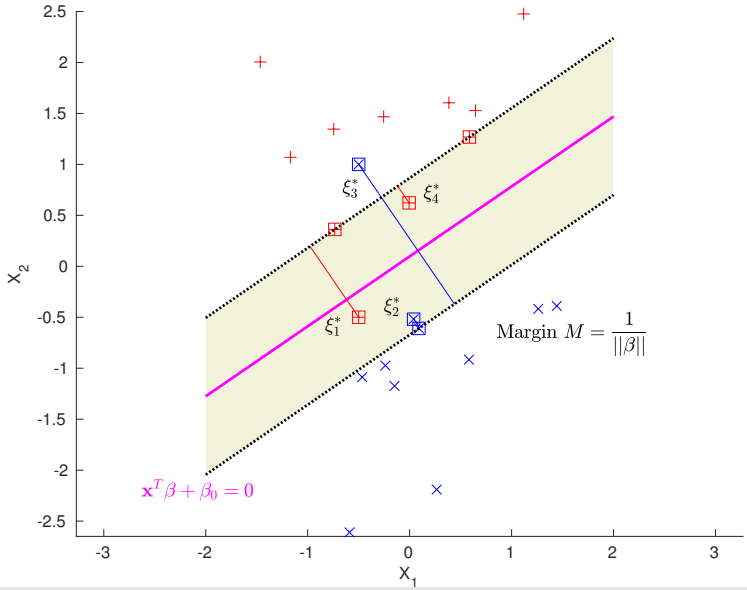
Support vectors include now the wrong classified points, and the points inside the margins ($\xi_i > 0$)

- Primal problem: adding a constraint on the ξ_i's

$$\begin{cases} \max_{\boldsymbol{\beta},\beta_0,\xi} & M, \\ \text{subject to} & y_i(\boldsymbol{x_i}^T\boldsymbol{\beta} + \beta_0) \geq 1 - \xi_i, \\ & C\sum_{i=1}^n \xi_i \leq 1. \end{cases}$$

where $C > 0$ is the "cost" parameter

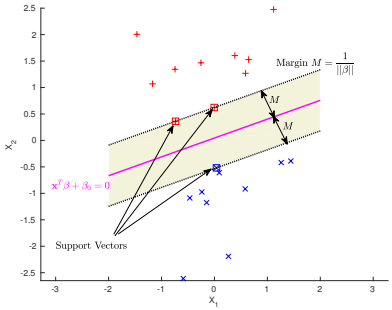
Example (nonseparable case)



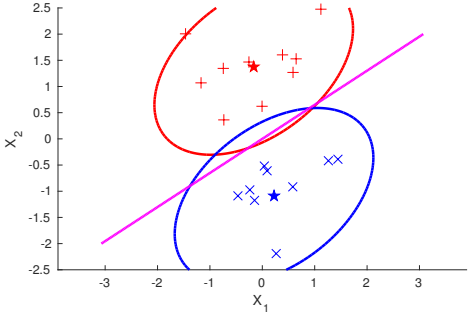
$\xi_i^* \equiv M\xi_i \leftarrow$ distance between a support vector and the margin

Linear discrimination

- Linear Discriminant Analysis (LDA): Gaussian generative model
- SVM: criterion optimization (maximizing the margin)

