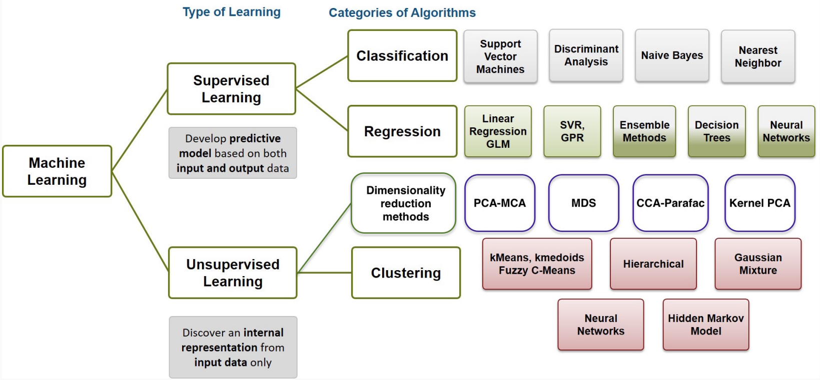
MSc Big Data for Business - *MAP 534*
Introduction to machine learning

Supervised classification

Linear/Quadratic discriminant analysis (LDA/QDA) & Support Vector Machines (SVM)

Machine Learning



Outline

Introduction to supervised learning

Bayes and Plug-in classifiers

Naive Bayes

Discriminant analysis (linear and quadratic)

Support Vector Machine

Supervised Learning Framework

→ Input measurement $\mathbf{X} \in \mathcal{X}$ (often $\mathcal{X} \subset \mathbb{R}^d$), output measurement $Y \in \mathcal{Y}$.

→ The joint distribution of $(\mathbf{X}, Y)$ is unknown.

→ $Y \in \{-1, 1\}$ (classification) or $Y \in \mathbb{R}^m$ (regression).

→ A predictor is a measurable function in $\mathcal{F} = \{f : \mathcal{X} \to \mathcal{Y}\}$.

Training data

→ $\mathcal{D}_n = \{(\mathbf{X}_1, Y_1), \ldots, (\mathbf{X}_n, Y_n)\}$ i.i.d. with the same distribution as $(\mathbf{X}, Y)$.

Goal

→ Construct a good predictor $\widehat{f}_n$ from the training data.

→ Need to specify the meaning of good.

Loss and Probabilistic Framework

Loss function

→ $\ell(Y, f(\mathbf{X}))$ measures the goodness of the prediction of Y by $f(\mathbf{X})$.

→ Prediction loss: $\ell(Y, f(\mathbf{X})) = \mathbf{1}_{Y \neq f(\mathbf{X})}$.

→ Quadratic loss: $\ell(Y, \mathbf{X}) = \|Y - f(\mathbf{X})\|^2$.

Risk function

→ Risk measured as the average loss:

$$\mathcal{R}(f) = \mathbb{E}\left[\ell(Y, f(\mathbf{X}))\right] .$$

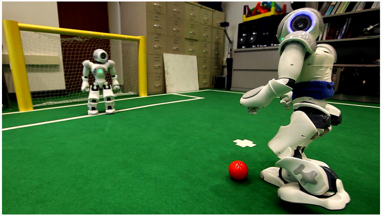
→ Prediction loss: $\mathbb{E}\left[\ell(Y, f(\mathbf{X}))\right] = \mathbb{P}\left(Y \neq f(\mathbf{X})\right)$.

→ Quadratic loss: $\mathbb{E}\left[\ell(Y, f(\mathbf{X}))\right] = \mathbb{E}\left[\|Y - f(\mathbf{X})\|^2\right]$.

→ **Beware:** As $\widehat{f}_n$ depends on $\mathcal{D}_n$, $\mathcal{R}(\widehat{f}_n)$ is a random variable!

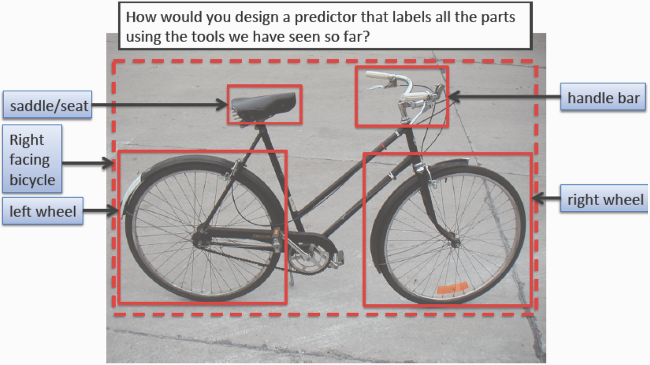
A robot that learns

A robot endowed with a set of sensors and an online learning algorithm.



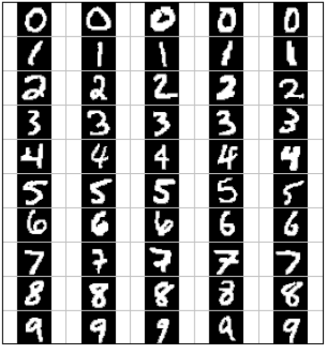
- Task: play football.
- Performance: score.
- Experience: current environment and outcome, past games...

Object recognition in an image



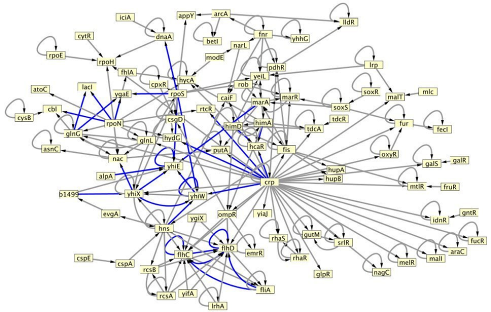
- Task: say if an object is present or not in the image.
- Performance: number of errors.
- Experience: set of previously seen labeled image.

Number



- → Task: Read a ZIP code from an envelop.
- → Performance: give a number from an image.
- → Prediction problem with $\mathbf{X}$: image and Y: corresponding number.

Applications in biology

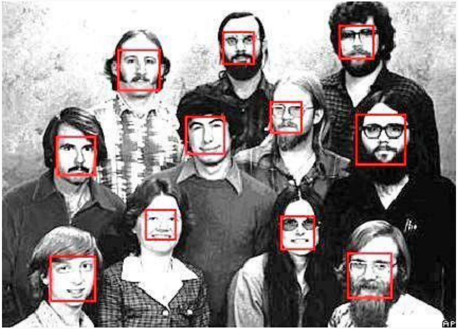


→ Task: protein interaction network prediction.

→ Goal: predict (unknown) interactions between proteins.

→ Prediction problem with **X**: pair of proteins and Y: existence or no of interaction.

