Data Science for Geosciences

Data classification

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Outline

Model based approaches for classification

Model free approaches for classification

Model Selection and Model Assessment

Conclusions

Model based approaches for classification

Model based approaches for classification

Bayes Classifier

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

- $f^*(X) \equiv$ *maximum a posteriori* (MAP) estimate
- 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: $Y \in \mathcal{Y} = \{1, \dots, K\}$,
- 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

Quadratic Discriminant Analysis (QDA)

Supervised classification assumptions

- $X \in \mathbb{R}^p$, $Y \in \mathcal{Y} = \{1, \dots, K\}$,
- 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 parametric and Gaussian distribution:

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

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

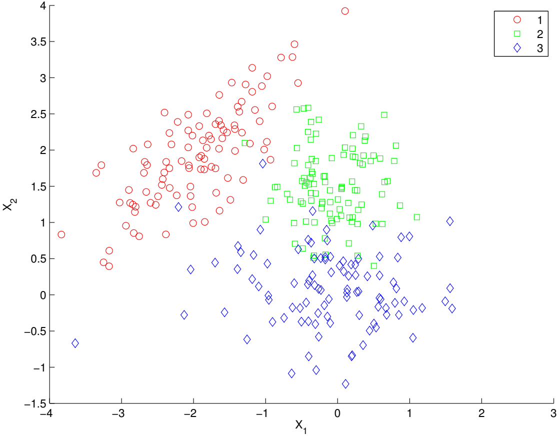
- mean vectors $\mu_k \in \mathbb{R}^p$,
- covariance matrices $\boldsymbol{\Sigma}_k \in \mathbb{R}^{p \times p}$,

☞ set of parameters $\theta_k \equiv \{\mu_k, \boldsymbol{\Sigma}_k\}$, plus the weights π_k, for $k = 1, \dots, K$.

Example

Mixture of $K = 3$ Gaussians

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



Example

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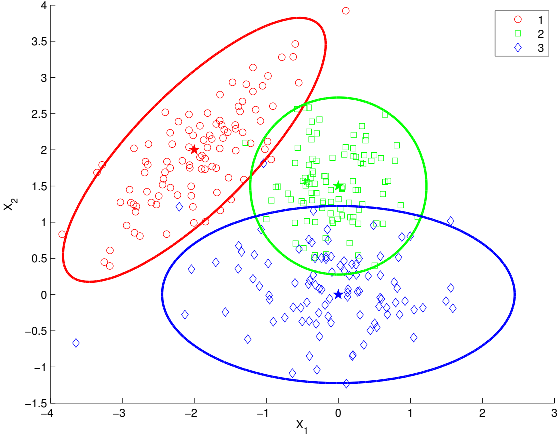


QDA parameter estimation

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)

- $\widehat{\pi}_k = \dfrac{n_k}{n}$, $\leftarrow$ 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 $\frac{1}{n_k}$)

DISCRIMINANT FUNCTIONS

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 $k_0 = \arg\max_{k \in \mathcal{Y}} \delta_k(x)$