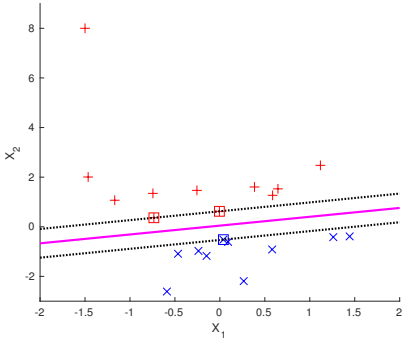


SVM

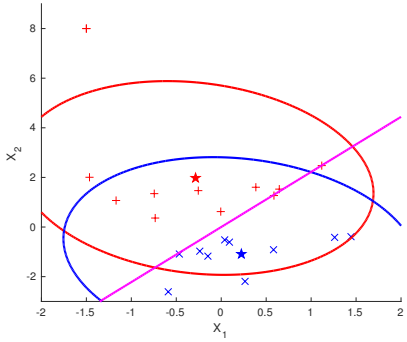


LDA

Adding one atypical data



SVM



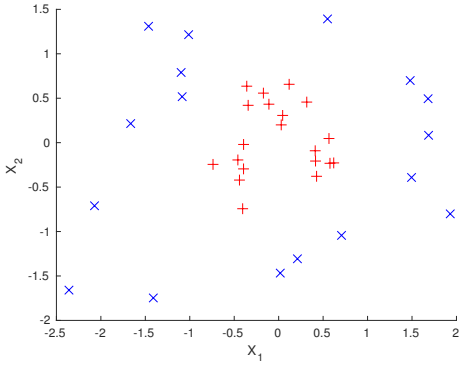
LDA

SVM property

- Nonsensitive to atypical points (outliers) far from the margin

☞ sparse method (information ≡ support vectors)

Nonlinear discrimination in the input space



Transformed space $\mathcal{F}$

- Choice of a transformed space $\mathcal{F}$ (expansion space) where the linear separation assumption is more relevant
- Nonlinear expansion map $\phi : \mathbb{R}^p \to \mathcal{F}$, $\boldsymbol{x} \mapsto \phi(\boldsymbol{x})$ (enlarged features)

Nonlinear discrimination in the input space

- Projection in the space of monomials of order 2.

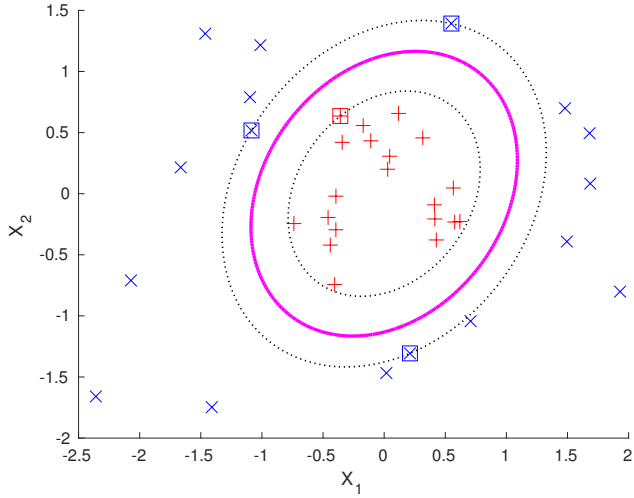
$$\begin{aligned} \phi : \mathbb{R}^2 &\to \mathbb{R}^3 \\ \mathbf{x} &\mapsto \phi(\mathbf{x}) \\ (\mathbf{x}_1, \mathbf{x}_2) &\mapsto (\mathbf{x}_1^2, \mathbf{x}_2^2, \sqrt{2}\mathbf{x}_1\mathbf{x}_2) \end{aligned}$$

- In $\mathbb{R}^3$, the inner product can be expressed as

$$\begin{aligned} \langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle_{\mathbb{R}^3} &= \sum_{i=1}^{3} \phi(\mathbf{x})_i \phi(\mathbf{x}')_i \\ &= \phi(\mathbf{x})_1 \phi(\mathbf{x}')_1 + \phi(\mathbf{x})_2 \phi(\mathbf{x}')_2 + \phi(\mathbf{x})_3 \phi(\mathbf{x}')_3 \\ &= \mathbf{x}_1^2 \mathbf{x}'^2_1 + \mathbf{x}_2^2 \mathbf{x}'^2_2 + 2\mathbf{x}_1\mathbf{x}_2\mathbf{x}'_1\mathbf{x}'_2 \\ &= (\mathbf{x}_1\mathbf{x}'_1 + \mathbf{x}_2\mathbf{x}'_2)^2 \\ &= \langle \mathbf{x}, \mathbf{x}' \rangle^2_{\mathbb{R}^2} \\ &= k(\mathbf{x}, \mathbf{x}'). \end{aligned}$$