Detection



→ Goal: detect the position of faces in an image.

→ $\mathbf{X}$: mask in the image and Y: presence or no of a face...

Classification

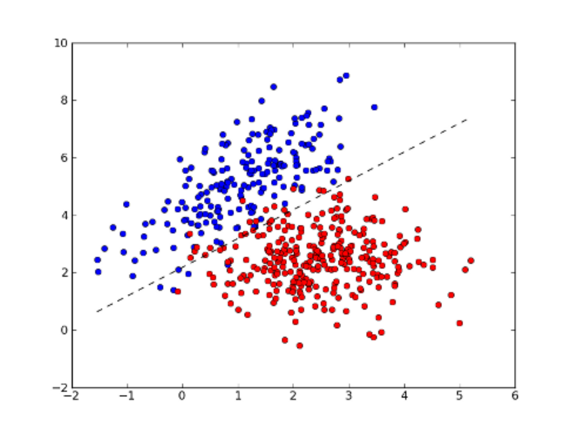
Setting

- Historical data about individuals $i = 1, \ldots, n$.
- **Features** vector $\mathbf{X}_i \in \mathbb{R}^d$ for each individual i.
- For each i, the individual belongs to a group $(Y_i = 1)$ or not $(Y_i = -1)$.
- $Y_i \in \{-1, 1\}$ is the **label** of i.

Aim

- Given a new $\mathbf{X}$ (with no corresponding label), predict a label in $\{-1, 1\}$.
- Use data $\mathcal{D}_n = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$ to construct a **classifier**.

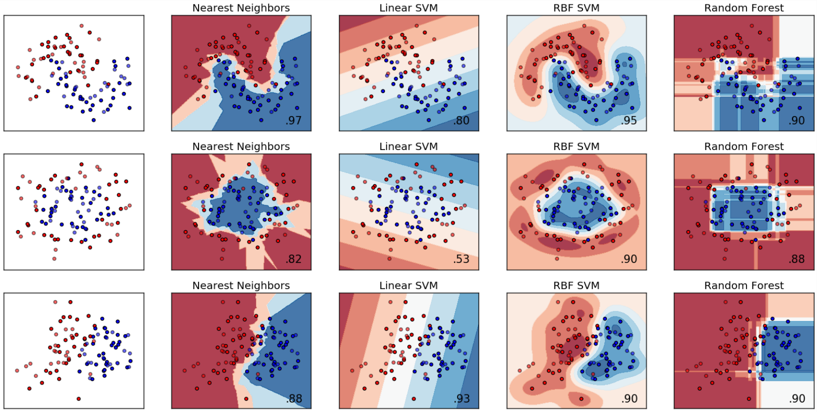
Geometrically



Learn a boundary to separate two “groups” of points.

Classification

...many ways to separate points!



Supervised learning methods

Support Vector Machine

Linear Discriminant Analysis

Logistic Regression

Trees/ Random Forests

Kernel methods

Neural Networks

Many more...

Outline

Best Solution

The best solution f^* (which is independent of $\mathcal{D}_n$) is

$$\boxed{f^* = \arg\min_{f\in\mathcal{F}} R(f) = \arg\min_{f\in\mathcal{F}} \mathbb{E}\left[\ell(Y, f(\mathbf{X}))\right] .}$$

Bayes Predictor (explicit solution)

→ Binary classification with $0-1$ loss:

$$f^*(\mathbf{X}) = \begin{cases} +1 & \text{if } \mathbb{P}\left(Y=1|\mathbf{X}\right) \geqslant \mathbb{P}\left(Y=-1|\mathbf{X}\right) \\ & \quad \Leftrightarrow \mathbb{P}\left(Y=1|\mathbf{X}\right) \geqslant 1/2\,, \\ -1 & \text{otherwise}\,. \end{cases}$$

→ Regression with the quadratic loss

$$f^*(\mathbf{X}) = \mathbb{E}\left[Y|\mathbf{X}\right] .$$

The explicit solution requires to know $\mathbb{E}\left[Y|\mathbf{X}\right]$...

Plugin Classifier

$\rightharpoondown$ In many cases, the conditional law of Y given $\mathbf{X}$ is not known... or relies on parameters to be estimated.

$\rightharpoondown$ An empirical surrogate of the Bayes classifier is obtained from a possibly nonparametric estimator $\widehat{\eta}_n(\mathbf{X})$ of

$$\boxed{\eta(\mathbf{x}) = \mathbb{P}(Y = 1|\mathbf{X})}$$

using the training dataset.

$\rightharpoondown$ This surrogate is then plugged into the Bayes classifier.

Plugin Bayes Classifier

$\rightharpoondown$ Binary classification with $0-1$ loss:

$$\widehat{f}_n(\mathbf{X}) = \begin{cases} +1 & \text{if } \quad \widehat{\eta}_n(\mathbf{X}) \geqslant 1/2\,, \\ -1 & \text{otherwise}\,. \end{cases}$$

Plugin Classifier

Input: a data set $\mathcal{D}_n$.

Learn the ditribution of Y given $\mathbf{X}$ (using the data set) and plug this estimate in the Bayes classifier.

Output: a classifier $\widehat{f}_n : \mathbb{R}^d \to \{-1, 1\}$

$$\widehat{f}_n(\mathbf{X}) = \begin{cases} +1 & \text{if } \widehat{\eta}_n(\mathbf{X}) \geqslant 1/2\,, \\ -1 & \text{otherwise}\,. \end{cases}$$

$\rightharpoondown$ Can we certify that the plug-in classifier is good ?

Classification Risk Analysis

The missclassification error satisfies (see exercices):

$$0 \leqslant \mathbb{P}(\widehat{f}_n(\mathbf{X}) \neq Y) - L^\star \leqslant 2\mathbb{E}\left[|\eta(\mathbf{X}) - \hat{\eta}_n(\mathbf{X})|^2\right]^{1/2},$$

where

$$L^\star = \mathbb{P}(f^\star(\mathbf{X}) \neq Y)$$

and $\widehat{\eta}_n(\mathbf{x})$ is an empirical estimate based on the training dataset of

$$\eta(\mathbf{x}) = \mathbb{P}(Y = 1 | \mathbf{X} = \mathbf{x}).$$

How to estimate the conditional law of Y?

Fully parametric modeling.

Estimate the law of $(\mathbf{X}, Y)$ and use the **Bayes formula** to deduce an estimate of the conditional law of Y: *LDA/QDA, Naive Bayes...*

Parametric conditional modeling.

Estimate the conditional law of Y by a **parametric** law: *linear regression, logistic regression, Feed Forward Neural Networks...*

Nonparametric conditional modeling.

