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Machine Learning in Finance

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Calibration versus Prediction

We distinguish several type of statistical problems :

- Regression problems where Y and X are quantitative variables and where Y is inferred by a function $f(X)$
- Classification problems where Y is a qualitative variable and where the class of Y is inferred from X
- Clusterization problems where a quantitative variable X is observed and classified into groups of similar features.

Remarks: Often a qualitative variable will be "coded" for modelisation purposes into a quantitative variable but usually without any implicit order relationship or proximity notion between the values coded, and this contrarily to what would happen for "native" quantitative variables.

Calibration versus Prediction

We will focus mainly on classification problems where:

- Y is a binary variable and X is a quantitative variable in \mathbb{R}^d .
- $(X^1, Y^1), (X^2, Y^2), \dots, (X^n, Y^n)$ are observations

The issue is to choose:

- a particular class of models $\mathcal{F} \in \{\mathcal{F}_\alpha\}$
- a function f within \mathcal{F} to estimate Y by $f(X)$

We define a measure of error between Y and $f(X)$ as :

- $\|Y - f(X)\|$ for a regression problem
- $1_{Y \neq f(X)}$ for a classification problem

Mathematically in a classification problem the goal is to find f which minimizes the risk $E[1_{f(X) \neq Y}]$

Definition: Calibration Error and Expected Error

For any f in \mathcal{F} we note:

- $R(f) := E[1_{f(X) \neq Y}]$
- $R_n(f) := \frac{1}{n} \sum_{i=1}^{i=n} 1_{f(X_i) \neq Y_i}$

Calibration associates to a sample $(X_i, Y_i)_{i \in \llbracket 1, n \rrbracket}$ an element f_n of \mathcal{F} which minimizes $R_n(f)$. By doing so f_n is a random variable taking its value in \mathcal{F} and we define by extension for f_n :

- $R_n(f_n) := \frac{1}{n} \sum_{i=1}^{i=n} 1_{f_n(X_i) \neq Y_i}$ the calibration error for f_n
- $R(f_n) := E[1_{f_n(X_{n+1}) \neq Y_{n+1}}]$ the expected error for f_n

Proposition: Calibration Error and Expected Error

$E[R_n(f_n)] \leq R(f_n)$ which means (not surprisingly) that the expected error on calibration is less than the expected error on prediction, i.e that it is easier to calibrate than to predict...

Demonstration: $R_n(f_n) = \min_{f \in \mathcal{F}} R_n(f)$ so, $E[R_n(f_n)] = E[\min_{f \in \mathcal{F}} R_n(f)]$

but $E[\min_{f \in \mathcal{F}} R_n(f)] \leq \min_{f \in \mathcal{F}} E[R_n(f)] = \min_{f \in \mathcal{F}} E[1_{f(X_{n+1}) \neq Y_{n+1}}]$

$\forall (X_i, Y_i)_{i \in \llbracket 1, n \rrbracket} f_n \in \mathcal{F}$ so:

$E[1_{f_n(X_{n+1}) \neq Y_{n+1}} / (X_i, Y_i)_{i \in \llbracket 1, n \rrbracket}] \geq \min_{f \in \mathcal{F}} E[1_{f(X_{n+1}) \neq Y_{n+1}}]$

by taking the expectation we get:

$E[1_{f_n(X_{n+1}) \neq Y_{n+1}}] \geq \min_{f \in \mathcal{F}} E[1_{f(X_{n+1}) \neq Y_{n+1}}]$ so in conclusion

$R(f_n) = E[1_{f_n(X_{n+1}) \neq Y_{n+1}}] \geq \min_{f \in \mathcal{F}} E[1_{f(X_{n+1}) \neq Y_{n+1}}] \geq E[\min_{f \in \mathcal{F}} R_n(f)] =$

$E[R(f_n)]$. Q.E.D

Calibration versus Prediction - Risk Measure

Example: Let (X, Y) be random variables with $X \sim \mathcal{U}([0, 1])$ and $Y = 1_{X \leq a}$ with $a \in]0, 1[$.

We assume that we do not know the existing relationship between X and Y but want to build a classifier based on some sampling $(X_i, Y_i)_{i \in \llbracket 1, n \rrbracket}$ and a machine $\mathcal{F} = \{1_{X \leq \alpha}, 1_{X \geq \alpha}\}_{\alpha \in \mathbb{R}}$.

If we assume that when observing $(X_i, Y_i)_{i \in \llbracket 1, n \rrbracket}$ we choose the classifier $f_n = 1_{X \leq \text{Max}(X_1 1_{\{Y_1=1\}}, X_2 1_{\{Y_2=1\}}, \dots, X_n 1_{\{Y_n=1\}})}$ of \mathcal{F} then show that:

- $R_n(f_n) = 0$
- $R(f_n) = \frac{1 - (1-a)^{n+1}}{n+1}$

Hint: $R(f_n) = \int_0^a P\left(\max_{i \in \llbracket 1, n \rrbracket} X_i 1_{\{X_i < a\}} < u\right) du$

Calibration versus Prediction

Our goal is:

- not so much to explain perfectly what has happened (calibration) but
- to be as precise as possible in the prediction

So we face a dilemma as:

- a model which has too many parameters may enable perfect calibration but lead to over-fitting and a poor quality of prediction
- a too simplistic model which fits only very poorly the sample data has no chance to predict accurately

The Vapnik Chernovenkis theorem enables to control $R(f_n)$ based on:

- $R_n(f_n)$
- the complexity, noted $VC(\mathcal{F})$, of the model \mathcal{F}

Remarks: in Machine Learning

- each family \mathcal{F}_α of estimators is called a machine
- the phase of calibration is called the learning phase
- if the Y_i are known in the sample and thus an error of calibration can be calculated, the learning is said to be supervised

Definition: VC dimension of \mathbb{R}^d classifiers

Let $\mathcal{F} = \{f_\alpha\}_{\alpha \in \mathcal{E}}$ be a family of classifiers, each f_α being a function from \mathbb{R}^d to $\{0, 1\}$.

The Vapnik Chervonenkis dimension of \mathcal{F} noted $VC(\mathcal{F})$ is the maximum number of points of \mathbb{R}^d that can be classified in all possible different ways by some classifiers of \mathcal{F} .

Calibration versus Prediction - VC dimension

Remarks: $VC(\mathcal{F}) = k$ if and only if it is possible to find k points $(x_i)_{i \in \llbracket 1, k \rrbracket}$ in \mathbb{R}^d such that for any of the 2^k possible labelling $(y_i)_{i \in \llbracket 1, k \rrbracket}$ in $\{0, 1\}^k$ it is possible to find f in \mathcal{F} such that $\forall i \in \llbracket 1, k \rrbracket, f(x_i) = y_i$.