QDA DECISION RULE

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

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

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

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

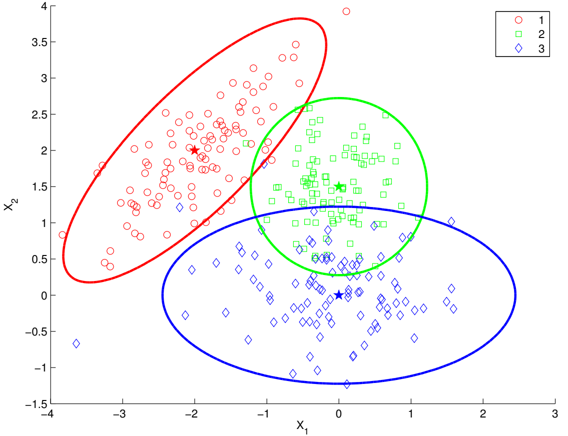
where

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

☞ Quadratic discriminant analysis

Mixture of $K = 3$ Gaussians

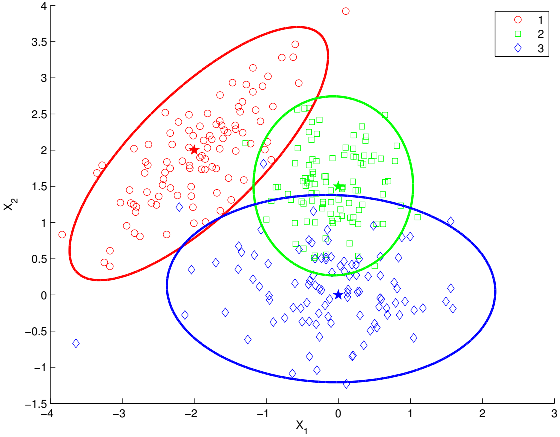
- Estimation of the parameters $\hat{\mu}_k$, $\hat{\Sigma}_k$ and $\hat{\pi}_k$, for $k = 1, 2, 3$



95% true confidence regions

Mixture of $K = 3$ Gaussians

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

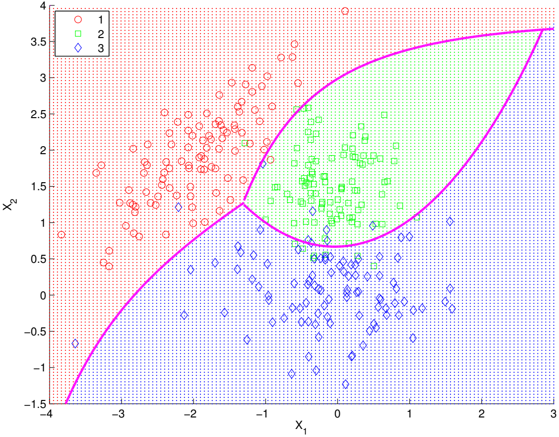


95% estimated confidence regions

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 PRINCIPLE

LDA Assumptions

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

(Unbiased) Maximum likelihood estimators (MLE)

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

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

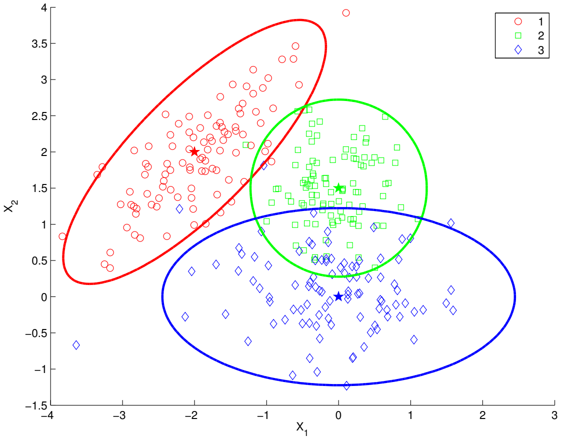
where

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

☞ Linear discriminant analysis

Mixture of $K = 3$ Gaussians

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

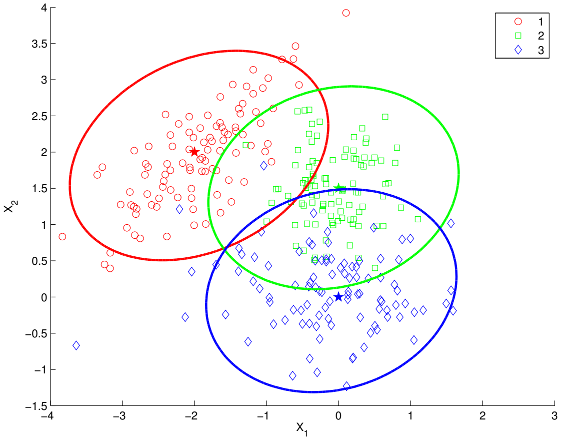


95% true confidence regions

LDA EXAMPLE

Mixture of $K = 3$ Gaussians

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

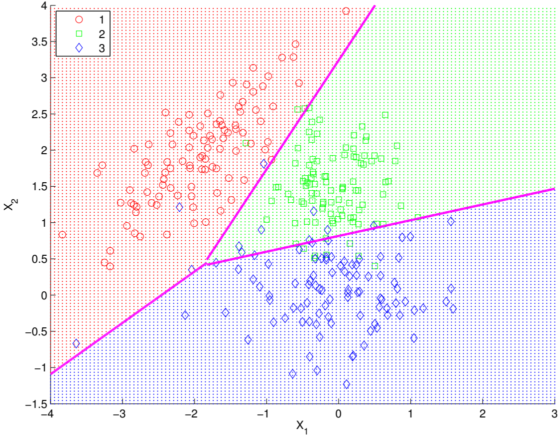


95% estimated confidence regions

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

Perspectives

Model free approaches: direct learning of the prediction rule f

Notebook

Model free approaches for classification

Model free approaches for classification

K Nearest Neighbors (K-NN)