Estimate the conditional law of Y by a **non parametric** estimate: *kernel methods, nearest neighbors...*

Fully Generative Modeling

If the law of $(\mathbf{X}, Y)$ **is known** everything can be easy!

Bayes formula

With a slight abuse of notation, if the law of $\mathbf{X}$ has a density g with respect to a reference measure,

$$\boxed{\mathbb{P}\left(Y = k|\mathbf{X}\right) = \frac{g_k(\mathbf{X})\mathbb{P}(Y=k)}{g(\mathbf{X})}\ ,}$$

where g_k is the density of the distribution of $\mathbf{X}$ given $\{Y = k\}$.

Generative Modeling

Propose a model for $(\mathbf{X}, Y)$.

Plug the conditional law of Y given $\mathbf{X}$ in the Bayes *classifier*.

Remark: require to model the joint law of $(\mathbf{X}, Y)$ rather than only the conditional law of Y.

Great flexibility in the model design but may lead to complex computation.

Outline

Naive Bayes

Classical algorithm using a crude modeling for $\mathbb{P}(\mathbf{X}|Y)$:

$\rightharpoondown$ Feature independence assumption:

$$\mathbb{P}(\mathbf{X}|Y) = \prod_{i=1}^{d} \mathbb{P}\left(X^{(i)}\middle|Y\right) .$$

$\rightharpoondown$ Simple featurewise model: binomial if binary, multinomial if finite and Gaussian if continuous.

If all features are continuous, the law of $\mathbf{X}$ given Y is Gaussian with a **diagonal covariance matrix**!

Very simple learning even in very high dimension!

Gaussian Naive Bayes

$\rightharpoondown$ Feature independence assumption:

$$\mathbb{P}\left(\mathbf{X}|Y\right) = \prod_{j=1}^{d} \mathbb{P}\left(X^{(j)}\middle|Y\right) .$$

For $k \in \{-1, 1\}$, $\mathbb{P}\left(Y = k\right) = \pi_k$ and the conditional density of $X^{(j)}$ given $\{Y = k\}$ is

$$\boxed{g_k(\mathbf{x}^{(j)}) = (2\pi\sigma_{j,k}^2)^{-1/2} \exp\left\{-(\mathbf{x}^{(j)} - \mu_{j,k})^2/(2\sigma_{j,k}^2)\right\} .}$$

The conditional distribution of $\mathbf{X}$ given $\{Y = k\}$ is then

$$\boxed{g_k(\mathbf{x}) = (\det(2\pi\Sigma_k))^{-1/2} \exp\left\{-(\mathbf{x} - \mu_k)^T \Sigma_k^{-1} (\mathbf{x} - \mu_k)/2\right\} ,}$$

where $\Sigma_k = \mathrm{diag}(\sigma_{1,k}^2, \ldots, \sigma_{d,k}^2)$ and $\mu_k = (\mu_{1,k}, \ldots, \mu_{d,k})^T$.

Gaussian Naive Bayes

In a two-classes problem, the optimal classifier is (see linear discriminant analysis below):

$$\boxed{f^* : \mathbf{X} \mapsto 2\mathbb{1}\{\mathbb{P}(Y = 1|\mathbf{X}) > \mathbb{P}(Y = -1|\mathbf{X})\} - 1\,.}$$

$\rightharpoondown$ When the parameters are unknown, they may be replaced by their maximum likelihood estimates.

This yields, for $k \in \{-1, 1\}$,

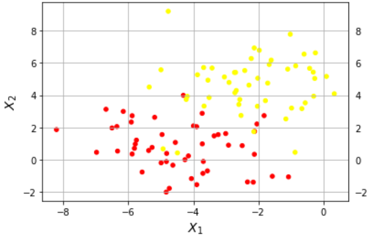
$$\widehat{\pi}_{\mathbf{k}}^{\mathbf{n}} = \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}_{Y_i=k}\,,$$

$$\widehat{\mu}_{\mathbf{k}}^{\mathbf{n}} = \frac{1}{\sum_{i=1}^{n} \mathbb{1}_{Y_i=k}} \sum_{i=1}^{n} \mathbb{1}_{Y_i=k} X_i\,,$$

$$\widehat{\Sigma}_k^n = \mathrm{diag}\left(\frac{1}{n}\sum_{i=1}^{n} (X_i - \widehat{\mu}_k^n)(X_i - \widehat{\mu}_k^n)^T \mathbb{1}_{Y_i=k}\right)\,.$$

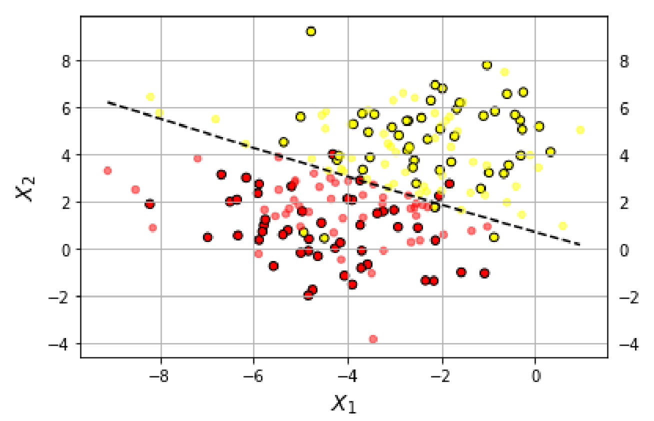
Gaussian Naive Bayes

```python
import numpy as np
import matplotlib.pyplot as plt
from sklearn.datasets import make_blobs

X, y = make_blobs(100, 2, centers = 2, cluster_std=1.5)
plt.scatter(X[:, 0], X[:, 1], c=y, s=20, cmap='autumn')
plt.ylabel(r"$X_2$", fontsize=14)
plt.xlabel(r"$X_1$", fontsize=14)
plt.tick_params(labelright=True)
plt.grid('True')
```