VC Theorem (admitted): Confidence interval for the risk of prediction

We note $(X_i, Y_i)_{i \in \llbracket 1, n \rrbracket}$ a i.i.d sample of (X, Y)

Let $\mathcal{F} = \{f_\alpha\}_{\alpha \in \mathcal{E}}$ be a machine with $VC(\mathcal{F}) < n$

Let f_n be defined by $R_n(f_n) = \min_{f \in \mathcal{F}} R_n(f)$ for the learning sample

$(X_i, Y_i)_{i \in \llbracket 1, n \rrbracket}$, then:

$$\forall \eta \in [0, 1], P \left(R(f_n) > R_n(f_n) + \phi_{n, \eta} \left(\frac{VC(\mathcal{F})}{n} \right) \right) \leq \eta$$

where $\phi_{n, \eta}(x) = \sqrt{x(1 + \ln(\frac{2}{x}))} + \frac{1}{n} \ln(\frac{4}{\eta})$ so

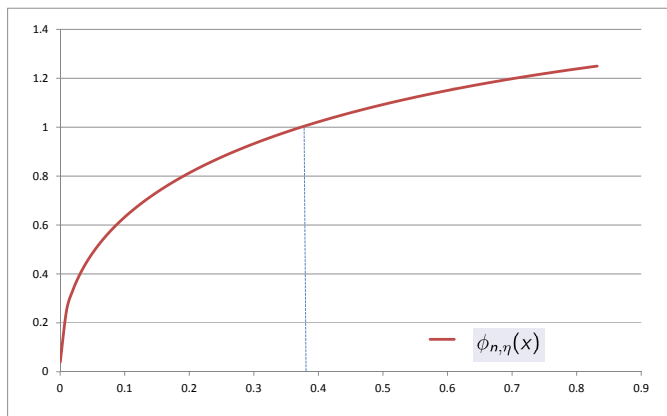
$\left[0, R_n(f_n) + \phi_{n, \eta} \left(\frac{VC(\mathcal{F}_d)}{n} \right) \right]$ is an interval at confidence level $1 - \eta$ for $R(f_n)$

Example 1: If we assume $VC(\mathcal{F}) = 20$, $n = 10,000$ then with $\eta = 1\%$ we obtain $P(R(f_n) > R_n(f_n) + 12.81\%) \leq 1\%$

Example 2: In the previous example of classification with $\mathcal{F} = \{1_{x < \alpha}, 1_{x \geq \alpha}\}_{\alpha \in \mathbb{R}}$ it is easy to check that $VC(\mathcal{F}) = 2$. With 10,000 observations the VC-theorem then guarantees that at 95% confidence level $R(f_n)$ (for estimators with minimum empirical risks) should be within the interval $[0, 4.98\%]$ (as $R_n(f_n) = 0$ and $\phi_{10,000,5\%}(\frac{2}{10,000}) = 4.98\%$). We note that the estimation of the confidence interval for this particular problem is quite loose because as seen previously

$$R(f_n) = \frac{1 - (1 - a)^{n+1}}{n+1} \leq \frac{1}{n+1} = 0.01\%.$$

Calibration versus Prediction - VC dimension



Example: We consider the following machine (of $\{0, 1\}$ -classifiers) in \mathbb{R}^2 :

$$\mathcal{F} = \{1_{ax+by+c \geq 0}, (a, b) \in \mathbb{R}^2 \setminus \{0\}, c \in \mathbb{R}\}.$$

Each classifier, classifies points in \mathbb{R}^2 according to their positions relatively to the line $ax + by + c = 0$.

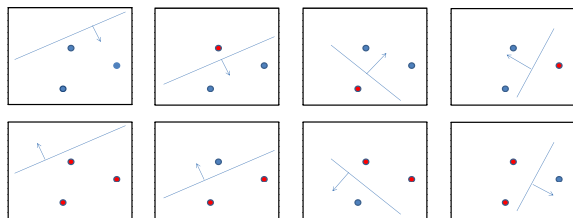
We notice that:

- we can find 3 points in \mathbb{R}^2 that can be $\{0, 1\}$ -classified in all possible ways with classifiers from \mathcal{F}
- it seems impossible to find 4 points in \mathbb{R}^2 that can be $\{0, 1\}$ -classified in all possible ways

If the later assumption is true, it will prove that $VC(\mathcal{F}) = 3$.

We are going to prove this result as a particular case of a more general result.

Calibration versus Prediction - VC dimension



Three points from \mathbb{R}^2 being $\{0, 1\}$ -classified in all possible ways by the machine \mathcal{F} (blue=1, red=0)

Calibration versus Prediction - VC dimension

Theorem : VC dimension of oriented hyperplanes of \mathbb{R}^d

Let x_1, x_2, \dots, x_n be n points of \mathbb{R}^d

Let $\mathcal{F}_d = \{1_{\{\langle w, x \rangle + c \geq 0\}}, w \in \mathbb{R}^d \setminus \{0\}, c \in \mathbb{R}\}$ be the family of $\{0, 1\}$ -classifiers defined by the oriented hyperplanes of \mathbb{R}^d .

Then, x_1, x_2, \dots, x_n can be $\{0, 1\}$ -classified in all possible ways by \mathcal{F}_d if and only if $x_2 - x_1, x_3 - x_1, \dots, x_n - x_1$ are linearly independent.

Corollary

$$VC(\mathcal{F}_d) = d + 1$$

Remarks: From the corollary, for an "affine classifier" in \mathbb{R}^d the VC dimension is the number of parameters.