k Nearest-Neighbors (k-NN) for classification

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

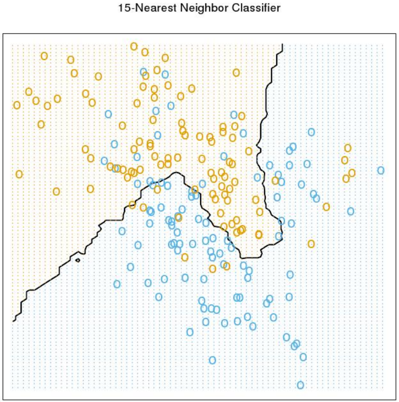
The binary classification problem can be directly extended for an arbitray number of class K:

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

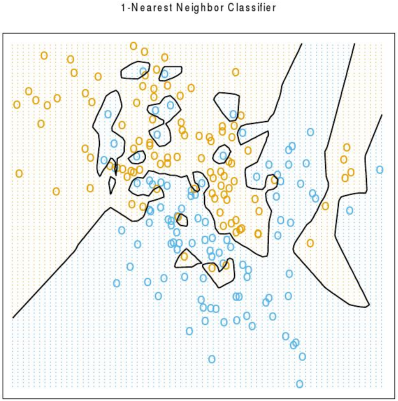
K Nearest-Neighbors

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



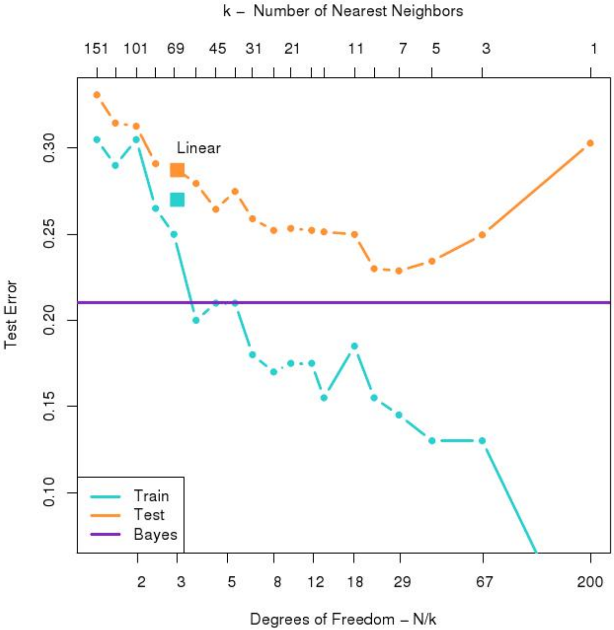
$k = 15$, $N_{\text{eff}} \approx 13$



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

- $k = 1 \rightarrow$ 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

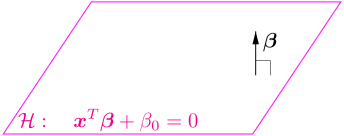
Linear discrimination and Separating hyperplane

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

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


$\boldsymbol{\beta}$
$\mathcal{H}: \quad \boldsymbol{x}^T \boldsymbol{\beta} + \beta_0 = 0$

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

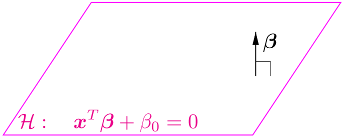
☞ $\mathcal{H}$ is an *affine subspace* of dimension $p - 1$

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

Separating hyperplane and prediction rule

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

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


$\boldsymbol{\beta}$
$\mathcal{H}: \quad \boldsymbol{x}^T\boldsymbol{\beta} + \beta_0 = 0$

the prediction rule can be expressed as

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

or in an equivalent way:

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

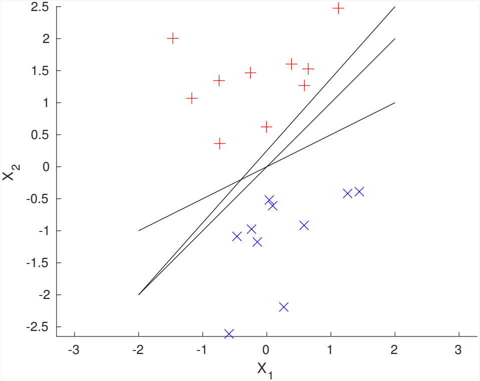
Rk: $\boldsymbol{x}$ is in class $y \in \{-1, 1\}$: prediction $G(\boldsymbol{x})$ is correct iff $y\left(\boldsymbol{x}^T\boldsymbol{\beta} + \beta_0\right) \geq 0$

Separating Hyperplane: separable case

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:

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

Separable case ($p = 2$ example)



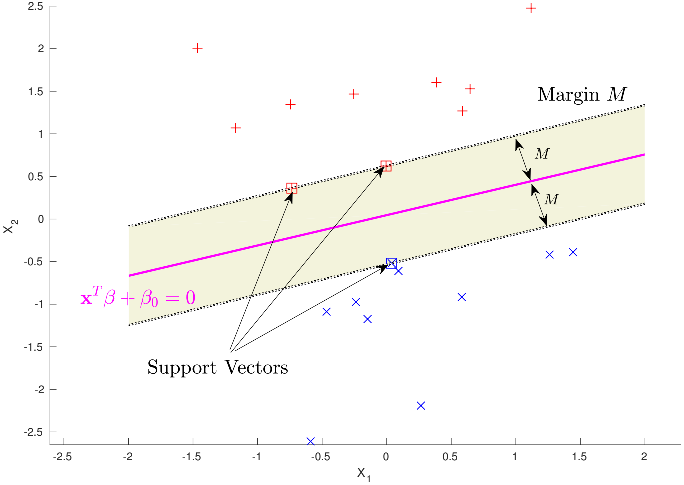
Pb: infinitely many possible perfect separating hyperplanes $\boldsymbol{x}^T \boldsymbol{\beta} + \beta_0 = 0$

☞ Find the 'optimal' separating hyperplane

Maximum margin separating hyperplane (separable case)

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

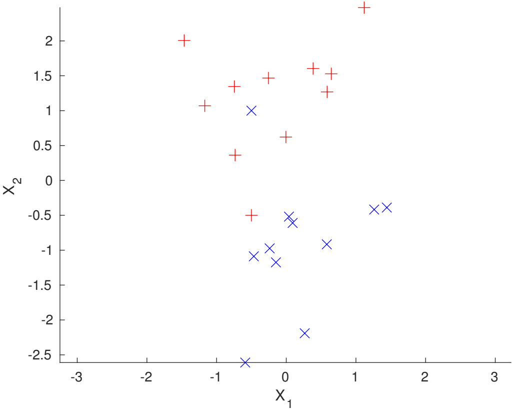
$$M = \min_{1 \le k \le n} \{d(x_k, \mathcal{H})\}$$

is maximized. Subject to

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

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”

Maximum margin separating hyperplane (nonseparable case)

Solution for the nonseparable case

Considering a *soft-margin* that allows wrong classifications

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

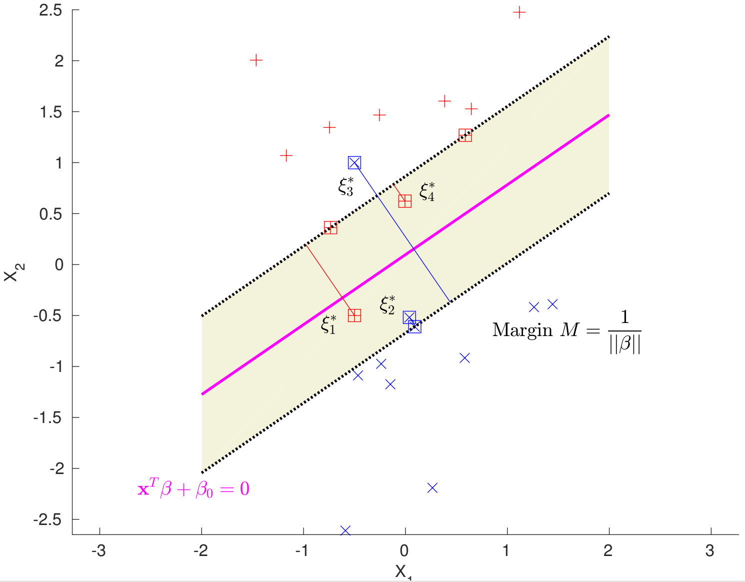
  $$y_i({\mathbf{x}_i}^T\boldsymbol{\beta} + \beta_0) \geq (1 - \xi_i)$$