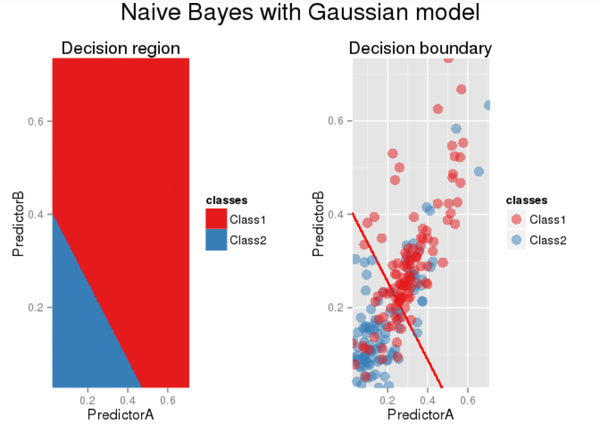
Gaussian Naive Bayes

```python
from sklearn.naive_bayes import GaussianNB
# Fit Naive Bayes to obtain the classifier
model = GaussianNB()
model.fit(X, y);

# Generate new data
Xnew = np.random.multivariate_normal([np.mean(X[:,0]),np.mean(X[:,1])], 4*np.eye(2), 100)
# Predict labels of new data from the classifier
ynew = model.predict(Xnew)

# Predict the classification probabilities on a grid
xgrid = (np.min(Xnew[:,0]), np.max(Xnew[:,0]))
ygrid = (np.min(Xnew[:,1]), np.max(Xnew[:,1]))
xx, yy = np.meshgrid(np.linspace(xgrid[0], xgrid[1], 100), np.linspace(ygrid[0], ygrid[1], 100))
Z = model.predict_proba(np.c_[xx.ravel(), yy.ravel()])
Z = Z[:, 1].reshape(xx.shape)

# Plot training data
plt.scatter(X[:, 0], X[:, 1], c = y, s = 30, edgecolors = 'black', cmap='autumn')
# Plot new data
plt.scatter(Xnew[:, 0], Xnew[:, 1], c = ynew, s = 20, cmap = 'autumn', alpha = 0.5)
# Plot classifier boundary
plt.contour(xx, yy, Z, [0.5], colors = 'k', linestyles = 'dashed')
plt.ylabel(r"$X_2$", fontsize=14)
plt.xlabel(r"$X_1$", fontsize=14)
plt.tick_params(labelright=True)
plt.grid(True)
```

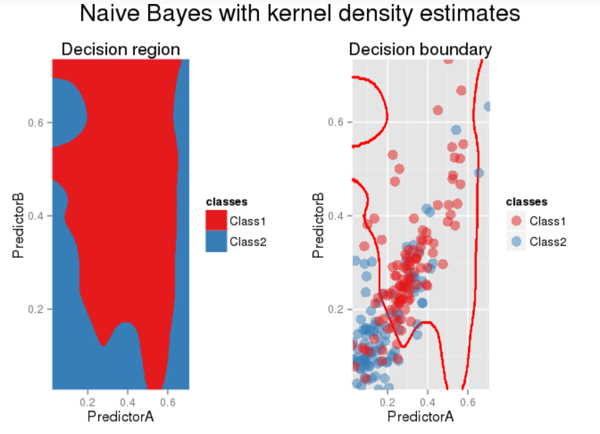


8
6
4
2
0
−2
−4
−8
−6
−4
−2
0
X_1
X_2

Gaussian Naive Bayes



Kernel density estimate based Naive Bayes



Outline

Discriminant Analysis (Gaussian model)

The conditional densities are modeled as multivariate normal. For all class k, conditionally on $\{Y = k\}$,

$$\mathbf{X} \sim \mathcal{N}(\mu_k, \Sigma_k)\,.$$

Discriminant functions:

$$g_k(\mathbf{X}) = \ln(\mathbb{P}\{\mathbf{X}|Y = k\}) + \ln(\mathbb{P}\,(Y = k))\,.$$

In a two-classes problem, the optimal classifier is (see exercises):

$$\boxed{f^* : x \mapsto 2\mathbb{1}\{g_1(x) > g_{-1}(x)\} - 1\,.}$$

QDA (differents Σ_k in each class) and LDA ($\Sigma_k = \Sigma$ for all k)

lightr: this model can be false but the methodology remains valid!

Estimation

In practice, μ_k, Σ_k and $\pi_k := \mathbb{P}\left(Y = k\right)$ have to be estimated.

$\rightharpoondown$ Estimated proportions $\widehat{\pi}_k = \frac{n_k}{n} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{1}_{\{Y_i = k\}}$.

$\rightharpoondown$ Maximum likelihood estimate of $\widehat{\mu_k}$ and $\widehat{\Sigma_k}$ (explicit formulas).

The DA classifier then becomes

$$\widehat{f}_n(\mathbf{X}) = \begin{cases} +1 & \text{if } \widehat{g}_1(\mathbf{X}) \geq \widehat{g}_{-1}(\mathbf{X})\,, \\ -1 & \text{otherwise}\,. \end{cases}$$

If $\Sigma_{-1} = \Sigma_1 = \Sigma$ then the **decision boundary is an affine hyperplane**.

The loglikelihood of the observations is given by

$$\log \mathbb{P}_\theta\left(X_{1:n}, Y_{1:n}\right) = \sum_{i=1}^{n} \log \mathbb{P}_\theta\left(X_i, Y_i\right) ,$$

$$= -\frac{nd}{2}\log(2\pi) - \frac{n}{2}\log\det(\Sigma) + \left(\sum_{i=1}^{n} \mathbb{1}_{Y_i=1}\right)\log\pi_1 + \left(\sum_{i=1}^{n} \mathbb{1}_{Y_i=-1}\right)\log(1-\pi_1)$$

$$-\frac{1}{2}\sum_{i=1}^{n}\mathbb{1}_{Y_i=1}(X_i-\mu_1)^T\Sigma^{-1}(X_i-\mu_1) - \frac{1}{2}\sum_{i=1}^{n}\mathbb{1}_{Y_i=-1}(X_i-\mu_{-1})^T\Sigma^{-1}(X_i-\mu_{-1}) .$$

This yields, for $k \in \{-1, 1\}$,

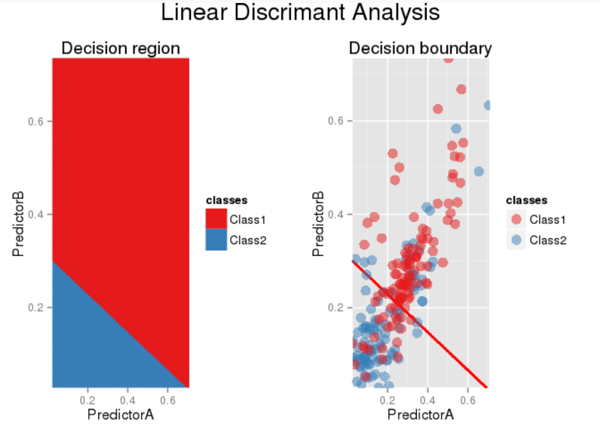
$$\widehat{\pi}^{\mathbf{n}}_{\mathbf{k}} = \frac{1}{n}\sum_{i=1}^{n}\mathbb{1}_{Y_i=k} ,$$

$$\widehat{\mu}^{\mathbf{n}}_{\mathbf{k}} = \frac{1}{\sum_{i=1}^{n}\mathbb{1}_{Y_i=k}}\sum_{i=1}^{n}\mathbb{1}_{Y_i=k}X_i ,$$

$$\widehat{\Sigma}^n = \frac{1}{n}\sum_{i=1}^{n}\left(X_i - \widehat{\mu}^n_{Y_i}\right)\left(X_i - \widehat{\mu}^n_{Y_i}\right)^T .$$

Remains to plug these estimates in the classification boundary.