Calibration versus Prediction - VC dimension

Demonstration theorem: Let's assume that $x_2 - x_1, x_3 - x_1, \dots, x_n - x_1$ are linearly independent and let $(y_i)_{i \in \llbracket 1, n \rrbracket}$ be a $\{0, 1\}$ -classification of the $(x_i)_{i \in \llbracket 1, n \rrbracket}$.

let I_1 be the indices of the x_i with the same classification as x_1

let I_2 be the indices of the x_i with a different classification from x_1

we want to prove that we can separate the $\{x_i\}_{i \in I_1}$ and the $\{x_i\}_{i \in I_2}$

Let \mathcal{C}_1 (resp \mathcal{C}_2) be the convex envelope of the $\{x_i\}_{i \in I_1}$ (resp $\{x_i\}_{i \in I_2}$)

Let's start proving that $\mathcal{C}_1 \cap \mathcal{C}_2 = \emptyset$

If this was not the case we could find $(\lambda_i)_{i \in I_1} (\lambda_j)_{j \in I_2}$ such that:

$$\forall i \in I_1 \lambda_i \geq 0, \forall j \in I_2 \lambda_j \geq 0, \sum_{i \in I_1} \lambda_i = 1, \sum_{j \in I_2} \lambda_j = 1$$

$$\text{and } \sum_{i \in I_1} \lambda_i x_i = \sum_{j \in I_2} \lambda_j x_j \quad (1)$$

by subtracting x_1 from both terms of (1) we would have :

$$\sum_{i \in I_1 \setminus \{1\}} \lambda_i (x_i - x_1) = \sum_{j \in I_2} \lambda_j (x_j - x_1) \text{ which would be in contradiction with}$$

the assumption of independence in the theorem

Calibration versus Prediction - VC dimension

So necessarily $\mathcal{C}_1 \cap \mathcal{C}_2 = \emptyset$.

By compactity we deduct that we can find $z_1 \in \mathcal{C}_1$ and $z_2 \in \mathcal{C}_2$ such that $|z_1 - z_2| = \text{distance}(\mathcal{C}_1, \mathcal{C}_2) > 0$. If now we consider the hyperplane orthogonal to $z_2 - z_1$ and containing $\frac{z_1+z_2}{2}$ it is easy to check that:

- this hyperplane separates \mathcal{C}_1 and \mathcal{C}_2 and has for equation $\langle x, z_2 - z_1 \rangle = \langle \frac{z_1+z_2}{2}, z_2 - z_1 \rangle$
- $\langle z_1, z_2 - z_1 \rangle < \langle \frac{z_1+z_2}{2}, z_2 - z_1 \rangle < \langle z_2, z_2 - z_1 \rangle$
- the points of \mathcal{C}_1 satisfy $\langle x, z_2 - z_1 \rangle \leq \langle z_1, z_2 - z_1 \rangle$
- the points of \mathcal{C}_2 satisfy $\langle x, z_2 - z_1 \rangle \geq \langle z_2, z_2 - z_1 \rangle$

So \mathcal{C}_1 and \mathcal{C}_2 are separated by an hyperplane and so the $(x_i)_{i \in I_1}$ $(x_i)_{i \in I_2}$. So the independence condition shows that the points can be classified in all possible ways.

Calibration versus Prediction - VC dimension

Let's prove now that:

(the points can be classified in all possible ways) \Rightarrow

($x_2 - x_1, x_3 - x_1, \dots, x_n - x_1$ are linearly independent).

For this we show the contraposition.

If we assume that $x_2 - x_1, x_3 - x_1, \dots, x_n - x_1$ are linearly dependent then

we can find $(\lambda_i)_{i \in \llbracket 2, n \rrbracket} \in \mathbb{R}^{n-1} \setminus \{0\}$ such that $\sum_{i=2}^{i=n} \lambda_i (x_i - x_1) = 0$ (2)

we then note:

$I = \{i \in \llbracket 2, n \rrbracket, \lambda_i \geq 0\}$ $J = \{i \in \llbracket 2, n \rrbracket, \lambda_i < 0\}$

$\lambda_i = \lambda_i^+$ if $\lambda_i \geq 0$ and $\lambda_i = -\lambda_i^-$ if $\lambda_i < 0$ and we can rewrite (2) as

$$\sum_{i \in I} \lambda_i^+ (x_i - x_1) - \sum_{j \in J} \lambda_j^- (x_j - x_1) = 0 \quad (3)$$

a) We assume in a first case that the λ_i are not all of the same sign and

without loss of generality that $\sum_{i \in I} \lambda_i^+ \geq \sum_{j \in J} \lambda_j^-$

Calibration versus Prediction - VC dimension

If the $(x_i)_{i \in \llbracket 2, n \rrbracket}$ can be separated with \mathcal{F}_d we can find w and c such that:

$\forall i \in I, \langle w, x_i \rangle \geq c$ and $\forall j \in J, \langle w, x_j \rangle < c$ but from (3):

$$\sum_{i \in I} \lambda_i^+ \langle w, x_i \rangle - \sum_{j \in J} \lambda_j^- \langle w, x_j \rangle = \left(\sum_{i \in I} \lambda_i^+ - \sum_{j \in J} \lambda_j^- \right) \langle w, x_1 \rangle \quad (4)$$

implies that x_1 cannot be separated from the $(x_i)_{i \in I}$ as

$$\sum_{i \in I} \lambda_i^+ \langle w, x_i \rangle - \sum_{j \in J} \lambda_j^- \langle w, x_j \rangle \geq \left(\sum_{i \in I} \lambda_i^+ - \sum_{j \in J} \lambda_j^- \right) c$$

implies from (4) that $\langle w, x_1 \rangle \geq c$ as well. Q.E.D

b) If we assume now that the λ_i are all of the same sign and without loss of generality that this sign is positive then (2) can be rewritten as

$$\sum_{i=1}^{i=n} \lambda_i x_i = \left(\sum_{i=1}^{i=n} \lambda_i \right) x_1 \quad (5) \text{ which proves that no classifier in } \mathcal{F}_d \text{ can separate}$$

the $(x_i)_{i \in \llbracket 2, n \rrbracket}$ from x_1 as:

$$\forall i \in \llbracket 2, n \rrbracket, \langle w, x_i \rangle \geq c \Rightarrow \sum_{i=1}^{i=n} \lambda_i \langle w, x_i \rangle \geq \left(\sum_{i=1}^{i=n} \lambda_i \right) c \text{ and from (5) this}$$

implies $\langle w, x_1 \rangle \geq c$ as well. Q.E.D

Demonstration corollary:

In \mathbb{R}^d if we take d vectors x_1, x_2, \dots, x_d independent then according to the theorem, the vectors: $0, x_1, x_2, \dots, x_d$ can be classified in all possible ways by \mathcal{F}_d . This proves that $VC(\mathcal{F}_d) \geq d + 1$.

Conversely we know that if x_1, x_2, \dots, x_n can be classified in all possible different ways by \mathcal{F}_d then the $n - 1$ vectors $x_d - x_1$ must be independent and therefore $n - 1 \leq d$ and $VC(\mathcal{F}_d) - 1 \leq d$.

Consequently $VC(\mathcal{F}_d) = d + 1$. Q.E.D

Calibration versus Prediction - VC dimension

Remarks: For hyperplane classifiers $VC(\mathcal{F}_d)$ is the number of parameters of the hyperplanes, but in general the VC dimension is something different from the number of parameters of the model.