Nonlinear discrimination in the input space

- $X \in \mathbb{R}^2$, $\phi(x) = (x_1^2, x_2^2, \sqrt{2}x_1x_2)^T$



Linear separation in the feature space $\mathcal{F} \Rightarrow$ Nonlinear separation in the input space

The SVM solution depends only on the inner product between the input features $\phi(\boldsymbol{x})$ and the support vectors $\phi(\boldsymbol{x}_{\text{margin}})$

Kernel trick

Use of a kernel function k associated with an expansion/feature map ϕ:

$$\begin{array}{rccc} k: & \mathbb{R}^p \times \mathbb{R}^p & \to & \mathbb{R} \\ & (\boldsymbol{x}, \boldsymbol{x}') & \mapsto & k(\boldsymbol{x}, \boldsymbol{x}') \equiv \langle \phi(\boldsymbol{x}), \phi(\boldsymbol{x}') \rangle \end{array}$$

Advantages

- Computations are performed in the original input space: less expansive than in a high dimensional transformed space $\mathcal{F}$
- Explicit representations of the feature map ϕ and enlarged feature space $\mathcal{F}$ are not necessary, the only expression of k is required!

☞ Possibility of complex transformations in possible infinite space $\mathcal{F}$

☞ Standard trick in machine learning not limited to SVM (kernel ridge regression, gaussian process, kernel-PCA, spectral clustering ...)

Definition (Positive semi-definite kernel)

$k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is positive semi-definite is

- $\forall (\mathbf{x}, \mathbf{x}') \in \mathbb{R}^d \times \mathbb{R}^d, k(\mathbf{x}_i, \mathbf{x}_j) = k(\mathbf{x}_j, \mathbf{x}_i)$.
- $\forall n \in \mathbb{N}, \forall \xi_1 \dots \xi_n \in \mathbb{R}, \forall \mathbf{x}_1 \dots \mathbf{x}_n \in \mathbb{R}^d, \sum_{i,j}^n \xi_i \xi_j k(\mathbf{x}_i, \mathbf{x}_j) \geq 0$.

Theorem (Moore-Aronsjan (1950))

To every positive semi-definite kernel k, there exists a Hilbert space $\mathcal{H}$ and a feature map $\phi : \mathbb{R}^d \to \mathcal{H}$ such that for all $\mathbf{x}_i, \mathbf{x}_j$ we have $k(\mathbf{x}_i, \mathbf{x}_j) = \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle_{\mathcal{H}}$.

Operations on kernels

Let k_1 and k_2 be positive semi-definite, and $\lambda_{1,2} > 0$ then:

1. $\lambda_1 k_1$ is a valid kernel
2. $\lambda_1 k_1 + \lambda_2 k_2$ is positive semi-definite.
3. $k_1 k_2$ is positive semi-definite.
4. $\exp(k_1)$ is positive semi-definite.
5. $g(\mathbf{x}_i)g(\mathbf{x}_j)$ is positive semi-definite, with $g : \mathbb{R}^d \to \mathbb{R}$.

Usual kernel functions

- Linear kernel ($\mathcal{F} \equiv \mathbb{R}^p$) : $k(x, x') = x^T x'$
- Polynomial kernel (dimension of $\mathcal{F}$ increases with the order d)

$$k(x, x') = (x^T x' + q)^d = \sum_{l=1}^{d} \binom{d}{l} q^{d-l} (x^T x')^l.$$

- Gaussian radial function ($\mathcal{F}$ with infinite dimension)