Example: LDA

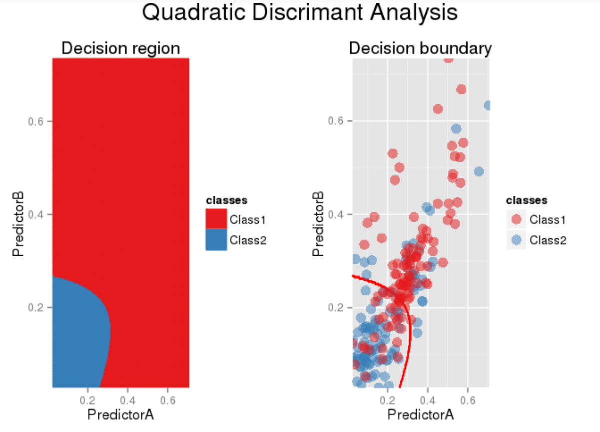


Linear Discriminant Analysis
Decision region
Decision boundary
PredictorB
PredictorA
0.2
0.4
0.6
classes
Class1
Class2

Example: LDA

```r
boundary_true_parameters = function(x, mu0, mu1, Sigma, pi0){
  u = t(as.matrix(mu1-mu0)) %*% inv(Sigma)
  v = (u %*% (matrix(x - ((mu1+mu0)/2)) )) - log(pi0/(1-pi0))
  return(as.numeric(v))
}
```

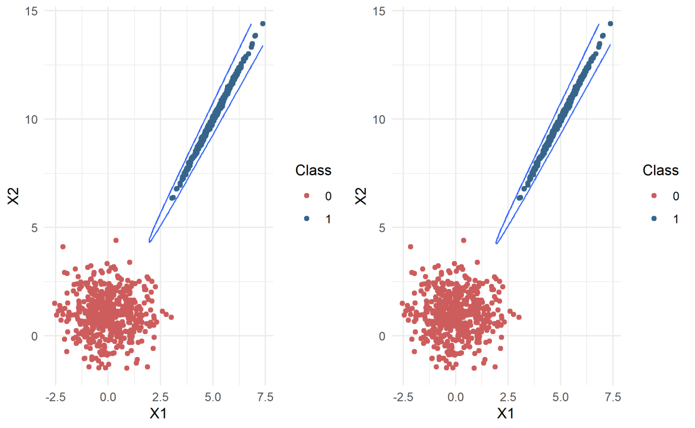
Example: QDA



Quadratic Discrimant Analysis
Decision region
Decision boundary
PredictorB
PredictorA
0.2
0.4
0.6
classes
Class1
Class2

Example: QDA

```r
boundary_true_parameters_quadratic = function(x, mu0, mu1, Sigma0, Sigma1, pi0){

  u1 =  -0.5*(t(as.matrix(x-mu1))) %*% inv(Sigma1) %*% as.matrix((x - mu1))
  u0 =  0.5*(t(as.matrix(x-mu0))) %*% inv(Sigma0) %*% as.matrix((x - mu0))
  cste = - log(pi0/(1-pi0))
  bonus = -0.5*log(abs(det(Sigma1))) + 0.5*log(abs(det(Sigma0)))

  return(as.numeric(u1+u0+cste+bonus))
}
```



Packages in R

Function `svm` in package `e1071`.

Function `lda` and `qda` in package `MASS`.

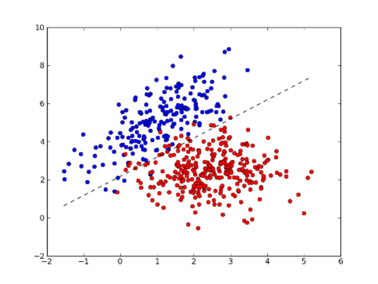
Function `naive_bayes` in package `naivebayes`.

Outline

Linear classification

→ Simple to interpret and to implement.

→ On very large datasets ($n \geqslant 10^6$), no other choice (training complexity).



→ Learn $\hat{\mathbf{w}} \in \mathbb{R}^d$ and $\hat{b}$ to build the classifier:

$$\boxed{\hat{Y} = \mathrm{sign}(\langle \mathbf{X}, \hat{\mathbf{w}} \rangle + \hat{b})\,.}$$

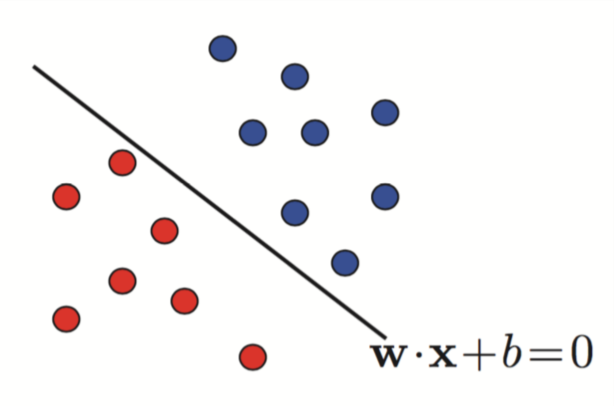
Linearly separable data

A dataset is **linearly separable** if there exists an hyperplane H (linear classification rule) such that the following assumptions hold.

→ Points $\mathbf{X}_i \in \mathbb{R}^d$ such that $Y_i = 1$ are on one side of the hyperplane.

→ Points $\mathbf{X}_i \in \mathbb{R}^d$ such that $Y_i = -1$ are on the other side.

→ H does not pass through any point $\mathbf{X}_i$.



Some geometry

A **hyperplane** is a translation of a set of vectors orthogonal to $\mathbf{w}$.

$$\boxed{H_{\mathbf{w},b} = \{\mathbf{x} \in \mathbb{R}^d : \langle \mathbf{w}, \mathbf{x} \rangle + b = 0\}\,.}$$

$\rightharpoonup$ $\mathbf{w} \in \mathbb{R}^d$ is a **non-zero vector normal** to the hyperplane. $\rightharpoonup$ $b \in \mathbb{R}$ is a scalar.