  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

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

  where $C > 0$ is the “cost” parameter

Example (nonseparable case)

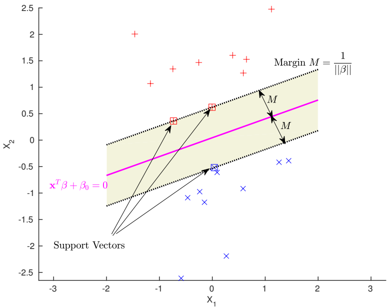


$\xi_i^* \equiv M\xi_i \leftarrow$ distance between a support vector and the margin

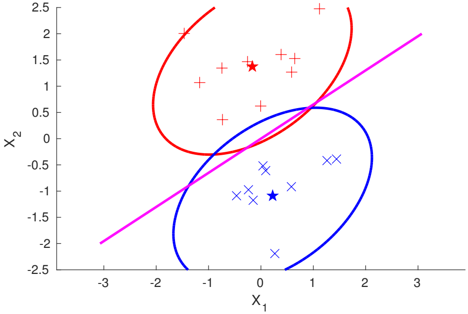
Linear discrimination: SVM vs LDA

Linear discrimination

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



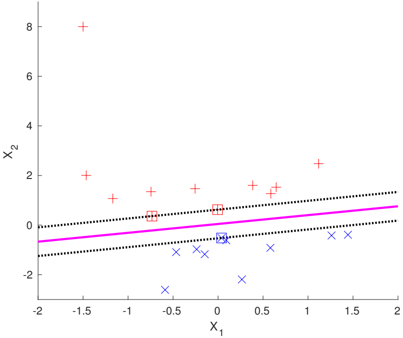
SVM



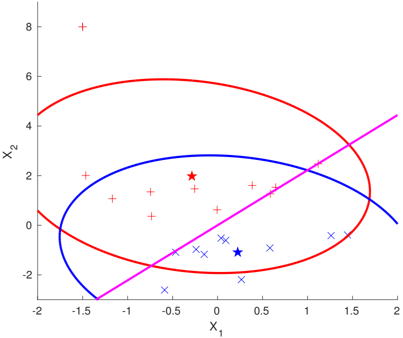
LDA

Linear discrimination: SVM vs LDA (Cont'd)

Adding one atypical data



SVM



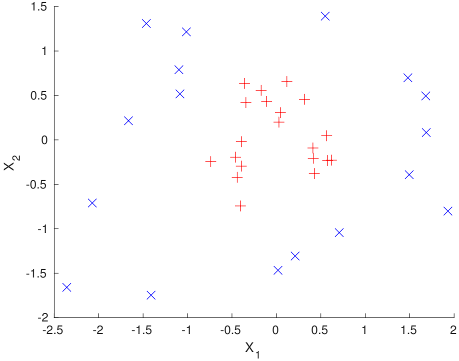
LDA

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 $\phi : \mathbb{R}^p \to \mathcal{F}, \mathbf{x} \mapsto \phi(\mathbf{x})$ (enlarged features)

- Projection in the space of monomials of order 2.