Exercise:

We consider on \mathbb{R} the machine $\mathcal{F} = \{1_{\sin(\alpha x) > 0}, \alpha \in \mathbb{R}\}$

and the $(x_i)_{i \in \llbracket 1, l \rrbracket}$ defined by $x_i = 10^{-i}$.

Show that for any $\{0, 1\}$ -classification $(y_i)_{i \in \llbracket 1, l \rrbracket}$ of the $(x_i)_{i \in \llbracket 1, l \rrbracket}$ the

classifier $1_{\sin(\alpha x) > 0}$ with $\alpha = \pi \left(1 + \sum_{i=1}^{i=l} (1 - y_i) 10^i \right)$ classifies perfectly all the points. Conclude that $VC(\mathcal{F}) = +\infty$

Demonstration:

For any indice $1 < j < l$ we have:

$$\alpha x_j = \pi \left(1 + \sum_{i=1}^{i=j-1} (1 - y_i) 10^i \right) 10^{-j} + \pi(1 - y_j) + \pi \sum_{i=j+1}^{i=l} (1 - y_i) 10^{i-j}$$

Calibration versus Prediction - VC dimension

We notice that the last term is a multiple of 2π and thus can be noted $2k\pi$ and that the first term is always between 0 and π and thus can be noted $\beta\pi$ with $0 < \beta < 1$ so:

if $y_j = 1$, $\sin(\alpha x) = \sin(\beta\pi + 0 + 2k\pi) = \sin(\beta\pi) > 0$

if $y_j = 0$, $\sin(\alpha x) = \sin(\beta\pi + \pi + 2k\pi) = \sin(\beta\pi + \pi) < 0$

so $1_{\sin(\alpha x) > 0}$ classifies x_j correctly.

We can prove the same for x_1 and x_l which proves that whatever the labels are for the $(x_i)_{i \in \llbracket 1, l \rrbracket}$ we can classify them correctly.

Now $\forall l$, $VC(\mathcal{F}) \geq l \Rightarrow VC(\mathcal{F}) = +\infty$. Q.E.D

Remarks: In the exercise above the classifiers depends only on one parameter but the VC dimension of the machine is infinite. So the complexity of a model, as measured by its VC dimension, and the number of parameters can be quite different in the non-linear case.

Maximum Margin Classifiers

Maximum Margin Classifiers

Definition

Let $(x_i, y_i)_{i \in \llbracket 1, n \rrbracket}$ be a sample of (X, Y) with $x_i \in \mathbb{R}^d$ and $y_i \in \{0, 1\}$

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

We say that $H_{w,b}$ separates totally the $(x_i, y_i)_{i \in \llbracket 1, n \rrbracket}$ iff

for one class of points $\langle w, x \rangle + b \geq 0$ while for the other class

$\langle w, x \rangle + b < 0$.

Proposition

Let $H_{w,b}$ be an hyperplane of \mathbb{R}^d then for any $x \in \mathbb{R}^d$,

$$d(x, H_{w,b}) = \frac{|\langle w, x \rangle + b|}{\|w\|}$$

Notation:

We note $\mathcal{X}_0 = \{x_i, i \in \llbracket 1, n \rrbracket \text{ such that } y_i = 0\}$,

$\mathcal{X}_1 = \{x_i, i \in \llbracket 1, n \rrbracket \text{ such that } y_i = 1\}$ and $\mathcal{S} = \{(x_i, y_i)\}_{i \in \llbracket 1, n \rrbracket}$

Demonstration:

Let $y = p_{H_{w,b}}(x)$ be the orthogonal projection of x onto $H_{w,b}$ then,

$\exists \lambda \in \mathbb{R}, y - x = \lambda w$ and $d(x, H_{w,b}) = |\lambda| \|w\|$

but, $y - x = \lambda w \Rightarrow \langle w, y - x \rangle = \lambda \|w\|^2 \Rightarrow -b - \langle w, x \rangle = \lambda \|w\|^2$

this implies $\lambda = \frac{-b - \langle w, x \rangle}{\|w\|^2}$ and $|\lambda| \|w\| = \frac{|b + \langle w, x \rangle|}{\|w\|}$ Q.E.D

Exercise: Show that

- $d(H_{w,b_1}, H_{w,b_2}) = \frac{|b_2 - b_1|}{\|w\|}$
- $H_{w,b} = H_{-w,-b}$
- $d(H_{w,b_1}, H_{-w,-b_2}) = \frac{|b_2 - b_1|}{\|w\|}$

Definition: Margin, Maximum Margin Hyperplane

Let $(x_i, y_i)_{i \in \llbracket 1, n \rrbracket}$ be a sample of (X, Y) with $x_i \in \mathbb{R}^d$ and $y_i \in \{0, 1\}$.
if $H_{w,b}$ separates totally the $(x_i, y_i)_{i \in \llbracket 1, n \rrbracket}$.

- We call margin of $H_{w,b}$ and note $\Delta(H_{w,b})$ the quantity :
$$\begin{cases} \max_{c_1, c_2} d(H_{w, c_1}, H_{-w, -c_2}) \\ H_{w, c_1}, H_{-w, -c_2} \text{ separates totally the } (x_i, y_i)_{i \in \llbracket 1, n \rrbracket} \end{cases}$$
- We say that $H_{w,b}$ has maximum margin iff any other hyperplane H separating totally the $(x_i, y_i)_{i \in \llbracket 1, n \rrbracket}$, verifies $\Delta(H) \leq \Delta(H_{w,b})$

Exercise: Show that if the $(x_i, y_i)_{i \in \llbracket 1, n \rrbracket}$ are a sample of (X, Y) separable by an hyperplane, then the margin of the maximum margin hyperplane is $d(\mathcal{C}_0, \mathcal{C}_1)$ where \mathcal{C}_0 and \mathcal{C}_1 are the convex envelopes of the two classes.

Maximum Margin Classifiers

Exercise: Let $(x_i, y_i)_{i \in \llbracket 1, n \rrbracket}$ be a sample of (X, Y) . Let $H_{w,c}$ be an hyperplane which separates the convex envelopes \mathcal{C}_0 and \mathcal{C}_1 .