$$k(x, x') = \exp\left(-\gamma ||x - x'||^2\right)$$

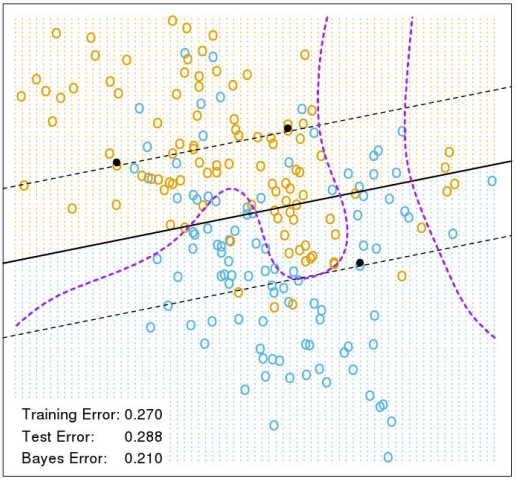
- Neural net kernel ($\mathcal{F}$ with infinite dimension)

$$k(x, x') = \tanh\left(\kappa_1 x^T x' + \kappa_2\right)$$

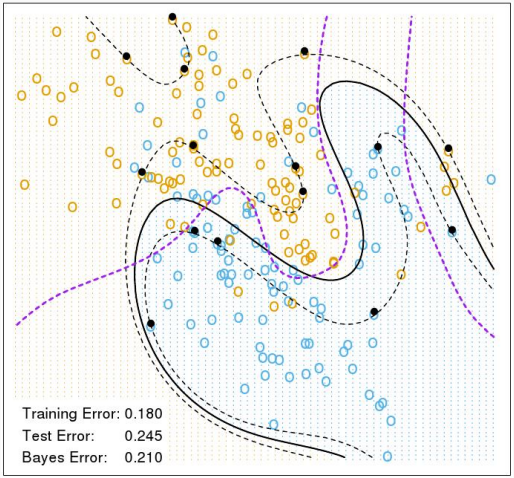
☞ standard practice is to estimate optimal values of kernel parameters by cross validation

Application: binary data (cf introduction course)

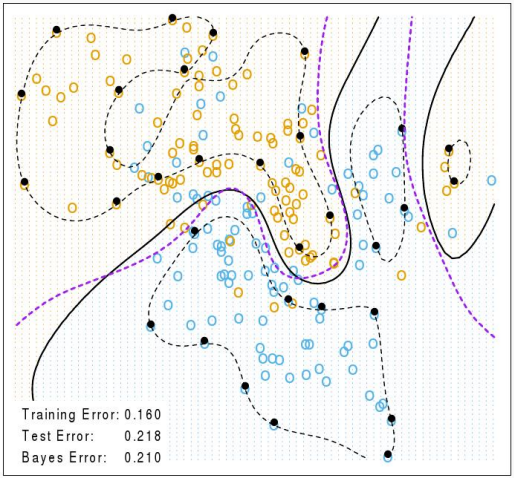
Linear kernel



Polynomial kernel ($d = 4$)



Gaussian radial kernel ($\gamma = 1$)



SCALE YOUR DATA!!

- With Gaussian kernel

$$\begin{aligned} k(x, x') &= \exp\left(-\gamma ||x - x'||^2\right) \\ &= \exp\left(-\gamma \sum_{i=1}^{p} (x_i - x_i')^2\right) \end{aligned}$$

- Scaling:

$$\begin{aligned} \tilde{x}_i &= \frac{x_i - \mu_i}{\sigma_i} \\ \tilde{x}_i &= \frac{x_i - \min_i}{\max_i - \min_i} \end{aligned}$$

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- $Y \in \{1, \ldots, K\} \leftarrow K$ classes

Standard approach: direct generalization by using multiple binary SVMs

OVA: one-versus-all strategy

- K classifiers between one class ($+1$ label) versus all the other classes (-1 label)

☞ classifier with the highest confidence value (e.g. the maximum distance to the separator hyperplane) assigns the class