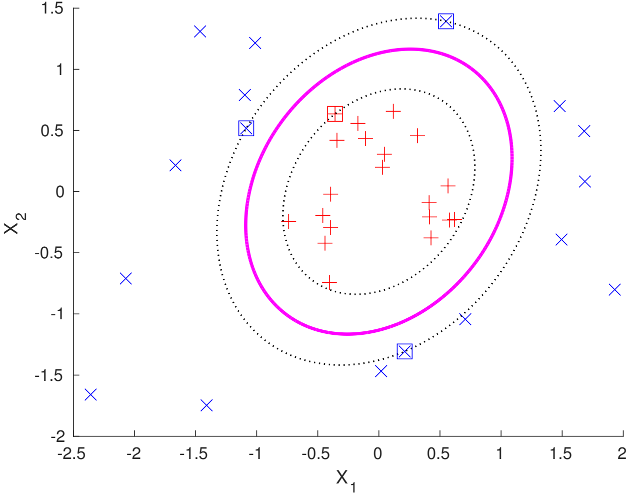
$$\begin{aligned} \phi : \mathbb{R}^2 &\to \mathbb{R}^3 \\ \mathrm{x} &\mapsto \phi(\mathrm{x}) \\ (\mathrm{x}_1, \mathrm{x}_2) &\mapsto (\mathrm{x}_1^2, \mathrm{x}_2^2, \sqrt{2}\mathrm{x}_1\mathrm{x}_2) \end{aligned}$$

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

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

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 $\mathcal{F}$ ⇒ Nonlinear separation in the input space

Kernel trick

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

Kernel trick

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

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

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 . . .)

Kernel function

Definition (Positive semi-definite kernel)

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

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

Theorem (Moore-Aronsjan (1950))

To every positive semi-definite kernel k, there exists a Hilbert space $\mathcal{H}$ and a feature map $\phi : \mathbb{R}^d \rightarrow \mathcal{H}$ 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 $g : \mathbb{R}^d \to \mathbb{R}$.

Choosing the Kernel function

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)

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

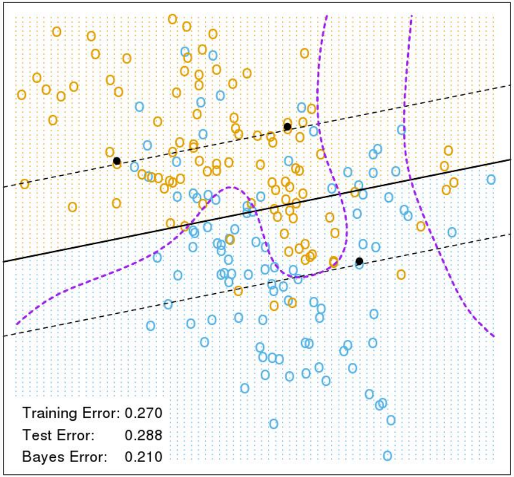
- Neural net kernel ($\mathcal{F}$ with infinite dimension)

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

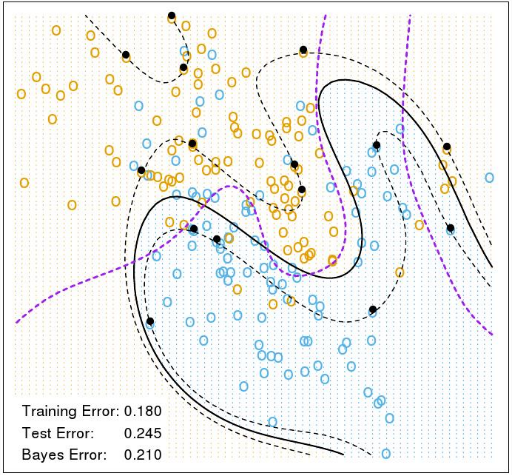
☞ standard practice is to estimate optimal values of kernel parameters by cross validation

Application: binary data (cf introduction course)

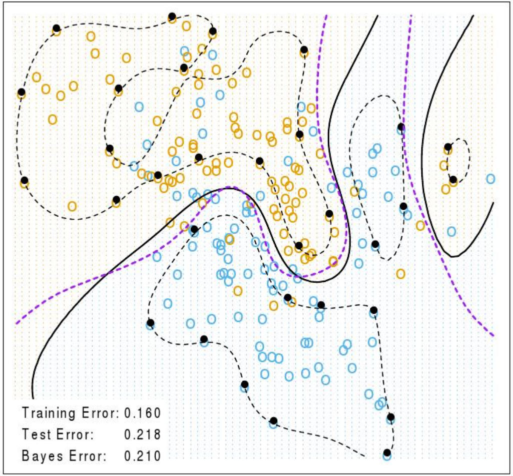
Linear kernel



Polynomial kernel ($d = 4$)



Gaussian radial kernel ($\gamma = 1$)



Practical tips

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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MULTICLASS SVM