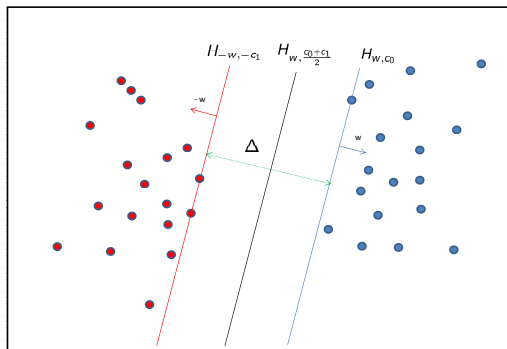
a) show that $\exists c_0$ and c_1 ,

- $\forall x \in \mathcal{C}_0, \langle w, x \rangle + c_0 \geq 0$
- $\forall x \in \mathcal{C}_1, \langle -w, x \rangle - c_1 \geq 0$ and
- $\Delta(H_{w,c}) = \frac{|c_1 - c_0|}{\|w\|}$

b) show that,

- $d(H_{w, \frac{c_0+c_1}{2}}, H_{w, c_0}) = \frac{|\frac{c_0+c_1}{2} - c_0|}{\|w\|} = \frac{|\frac{c_1 - c_0}{2}|}{\|w\|}$
- $d(H_{w, \frac{c_0+c_1}{2}}, H_{-w, -c_1}) = \frac{|\frac{c_0+c_1}{2} - c_1|}{\|w\|} = \frac{|\frac{c_0 - c_1}{2}|}{\|w\|}$
- $\forall x \in \mathcal{C}_0, \langle w, x \rangle + \frac{c_0+c_1}{2} \geq \frac{\Delta(H_{w,c})}{2} \|w\|$ (5)
- $\forall x \in \mathcal{C}_1, \langle w, x \rangle + \frac{c_0+c_1}{2} \leq -\frac{\Delta(H_{w,c})}{2} \|w\|$ (6)

Maximum Margin Classifiers



Maximum Margin Hyperplane H_w

Maximum Margin Classifiers

Remarks:

- $H_{w, \frac{c_0+c_1}{2}}$ lies at equal distance from the two hyperplanes, orthogonal to w , separating, with maximum distance between them, \mathcal{C}_0 and \mathcal{C}_1 . We note this hyperplane H_w

- If we define $\omega = \frac{w}{\|w\|} \frac{2}{\Delta}$ and $b = \frac{c_0+c_1}{\Delta\|w\|}$ we can write (5) and (6) in the standard form:

$$\forall x \in \mathcal{C}_0, \langle \omega, x \rangle + b \geq 1 \quad (5)$$

$$\forall x \in \mathcal{C}_1, \langle \omega, x \rangle + b \leq -1 \quad (6)$$

The three (parallel) hyperplanes defined previously can now be noted $H_{\omega, b-1}$, $H_{-\omega, -b-1}$ and $H_{\omega, b}$ and $d(H_{-\omega, -b-1}, H_{\omega, b-1}) = \frac{2}{\|\omega\|}$

- Therefore, in practice to search for an hyperplane with maximum margin search for ω and b which solve:

$$(P) \begin{cases} \max_{\omega, b} \frac{2}{\|\omega\|} \\ \forall x_i \in \mathcal{X}_0, \langle \omega, x \rangle + b \geq 1 \\ \forall x_i \in \mathcal{X}_1, \langle \omega, x \rangle + b \leq -1 \end{cases}$$

Remarks: ω and b also solve:

$$(P) \begin{cases} \min_{\omega, b} \|\omega\|^2 \\ \forall x_i \in \mathcal{X}_0, \langle \omega, x_i \rangle + b \geq 1 \\ \forall x_i \in \mathcal{X}_1, \langle \omega, x_i \rangle + b \leq -1 \end{cases}$$

which is a quadratic problem with affine constraints, which can be solved using the Karush-Kuhn-Tucker theorem.

Structural Risk Minimization and Gap Tolerant Classifiers

In the Structural Risk Minimization method:

- we define nested ensembles of classifiers (machines),
 $\mathcal{F}_1 \subset \mathcal{F}_2 \cdots \subset \mathcal{F}_k \cdots$, with $VC(\mathcal{F}_1) < VC(\mathcal{F}_2) < \cdots < VC(\mathcal{F}_k)$
- for the sample $(x_i, y_i)_{i \in \llbracket 1, n \rrbracket}$, we calculate for each machine \mathcal{F}_k the best classifier $f_{n,k}$ and its empirical risk $R_n(f_{n,k})$
- to control in the best possible way the error of prediction at confidence level 5%, we pick the estimator $f_{n,k}$ which minimizes $R_n(f_{n,k}) + \phi_{n,5\%}\left(\frac{VC(\mathcal{F}_k)}{n}\right)$

Definition: Δ -Gap Tolerant Classifier of Diameter D

For $w \in \mathbb{R}^d$, $b \in \mathbb{R}$ and B_D a ball in \mathbb{R}^d of diameter D we define $h_{w,b}^{B_D,\Delta}$ as:

$$h_{w,b}^{B_D,\Delta}(x) = 1 \text{ iff } x \in B_D \text{ and } \langle w, x \rangle + b \geq \frac{\Delta \|w\|}{2}$$

$$h_{w,b}^{B_D,\Delta}(x) = 0 \text{ iff } x \in B_D \text{ and } \langle w, x \rangle + b \leq -\frac{\Delta \|w\|}{2}$$

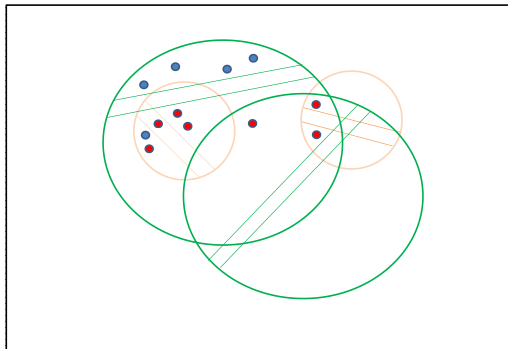
if $x \notin B_D$ or $|\langle w, x \rangle + b| < \frac{\Delta \|w\|}{2}$ then $h_{w,b}^{B_D,\Delta}$ is not defined

Such a $\{0, 1\}$ -classifier is called a Δ -Gap Tolerant classifier of diameter D

Remarks:

- For the Δ -Gap tolerant classifier of diameter D the two hyperplanes $H_{w,b-\frac{\Delta\|w\|}{2}}$ and $H_{w,b+\frac{\Delta\|w\|}{2}}$ which separates two distinct classes of points are distant of Δ .
- We allow in the definition that the classifier may classify some points incorrectly

SRM and Gap Tolerant Classifiers



Only one Gap Tolerant Classifier classifies all the points here

Theorem admitted: VC of Δ -Gap Tolerant Classifier of Diameter D

Let $\mathcal{F}_{\Delta,D} = \{h_{w,b}^{B_D,\Delta}, w \in \mathbb{R}^d, b \in \mathbb{R} \text{ and } B_D \text{ is a ball of diameter } D\}$
then $VC(\mathcal{F}_{\Delta,D}) \leq 1 + \text{Min}(\frac{D^2}{\Delta^2}, d)$

Remark:

- the notion of margin was introduced to classify as robustly as possible (i.e to minimize the risk of misclassification in case of a small errors in the measurements).
- using classifiers with a fixed margin may reduce significantly the VC dimension of the Machine when observing data in large dimension. For example if $d = 1,000,000$, $D = 1$, $\Delta = 0.1$, the VC dimension of hyperplane classifiers is 1,000,001 while the same hyperplane classifiers with a margin of 0.1 and a diameter of 1 have a VC dimension of no more than 101.