OVO: one-versus-one strategy

- $\binom{K}{2} = K(K-1)/2$ classifiers between every pair of classes

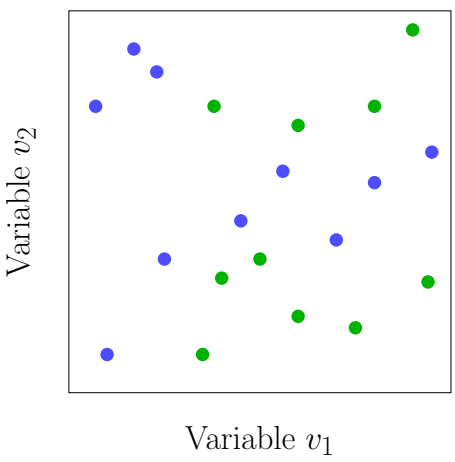
☞ majority vote rule: the class with the higher number of votes determines the instance classification

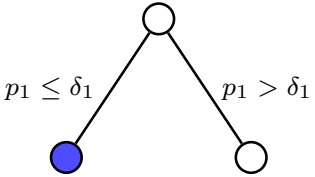
Which to choose? if K is not too large, choose OVO

Model free approaches for classification

Random Forests

- Introduced in 2001 (Breiman)
- Model free and non linear
- Build a large collection of de-correlated trees and average them
- Combination of weak learner





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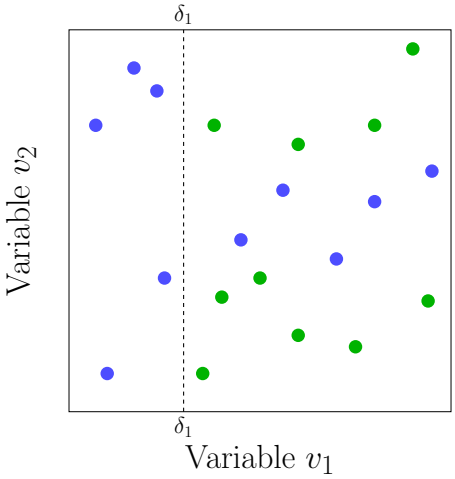

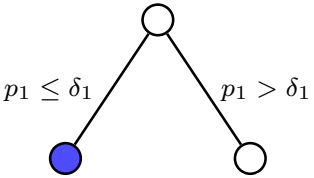

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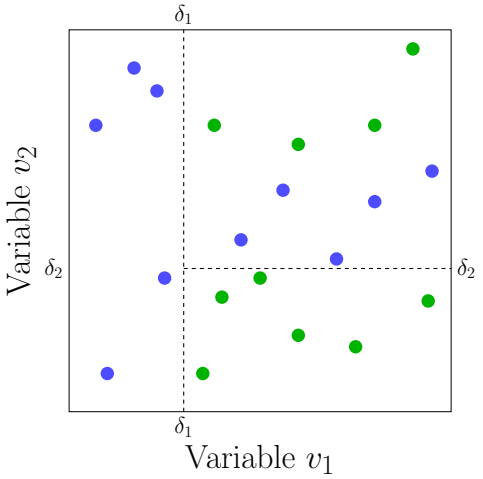

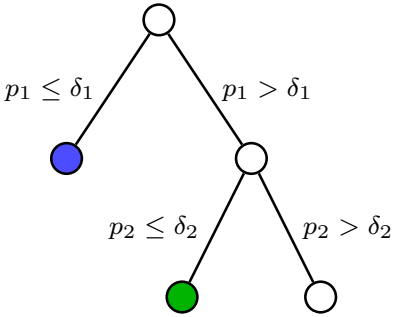

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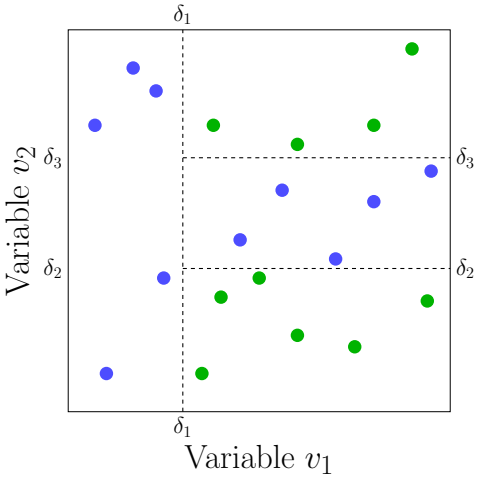