- $Y \in \{1, \dots, K\} \leftarrow K$ 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

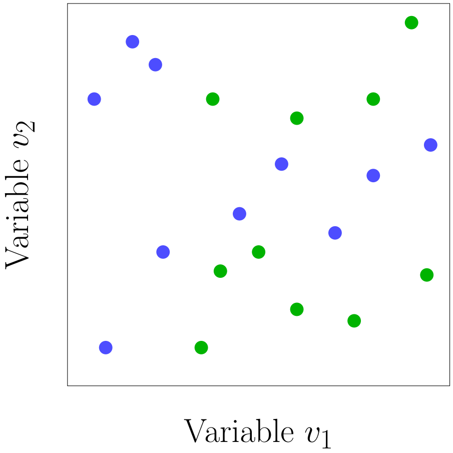
Which to choose? if K is not too large, choose OVO

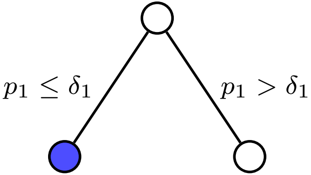
Model free approaches for classification

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

Decision trees





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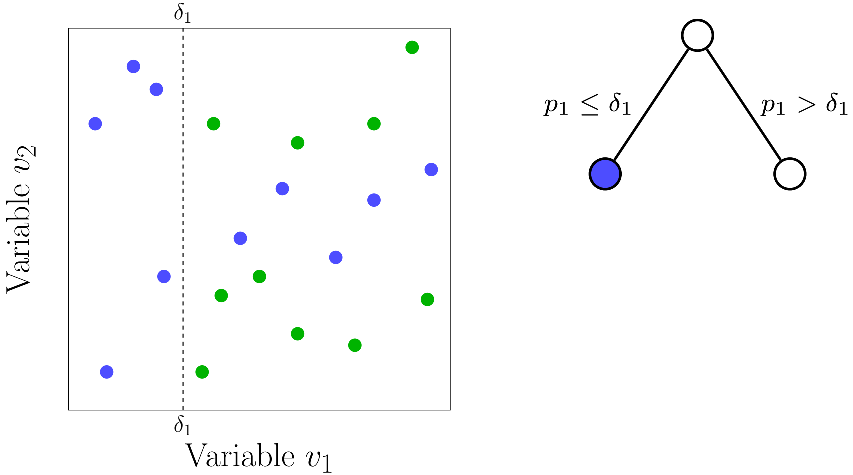
Decision trees



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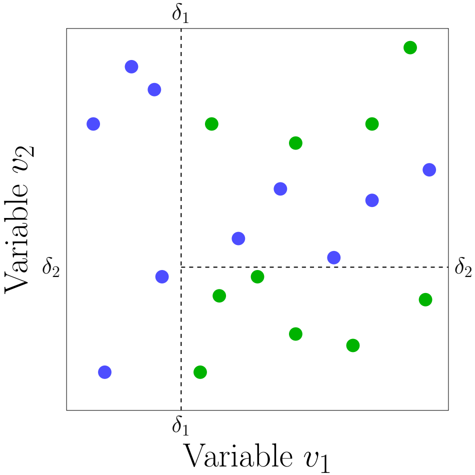
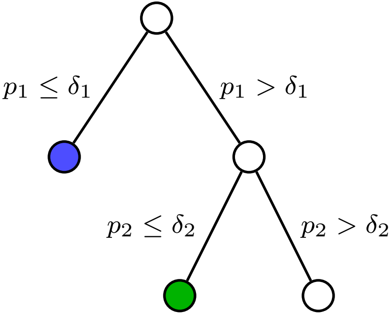
Decision trees