Theorem admitted: Max Margin (Husch Scovel)

In \mathbb{R}^k , the margin Δ at which a family of $k + 1$ points within a ball of radius 1 can be classified in all possible ways by a family of Δ - Gap tolerant classifiers (of radius 1) cannot be more than $\sqrt{\frac{k+1}{k}} \sqrt{\frac{1}{\lfloor \frac{k+1}{2} \rfloor} + \frac{1}{k+1 - \lfloor \frac{k+1}{2} \rfloor}}$ where $\lfloor \frac{k+1}{2} \rfloor$ denotes the integer part of $\frac{k+1}{2}$. This maximum can be attained for some particular choices of families of $k + 1$ points.

Remarks:

We know that it is possible to find $k + 1$ points of \mathbb{R}^k that can be classified in all possible ways by hyperplane classifiers. By renormalizing these points we can put them inside a ball of radius 1 and the hyperplanes renormalized will continue to classify them in all possible ways. This family of classifiers exhibits a certain margin and the theorem above gives us a limit in terms of the maximum margin we can expect. Later on we will show that the maximum margin is attained when the points form a simplex of the affine space \mathbb{R}^k i.e. can be seen as an orthonormal family of vectors of \mathbb{R}^{k+1} .

SRM and Gap Tolerant Classifiers

The strategy to predict with Gap Tolerant Classifiers after observing a (learning) sample $(x_i, y_i)_{i \in [1, n]}$ is as follows:

- define a ball B_D that is most likely to contain most realizations of X
- build a set of nested Gap Tolerant machines
 $\mathcal{F}_{\alpha_0, D} \subset \mathcal{F}_{\alpha_1, D} \subset \dots \subset \mathcal{F}_{\alpha_n, D}$ with decreasing margins
 $\alpha_0 > \alpha_1 > \dots > \alpha_n$
- for each machine select a gap tolerant classifier f_{n, α_n} with minimum empirical error $R(f_{n, \alpha_n})$ (when an observation is within the gap or outside the ball, the machine does not classify and the error of classification for this point is zero)
- using the fact that $VC(\mathcal{F}_{\alpha_i, D}) \leq 1 + \text{Min}(\frac{D^2}{\alpha_i^2}, d)$ choose a machine for which the error of calibration $R(f_{n, \alpha_n})$ and the complexity term, estimated by $1 + \text{Min}(\frac{D^2}{\alpha_i^2}, d)$ are providing the best control on the error of prediction.

Trade-off between Margin and Errors

Trade-off between Margin and Errors

Theorem and Definition:

The set $\{x \in \mathbb{R}^d, |\langle w, x \rangle + b| \leq 1\}$ consists of points in \mathbb{R}^d between $H_{w,b-1}$ and $H_{-w,-b-1}$.

As $d(H_{w,b-1}, H_{-w,-b-1}) = \frac{2}{\|w\|}$ this ensemble is called hyperplane of thickness $\frac{2}{\|w\|}$ and is noted $H_{w,b}^{\frac{2}{\|w\|}}$.

When the sample points $\{(x_i, y_i)\}_{i \in \llbracket 1, n \rrbracket}$ are separable (with $y_i \in \{-1, 1\}$) we search for an hyperplane of maximum thickness separating the points and solve

$$(P) \begin{cases} \min_{w,b} \|w\|^2 \\ \forall x_i \in \mathcal{X}_1, \langle w, x_i \rangle + b \geq 1 \\ \forall x_i \in \mathcal{X}_{-1}, \langle w, x_i \rangle + b \leq -1 \end{cases}$$

Trade-off between Margin and Errors

(P) can also be written as:

$$\begin{cases} \min_{w,b} \|w\|^2 \\ \forall (x_i, y_i) \in \mathcal{S}, y_i [\langle w, x_i \rangle + b] \geq 1 \end{cases}$$

When the points cannot be totally separated (i.e the domain of (P) is \emptyset) we search for w, b and $\xi = (\xi_i)_{i \in \llbracket 1, n \rrbracket} \in \mathbb{R}^n$ solutions of:

$$(P_C) \begin{cases} \min_{w,b,\{\xi_i\}_{i \in \llbracket 1, n \rrbracket}} \|w\|^2 + C \sum_{i=1}^{i=n} \xi_i \\ \forall (x_i, y_i) \in \mathcal{S}, y_i [\langle w, x_i \rangle + b] \geq 1 - \xi_i \\ \forall i \in \llbracket 1, n \rrbracket, \xi_i \geq 0 \end{cases}$$

Trade-off between Margin and Errors

Remarks:

- the $(\xi_i)_{i \in \llbracket 1, n \rrbracket}$ are (slack) variables which enable the relaxation of the constraints of strict separability of the $(x_i, y_i) \in \mathcal{S}$
- the parameter $C \geq 0$ is a cost of not separating a point correctly, based on the distance between this point and the frontier of the hyperplane defining its class
- other cost functions could have been used for mis-classification such as $C \sum_{i=1}^{i=n} \xi_i^2$ or $C \sum_{i=1}^{i=n} 1_{\xi_i > 0}$ but with slightly different solutions and interpretations for (P_C)
- at this point we have not defined what would be the strategy of classification for a new observation x lying between $H_{w, b-1}$ and $H_{-w, -b-1}$.