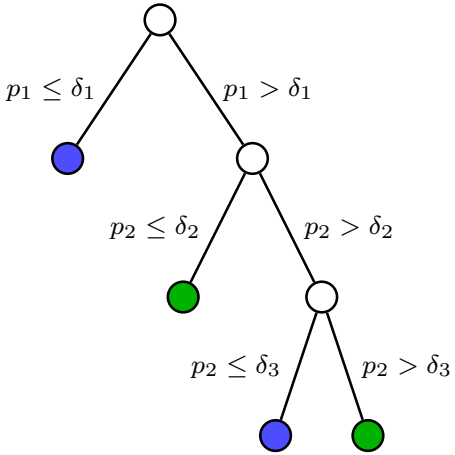

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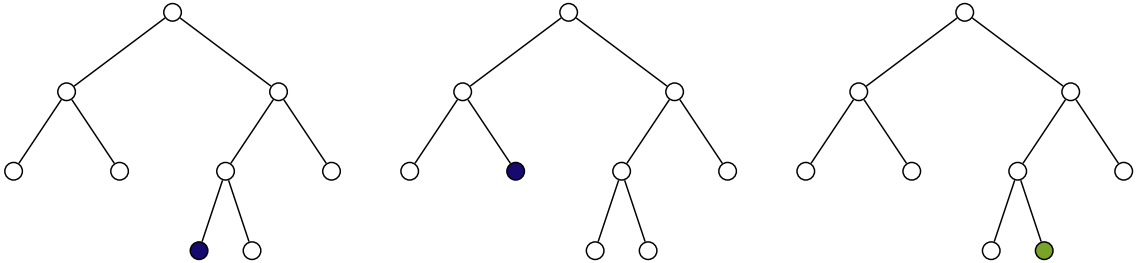
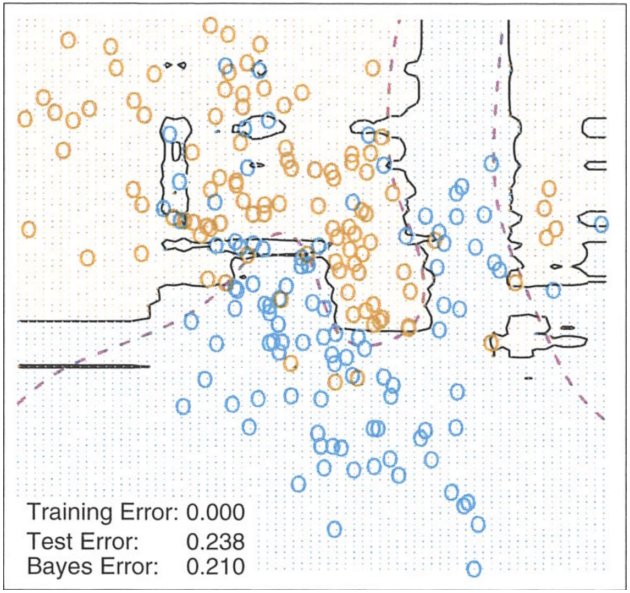
- For each tree:
  - Draw bootstrap sample X^b for training sample
  - Learn tree, for each node
    - ⋆ select m features from the initial p features
    - ⋆ Find the best split (e.g. Gini index, entropy ...)