Following for instance the results obtained for linear discriminant analysis and logistic regression, a hyperplane $H_{\mathbf{w},b}$ may be used as a classifier by defining

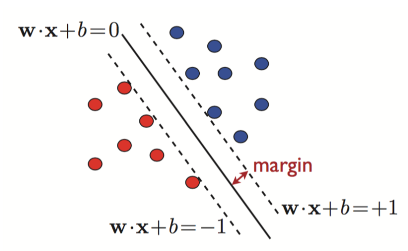
$$h_{\mathbf{w},b} : \mathbf{x} \mapsto \begin{cases} 1 & \text{if } \langle \mathbf{w}\,;\, \mathbf{x} \rangle + b > 0\,, \\ -1 & \text{otherwise}\,. \end{cases}$$

Some geometry

Definition of $H_{\mathbf{w},b}$ is invariant by multiplication of $\mathbf{w}$ and b by a non-zero scalar.

If $H_{\mathbf{w},b}$ does not pass through any sample point $\mathbf{x}_i$, $\mathbf{w}$ and b can be scaled so that

$$\boxed{\min_{(\mathbf{x},y)\in\mathcal{D}_n} |\langle \mathbf{w}, \mathbf{x}\rangle + b| = 1\,.}$$



For such $\mathbf{w}$ and b, we call H the *canonical* hyperplane.

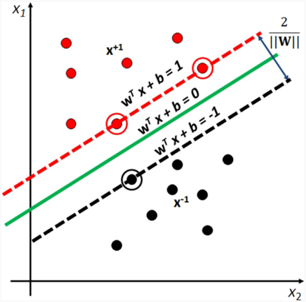
Some geometry

The distance of any point $\mathbf{x}' \in \mathbb{R}^d$ to $H_{\mathbf{w},b}$ is

$$\frac{|\langle \mathbf{w}, \mathbf{x}' \rangle + b|}{\|\mathbf{w}\|}$$

If $H_{\mathbf{w},b}$ is a canonical hyperplane, its margin is given by

$$\boxed{\min_{(\mathbf{x},y)\in\mathcal{D}_n} \frac{|\langle \mathbf{w},\mathbf{x} \rangle + b|}{\|\mathbf{w}\|} = \frac{1}{\|\mathbf{w}\|}\ .}$$



Linear separability and margin

If $\mathcal{D}_n$ is strictly linearly separable, there exists a canonical separating hyperplane

$$\boxed{H_{\mathbf{w},b} = \{\mathbf{x} \in \mathbb{R}^d : \langle \mathbf{w}, \mathbf{x} \rangle + b = 0\}}$$

that satisfies

$$|\langle \mathbf{w}, \mathbf{X}_i \rangle + b| \geqslant 1 \quad \text{for any} \quad i = 1, \ldots, n\,.$$

An individual $\mathbf{X}_i$ is correctly classified if

$$Y_i(\langle \mathbf{X}_i, \mathbf{w} \rangle + b) \geqslant 1\,.$$

The margin of $H_{\mathbf{w},b}$ is equal to $1/\|\mathbf{w}\|$.

Linear SVM: separable case

Hard Support Vector Machines is a classification procedure which aims at building a linear classifier with the largest possible margin, i.e. the largest minimal distance between a point in the training set and the hyperplane.

The hyperplane which **correctly separates all training data sets with the largest margin** is obtained with:

$$(\widehat{w}_n, \widehat{b}_n) \in \underset{\substack{(w,b)\in\mathbb{R}^d\times\mathbb{R}^d\,;\,\|w\|=1,\\ \forall i\in\{1,\ldots,n\},\, Y_i(\langle w\,;\,\mathbf{X}_i\rangle+b)>0}}{\mathrm{argmax}} \left\{\min_{1\leqslant i\leqslant n} |\langle w\,;\,\mathbf{X}_i\rangle + b|\right\}.$$

Linear SVM: separable case

The **hard Support Vector Machines** procedure is equivalent to solving the following optimization problem:

$$(\widehat{w}_n, \widehat{b}_n) \in \underset{(w,b)\in\mathbb{R}^d\times\mathbb{R}\,;\,\|w\|=1}{\operatorname{argmax}} \left\{ \min_{1\leqslant i\leqslant n} Y_i\left(\langle w\,;\, X_i\rangle + b\right)\right\}\,,$$

A solution to the hard Support Vector Machines optimization problem is obtained by setting $(\widehat{w}_n, \widehat{b}_n) = (w_\star/\|w_\star\|, b_\star/\|w_\star\|)$ where

$$(w_\star, b_\star) \in \underset{\substack{(w,b)\in\mathbb{R}^d\times\mathbb{R}\\ \forall i\in\{1,\ldots,n\},\, Y_i(\langle w\,;\,X_i\rangle+b)\geqslant 1}}{\operatorname{argmin}} \|w\|^2\,.$$

Linear SVM: separable case

A way of classifying $\mathcal{D}_n$ with maximum margin is to solve the following problem:

$$\boxed{(w_\star, b_\star) \in \underset{\substack{(w,b)\in\mathbb{R}^d\times\mathbb{R} \\ \forall i\in\{1,\dots,n\},\ Y_i(\langle w\,;X_i\rangle+b)\geqslant 1}}{\operatorname{argmin}} \|w\|^2 \,.}$$

→ This problem admits a **unique** solution.

→ It is a **quadratic programming** problem, which is easy to solve numerically.

→ Dedicated optimization algorithms can solve this on a large scale very efficiently.

Linear SVM: separable case

The optimization problem is solved using Karush-Kuhn-Tucker's theorem.

There are $\alpha_i \geqslant 0$, $i = 1, \ldots, n$, called dual variables, such that the solution $(\mathbf{w}, b)$ of this problem satisfies:

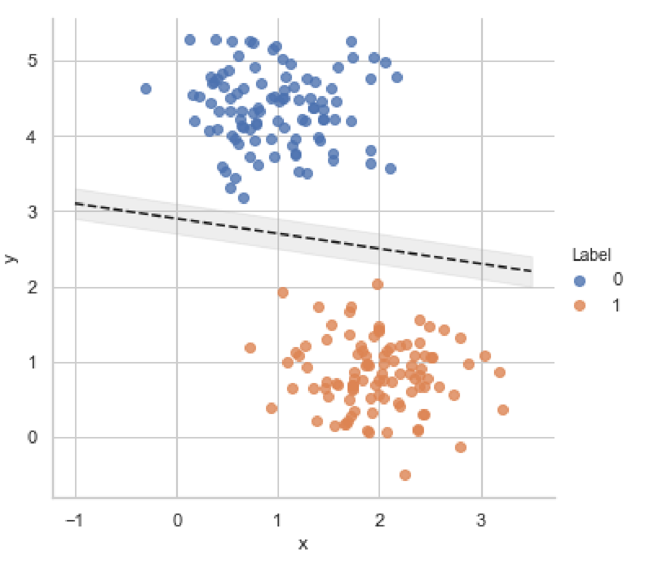
$$\boxed{\mathbf{w} = \sum_{i=1}^n \alpha_i Y_i \mathbf{X}_i \quad \text{and} \quad \alpha_i((Y_i\langle \mathbf{w}, \mathbf{X}_i\rangle + b) - 1) = 0 \;\; \text{for} \;\; i = 1, \ldots, n\,.}$$

$\rightharpoondown$ $\alpha_i \neq 0$ if and only if $Y_i\langle \mathbf{w}, \mathbf{X}_i\rangle + b = 1$, meaning that $\mathbf{X}_i$ is on the marginal hyperplane.