Trade-off between Margin and Errors: Resolution

to solve:

$$(P_C) \begin{cases} \min_{w, b, \xi \in \mathbb{R}^n} \|w\|^2 + C \sum_{i=1}^{i=n} \xi_i \\ \forall (x_i, y_i) \in \mathcal{S}, y_i[\langle w, x_i \rangle + b] \geq 1 - \xi_i \quad (1) \\ \forall i \in \llbracket 1, n \rrbracket, \xi_i \geq 0 \quad (2) \end{cases}$$

we consider the Lagrangian:

$$L(w, b, \xi, \alpha, \mu) = \|w\|^2 + C \sum_{i=1}^{i=n} \xi_i - \sum_{i=1}^{i=n} \alpha_i (y_i[\langle w, x_i \rangle + b] - 1 + \xi_i) - \sum_{i=1}^{i=n} \mu_i \xi_i$$

with $\xi = (\xi_1, \xi_2, \dots, \xi_n)'$, $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_n)'$ and $\mu = (\mu_1, \mu_2, \dots, \mu_n)'$

Lemma 1: (property of the Lagrangian)

$\max_{\alpha \in (\mathbb{R}^+)^n, \mu \in (\mathbb{R}^+)^n} L(w, b, \xi, \alpha, \mu)$ equals:

$$\begin{cases} +\infty & \text{if either (1) or (2) are not satisfied} \\ \|w\|^2 + C \sum_{i=1}^{i=n} \xi_i & \text{if both (1) and (2) are satisfied} \end{cases}$$

Demonstration:

$y_i[\langle w, x_i \rangle + b - 1 + \xi_i] < 0 \Rightarrow \lim_{\alpha_i \rightarrow +\infty} L(w, b, \xi, \alpha, \mu) = +\infty$ and

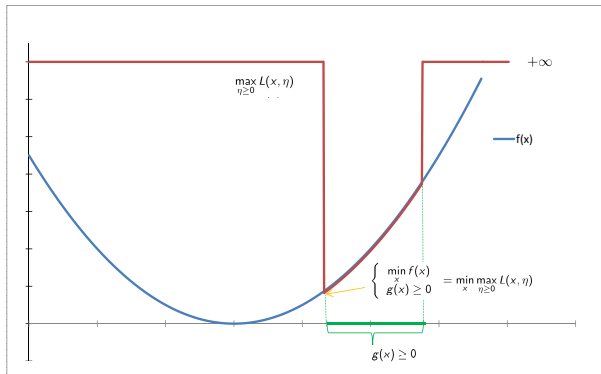
$\xi_i < 0 \Rightarrow \lim_{\mu_i \rightarrow +\infty} L(w, b, \xi, \alpha, \mu) = +\infty$. This proves the first part.

Now, if both (1) and (2) are satisfied then $\forall \alpha \in (\mathbb{R}^+)^n, \forall \mu \in (\mathbb{R}^+)^n$

$-\sum_{i=1}^{i=n} \alpha_i (y_i[\langle w, x_i \rangle + b - 1 + \xi_i]) - \sum_{i=1}^{i=n} \mu_i \xi_i \geq 0$ and so the minimum (of zero) is attained for $\alpha = \mu = 0$.

As $L(w, b, \xi, 0, 0) = \|w\|^2 + C \sum_{i=1}^{i=n} \xi_i$ this proves the result.

Trade-off between Margin and Errors: Resolution



Lagrangian principle illustrated

Lemma 2: (mini-max theorem)

For any domains \mathcal{Y} and \mathcal{Z} and real function g defined on $\mathcal{Y} \times \mathcal{Z}$:

$$\max_{z \in \mathcal{Z}} \left[\min_{y \in \mathcal{Y}} g(y, z) \right] \leq \min_{y \in \mathcal{Y}} \left[\max_{z \in \mathcal{Z}} g(y, z) \right]$$

Demonstration:

$$\min_{y \in \mathcal{Y}} g(y, z) \leq g(y, z) \Rightarrow \max_{z \in \mathcal{Z}} \left[\min_{y \in \mathcal{Y}} g(y, z) \right] \leq \max_{z \in \mathcal{Z}} g(y, z) \quad (1)$$

As (1) is true for all y the inequality stands for the *min* of the right term

of (1). So, $\max_{z \in \mathcal{Z}} \left[\min_{y \in \mathcal{Y}} g(y, z) \right] \leq \min_{y \in \mathcal{Y}} \left[\max_{z \in \mathcal{Z}} g(y, z) \right]$ Q.E.D

Trade-off between Margin and Errors: Resolution

Table: example for mini-max

$g(y,z)$	$y=1$	$y=2$	$y=3$
$z=3$	3	3	1
$z=2$	2	1	3
$z=1$	1	2	3

for the example here:

$$\max_{z \in \mathcal{Z}} \left[\min_{y \in \mathcal{Y}} g(y, z) \right] = 1$$

$$\min_{y \in \mathcal{Y}} \left[\max_{z \in \mathcal{Z}} g(y, z) \right] = 3$$

Trade-off between Margin and Errors: Resolution

Lemma 3: (Lagrangian method)

Solving P_C is equivalent to solving:

$$\min_{w, b, \xi \in \mathbb{R}^n} \left[\max_{\alpha \in (\mathbb{R}^+)^n, \mu \in (\mathbb{R}^+)^n} L(w, b, \xi, \alpha, \mu) \right]$$

Demonstration: this follows directly from lemma 1

Definition: Duality

$\min_{w, b, \xi \in \mathbb{R}^n} \left[\max_{\alpha \in (\mathbb{R}^+)^n, \mu \in (\mathbb{R}^+)^n} L(w, b, \xi, \alpha, \mu) \right]$ is called the primal problem

$\max_{\alpha \in (\mathbb{R}^+)^n, \mu \in (\mathbb{R}^+)^n} \left[\min_{w, b, \xi \in \mathbb{R}^n} L(w, b, \xi, \alpha, \mu) \right]$ is called the dual problem

The dual problem is noted P_C^*

Trade-off between Margin and Errors: Resolution

Remarks:

- if d is the value obtained for the dual problem and p for the primal problem then according to the mini-max lemma $d \leq p$
- according to the KKT theorem, a way to guarantee that $d = p$ is, when solving the dual problem, $\min_{w, b, \xi \in \mathbb{R}^n} L(w, b, \xi, \alpha, \mu)$ to impose some additional constraints, known as the "complementary slackness" conditions, defined here by:

$$\text{(KKT1): } \forall i \in \llbracket 1, n \rrbracket, \alpha_i (y_i [\langle w, x_i \rangle + b] - 1 + \xi_i) = 0$$

$$\text{(KKT2): } \forall i \in \llbracket 1, n \rrbracket, \mu_i \xi_i = 0.$$

The effect of these complementary constraints is to increase d up to d^* such that $d^* = p$.

- some convex analysis results guarantee that here (convex function optimized under affine constraints on a domain with a non empty interior) $d = d^* = p$. So (KKT1) and (KKT2) are automatically satisfied when solving P_C^* and will not be added to the constraints for P_C^* but will just be used as auxiliary equations when useful.