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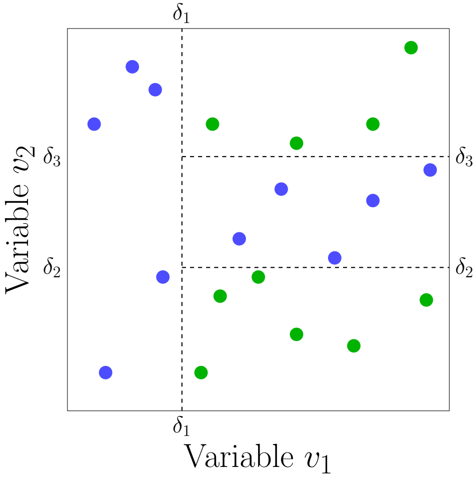
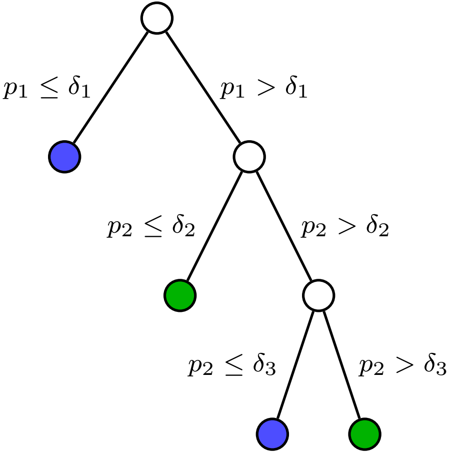
Decision trees





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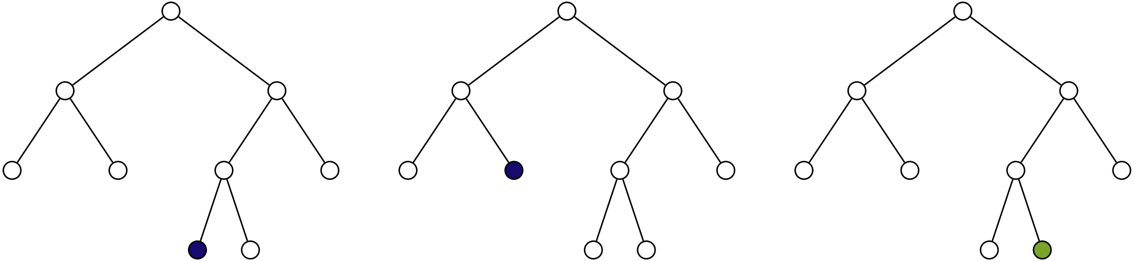
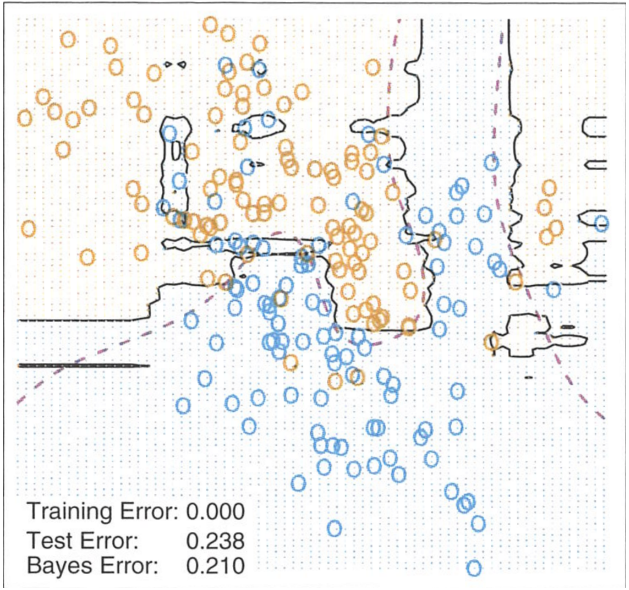
Random Forests

- 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 ← 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 → 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

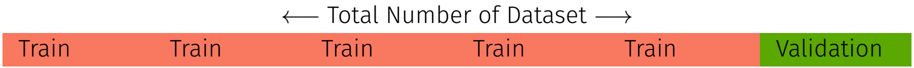
Model Selection vs Model Assessment

Model selection

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

Model Assessment

Estimate the generalization error on unseen/test sample



⟵ Total Number of Dataset ⟶

Train Train Train Train Train Validation

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:

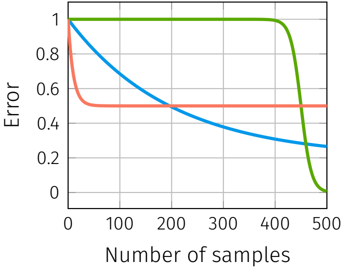
$$CV(\hat{f}, \theta) = \sum_{k=1}^{K} \text{Err}_k(\hat{f}, \theta)$$

PRATICAL ADVICES

- 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