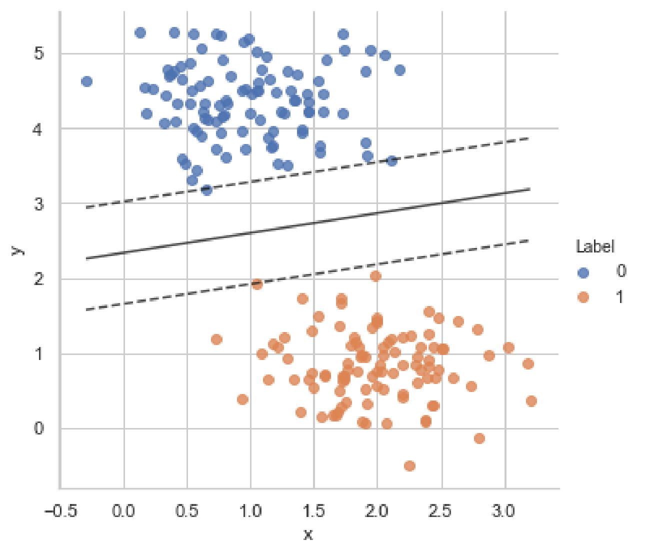
$\rightharpoondown$ Weights vector $\mathbf{w}$ is a linear combination of the vectors $\mathbf{x}_i$ that belong to a marginal hyperplane.

$\rightharpoondown$ Such points $\mathbf{x}_i$ are called **support vectors**.

```python
X, y = make_blobs(n_samples = 200, centers = 2, random_state = 0, cluster_std = 0.50)
simulated_data = pd.DataFrame(columns = ["X1","X2","Label"])

simulated_data["x"]     = X[:,0]
simulated_data["y"]     = X[:,1]
simulated_data["Label"] = y

# Use the 'Label' argument to provide a factor variable
sns.set_style("whitegrid")
sns.lmplot(x = "x", y = "y", data = simulated_data, fit_reg = False, hue = 'Label', legend = True)

slope  = 1.1
offset = 0.85
margin = 0.2

xfit = np.linspace(-1, 3.5)
yfit = m * xfit + b

plt.plot(xfit, yfit, '--k')
plt.fill_between(xfit, yfit - d, yfit + d, color = '#AAAAAA', alpha = 0.2)
```

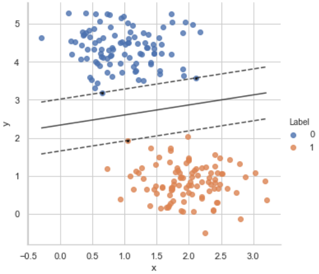

5
4
3
2
1
0
y
−1
0
1
2
3
x
Label
0
1

```python
# Classification based on a support vector classifier
model = SVC(kernel='linear', C=10)
model.fit(X, y)
sns.set_style("whitegrid")
sns.lmplot(x = "x", y = "y", data = simulated_data, fit_reg = False, hue = 'Label', legend = True)

xlim  = [np.min(X[:,0]), np.max(X[:,0])]
ylim  = [np.min(X[:,1]), np.max(X[:,1])]
xplot = np.linspace(xlim[0], xlim[1], 30)
yplot = np.linspace(ylim[0], ylim[1], 30)

Yplot, Xplot = np.meshgrid(yplot, xplot)
xy           = np.vstack([Xplot.ravel(), Yplot.ravel()]).T
P            = model.decision_function(xy).reshape(Xplot.shape)

# plot decision boundary and margins
plt.contour(Xplot, Yplot, P, colors = 'k', levels = [-1, 0, 1], alpha = 0.8,
            linestyles = ['--', '-', '--'])
```



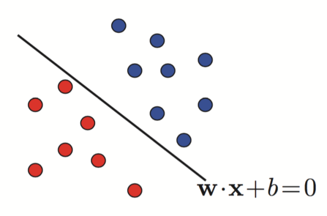
5
4
3
2
1
0
y
−0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
x
Label
0
1

```python
sns.set_style("whitegrid")
sns.lmplot(x = "x", y = "y", data = simulated_data, fit_reg = False, hue = 'Label', legend = True)
# plot decision boundary and margins
plt.contour(Xplot, Yplot, P, colors = 'k', levels = [-1, 0, 1], alpha = 0.8,
            linestyles = ['--', '-', '--'])
plt.scatter(model.support_vectors_[:, 0], model.support_vectors_[:, 1], s = 5, c = 'k');
```



Linear SVM: non-separable case

Have you ever seen a dataset that looks that this?



$\rightharpoondown$ Restricting the problem to linearly separable training data sets is a somehow strong assumption.

$\rightharpoondown$ Inequality constraints in the quadratic optimization problem can be relaxed.

$\rightharpoondown$ Introduction of nonnegative variables $(\xi_i)_{1\leqslant i\leqslant n}$ which quantify the nonfeasability of the constraint $Y_i(\langle \mathbf{w}\,;\,\mathbf{X}_i\rangle + b) \geqslant 1$.

$$Y_i(\langle \mathbf{w}, \mathbf{X}_i\rangle + b) \geqslant 1 - \xi_i\,.$$

Linear SVM: non-separable case

The original problem is then replaced by

$$(w_\star, b_\star, \xi_\star) \in \underset{\substack{(w,b,\xi)\in\mathbb{R}^d\times\mathbb{R}\times\mathbb{R}_+^d \\ \forall i\in\{1,\ldots,n\},\, Y_i(\langle w\,;X_i\rangle+b)\geqslant 1-\xi_i}}{\operatorname{argmin}} \left\{ \lambda\|w\|^2 + \frac{1}{n}\sum_{i=1}^n \xi_i \right\},$$

where $\lambda > 0$.

The **soft Support Vector Machines** algorithm minimizes simultaneously the margin of the linear classifier and the average value of these slack variables.

Note that, if $(w_\star, b_\star)$ is solution to

$$(w_\star, b_\star) \in \underset{(w,b)\in\mathbb{R}^d\times\mathbb{R}}{\operatorname{argmin}} \left\{ \lambda\|w\|^2 + \frac{1}{n}\sum_{i=1}^n (1 - Y_i\left(\langle w\,;X_i\rangle + b\right))_+ \right\},$$

then $(w_\star/\|w_\star\|, b_\star, \xi_\star/\|w_\star\|)$ is solution to the soft SVM problem.