Application: binary data



Conclusions on 'Black Box' approaches

k-NN

- non-parametric method which does not rely on a fixed model
- algorithm which is conceptually among the simplest of all machine learning algorithms
- badly behaved procedure in high dimension: dimension reduction, e.g. PCA, is usually performed prior to k-NN algorithm in order to avoid curse of dimensionality and to reduce computational complexity of the classification rule

SVM

- maximum margin learning criterion $\leftarrow$ model free
- classification algorithm nonlinear in the original input space by performing an implicit linear classification in a higher dimensional space
- sparse solutions characterized by the support vectors
- popular algorithms, with a large literature

Conclusions on 'Black Box' approaches (Cont'd)

Random Forests

- involve decision tree to split the prediction space in simple regions
- combine multiple decision trees to yield a single consensus prediction

☞ method able to scale efficiently to high dimensional data

Deep Neural Nets

- Neural Nets with multiple hidden layers between input and output ones
- many variants of deep architectures (Recurrent, Convolutional,...) used in specific domains (speech, vision, ...)

☞ supported by empirical evidence

☞ dramatic performance jump for several big data applications

Notebook

Model Selection and Model Assessment

Model Selection and Model Assessment

Introduction

Train and Prediction Errors

- Loss-function $L(y, \hat{y}) = 0$ if $y = \hat{y}$ else 1
- **Train error**: average loss over the training sample

$$\text{Err}_{\text{train}} = \frac{1}{n} \sum_{i=1}^{n} L(y_i, \hat{y}_i)$$

- **Test/Prediction error**: average loss over an independent test sample $\rightarrow$ Generalization error
- General picture:

$$\text{Err}_{\text{test}} \approx \text{Err}_{\text{train}} + O$$

O would be the average *optimism*.

Model Selection vs Model Assessment

Model selection

- Estimate the best set of hyperparameters
- Estimate the performance of differents models

Model Assessment

Estimate the generalization error on unseen/test sample

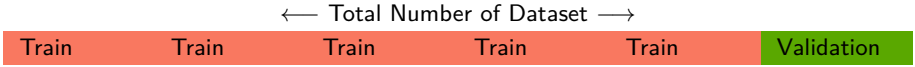
Model Selection vs Model Assessment

Model selection

- Estimate the best set of hyperparameters
- Estimate the performance of differents models

Model Assessment

Estimate the generalization error on unseen/test sample



Model Selection and Model Assessment

Cross-validation

Principle

- Method to estimate prediction error using the training sample
- Based on splitting the data in K-folds :

Model 1	Train	Train	Train	Train	Validation
Model 2	Train	Train	Train	Validation	Train
Model 3	Train	Train	Validation	Train	Train
Model 4	Train	Validation	Train	Train	Train
Model 5	Validation	Train	Train	Train	Train

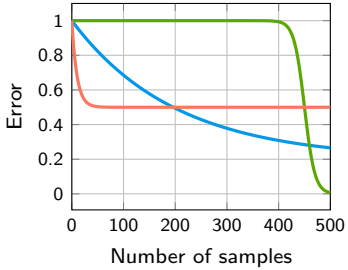
- Expected prediction error:

$$CV(\hat{f}, \theta) = \sum_{k=1}^{K} \text{Err}_k(\hat{f}, \theta)$$

- K ? Usually K=5 or 10 is a good trade-off (K=n is called leave-one-out)

	Bias	Variance
K low	High	Low
K high	Low	High
K = n	Low	Very High

- Be careful to the learning curve



- Model should be trained completely for each fold (i.e., data normalization, optimization, etc ...)
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Conclusions

Classifier comparison

Notebook

Conclusions

- There is no universal best classifier
- Needs to be chosen appropriately
- Pay attention to
  - Scale your data,
  - Try several algorithms, and optimize their hyperparameters
  - Extract/Select/Build relevant features
- In many situations, simple is actually good!
- Sklearn is a good try !

`https://scikit-learn.org/stable/index.html`

Thank you for your attention