Linear SVM: non-separable case

The **soft SVM problem boils down** to computing:

$$(w_\star, b_\star, \xi_\star) \in \underset{\substack{(w,b,\xi)\in\mathbb{R}^d\times\mathbb{R}\times\mathbb{R}_+^d \\ \forall i\in\{1,\ldots,n\},\, Y_i(\langle w\,;X_i\rangle+b)\geqslant 1-\xi_i}}{\operatorname{argmin}} \left\{ \lambda\|w\|^2 + \frac{1}{n}\sum_{i=1}^{n}\xi_i \right\},$$

where $\lambda > 0$.

→ This problem admits a **unique** solution.

→ It is a **quadratic programming** problem, which is easy to solve numerically.

→ Dedicated optimization algorithms can solve this on a large scale very efficiently.

The hinge loss

This problem can be reformulated as follows

$$\operatorname*{argmin}_{\mathbf{w}\in\mathbb{R}^d, b\in\mathbb{R}} \left\{ \frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{i=1}^{n} \max\Big(0, 1 - y_i(\langle \mathbf{x}_i, \mathbf{w}\rangle + b)\Big) \right\},$$

By introducing the hinge loss

$$\ell(y, y') = \max(0, 1 - yy') = (1 - yy')_+,$$

the problem can be written as

$$\operatorname*{argmin}_{\mathbf{w}\in\mathbb{R}^d, b\in\mathbb{R}} \left\{ \frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{i=1}^{n} \ell(y_i, \langle \mathbf{x}_i, \mathbf{w}\rangle + b) \right\}.$$

$\rightharpoondown$ Specific loss functions ℓ in a general setting.

The joint law of (X, Y) is **not assumed to belong to any parametric or semiparametric** family of models.

The classification risk **cannot be computed nor minimized**, it is instead estimated by the empirical classification risk defined as

$$\widehat{L}^n_{\mathrm{miss}}(f) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}_{Y_i \neq f(\mathbf{X}_i)}\,,$$

where $(X_i, Y_i)_{1\leqslant i\leqslant n}$ are independent with the same distribution as (X, Y).

The classification problem then boils down to solving

$$\widehat{f}^n \in \operatorname*{argmin}_{f\in\mathcal{F}} \widehat{L}^n_{\mathrm{miss}}(f)\,,$$

for a chosen class $\mathcal{F}$ of classifiers.

Introduction to nonparametric classification

Nonparametric classification based on the empirical risk minimization may seem appealing

It cannot be used to derive efficient practical classifiers due to **the computational cost of the optimization problem**.

The target loss function $\widehat{L}^n_{\mathrm{miss}}$ is replaced by **a convex surrogate and its minimization is constrained to a convex set of classifiers**.

For any convex function $\phi : \mathcal{X} \to \mathbb{R}$, it is possible to build a classifier f given by $f_\phi = \mathrm{sign}(\phi)$. The associated empirical classification is then

$$\widehat{L}^n_{\mathrm{miss}}(\phi) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}_{Y_i \neq f_\phi(X_i)} = \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}_{Y_i\phi(X_i)<0}\,.$$

Replacing the indicator function by **any convex loss funtion ℓ yields a convex surrogate**:

$$\widehat{L}^{n,\mathrm{conv}}_{\mathrm{miss}}(\phi) = \frac{1}{n}\sum_{i=1}^{n} \ell(Y_i \phi(X_i))\,.$$

Penalizing the smoothness of the function ϕ is penalized, $\widehat{L}^{n,\mathrm{conv}}_{\mathrm{miss}}$ may be replaced by

$$\widehat{L}^{n,\mathrm{conv}}_{\mathrm{miss}}(\phi) = \frac{1}{n}\sum_{i=1}^{n} \ell(Y_i \phi(X_i)) + \lambda \|\phi\|^2\,,$$

where $\lambda > 0$ and $\|\cdot\|$ is a norm on the space $\mathcal{H}$.

The soft Support Vector Machines algorithm fits this framework with the affine base function $\phi : \mathbf{x} \mapsto \langle \mathbf{w}\,;\,\mathbf{x}\rangle + b$ and ℓ chosen as the hinge loss $\ell : x \mapsto (1-x)_+$ when the target function is penalized by its margin $\|w\|^2$.

Kernel trick

A useful case in practice consists in choosing $\mathcal{H}$ as a **Reproducing Kernel Hilbert Space** with positive definite kernel k on $\mathcal{X} \times \mathcal{X}$.

A function k on $\mathcal{X} \times \mathcal{X}$ is said to be **a positive definite kernel** if and only if it is symmetric and if for all $n \geqslant 1$, $(x_1, \ldots, x_n) \in \mathcal{X}^n$ and all $(a_1, \ldots, a_n) \in \mathbb{R}^n$,

$$\sum_{1 \leqslant i,j \leqslant n} a_i a_j k(x_i, x_j) \geqslant 0\,.$$

The **Reproducing Kernel Hilbert Space** with kernel k is the only Hilbert space $\mathcal{H} \subset \mathbb{R}^{\mathcal{X}}$ such that for all $x \in \mathcal{X}$, $k(x, \cdot) \in \mathcal{H}$ and for all $x \in \mathcal{X}$ and all $f \in \mathcal{H}$,

$$f(x) = \langle f\,;\,k(x, \cdot)\rangle_{\mathcal{H}}\,.$$

Kernel trick

$k : \mathcal{X} \times \mathcal{X} :\to \mathbb{R}$ a positive definite kernel and $\mathcal{H}$ the RKHS with kernel k.

$$\widehat{\phi}^n_{\mathcal{H}} \in \underset{\phi \in \mathcal{H}}{\text{argmin}}\ \frac{1}{n} \sum_{i=1}^{n} \ell(Y_i \phi(X_i)) + \lambda \|\phi\|^2_{\mathcal{H}}\,,$$

where $\|\phi\|^2_{\mathcal{H}} = \langle \phi\,;\, \phi \rangle$, is given by

$$\widehat{\phi}^n_{\mathcal{H}} : x \mapsto \sum_{i=1}^{n} \widehat{\alpha}_i k(X_i, x)\,,$$

with

$$\widehat{\alpha} \in \underset{\alpha \in \mathbb{R}^n}{\text{argmin}} \left\{ \frac{1}{n} \sum_{i=1}^{n} \ell\left(\sum_{j=1}^{n} \alpha_j Y_i k(X_j, X_i) \right) + \lambda \sum_{1 \leqslant i,j \leqslant n} \alpha_i \alpha_j k(X_i, X_j) \right\}.$$