SVM and C-SVM

SVM and C-SVM: Solving the Dual Problem

To solve $\max_{\alpha \in (\mathbb{R}^+)^n, \mu \in (\mathbb{R}^+)^n} \left[\min_{w, b, \xi \in \mathbb{R}^n} L(w, b, \xi, \alpha, \mu) \right]$ we first solve

$\min_{w, b, \xi \in \mathbb{R}^n} L(w, b, \xi, \alpha, \mu)$ as a function of α and μ .

$$L(w, b, \xi, \alpha, \mu) =$$

$$= \|w\|^2 + \sum_{i=1}^{i=n} \xi_i (C - \alpha_i - \mu_i) - \langle w, \sum_{i=1}^{i=n} \alpha_i y_i x_i \rangle - b \sum_{i=1}^{i=n} \alpha_i y_i + \sum_{i=1}^{i=n} \alpha_i$$

$$\frac{\partial L}{\partial w} \text{ is defined as } \left(\frac{\partial L}{\partial w_1}, \frac{\partial L}{\partial w_2}, \dots, \frac{\partial L}{\partial w_n} \right)$$

$$\frac{\partial L}{\partial w} = 2w' - \sum_{i=1}^{i=n} \alpha_i y_i x_i \Rightarrow w = \frac{1}{2} \sum_{i=1}^{i=n} \alpha_i y_i x_i \quad (C1)$$

$$\frac{\partial L}{\partial b} = 0 \Rightarrow \sum_{i=1}^{i=n} \alpha_i y_i = 0 \quad (C2)$$

$$\frac{\partial L}{\partial \xi_i} = 0 \Rightarrow C - \alpha_i - \mu_i = 0 \quad (C3)$$

SVM and C-SVM: Solving the Dual Problem

so by duality:

$$(P_C) \Leftrightarrow \begin{cases} \max_{\alpha \in (\mathbb{R}^+)^n, \mu \in (\mathbb{R}^+)^n} -\frac{1}{4} \left\| \sum_{i=1}^{i=n} \alpha_i x_i \right\|^2 + \sum_{i=1}^{i=n} \alpha_i \\ C - \alpha_j - \mu_j = 0 \\ \sum_{i=1}^{i=n} \alpha_i y_i = 0 \end{cases}$$

$$\Leftrightarrow \begin{cases} \max_{\alpha \in \mathbb{R}^n} -\frac{1}{4} \left\| \sum_{i=1}^{i=n} \alpha_i x_i \right\|^2 + \sum_{i=1}^{i=n} \alpha_i \\ 0 \leq \alpha_j \leq C \\ \sum_{i=1}^{i=n} \alpha_i y_i = 0 \end{cases} \quad \text{which can be solved numerically}$$

we note α^* the solution of this system

Remarks:

- from (C1): $w^* = \frac{1}{2} \sum_{i=1}^{i=n} y_i \alpha_i^* x_i$
- from (KKT1), (KKT2) and (C3):
$$\begin{cases} \forall i \in \llbracket 1, n \rrbracket, (C - \alpha_i^*) \xi_i = 0 \text{ (as } \mu_i^* = C - \alpha_i^*) \\ \forall i \in \llbracket 1, n \rrbracket, \alpha_i^* (y_i [\langle w^*, x_i \rangle + b] - 1 + \xi_i) = 0 \end{cases}$$

so b^* can be determined by picking indices i for which $0 < \alpha_i^* < C$ as in this case: $\xi_i = 0$ and consequently $y_i [\langle w^*, x_i \rangle + b^*] - 1 = 0$, leading to : $b^* = y_i - \langle w^*, x_i \rangle$.

Note that in practice, as in the determination of α^* there may be some approximation errors, b^* is calculated as the average of $y_i - \langle w^*, x_i \rangle$ for the indices i for which $0 < \alpha_i < C$.
- we will see later (with ν -SVMs) how to control further the optimization problem to make sure that we get some α_i satisfying $0 < \alpha_i < C$.

SVM and C-SVM: Interpretation

Remarks:

two types of vectors x_i are used to determine w^*

- the x_i for which $0 < \alpha_i^* < C$
in this case (KKT2) and (C3) $\Rightarrow \xi_i = 0$ and $y_i[\langle w^*, x_i \rangle + b] - 1 = 0$
and these x_i are well classified and belongs to one the two separating hyperplanes $H_{w,b-1}$ and $H_{-w,-b-1}$
- the x_i for which $\alpha_i^* = C$ which can be misclassified, as in this case there is no constraint of nullity on ξ_i derived from (KKT2) and (C3)

Definition : Support Vector, Support Vector Machines

The vectors x_i for which $\alpha_i^* \neq 0$ (and which are used for the expression of w^*) are called "support vectors". The method of classification is then called "Support Vector Machines" and noted "SVM".

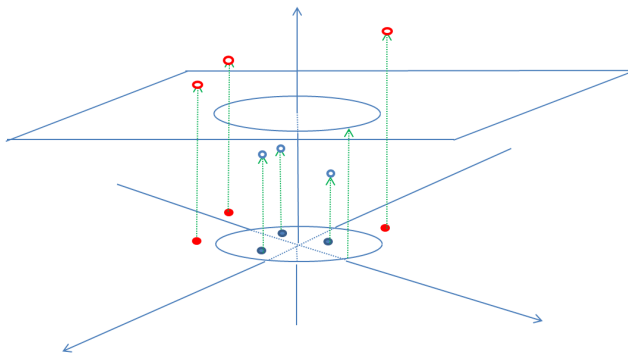
When some errors are permitted in the classification, with the introduction of the "slack variables" ξ and the cost C the method is called C-SVM.

Remarks:

When the points from the sample are perfectly separable the solution of (P) correspond to the solutions of (P_C) for C large enough. Indeed if the cost C is large enough the solution of (P_C) will maximize the margin while constricting the ξ_i to zero.

The Kernel Trick

The Kernel Trick



Classification after a change of variable

The Kernel Trick

In some situations the $(x_i, y_i)_{i \in \llbracket 1, n \rrbracket}$ cannot be separated by an hyperplane in \mathbb{R}^d but it is possible to find a transformation ϕ such that the $(\phi(x_i), y_i)_{i \in \llbracket 1, n \rrbracket}$ are separable.

Example: Consider in \mathbb{R}^2 the classification of (X, Y) where $X = (X^1, X^2)'$ and $Y = 1_{(X^1)^2 + (X^2)^2 \leq 1}$. In the graph we represent the x_i for a sample of 6 points $(x_i, y_i)_{i \in \llbracket 1, 6 \rrbracket}$. The blue points are the points for which $Y_i = 1$ and the red points the points for which $Y_i = 0$.

It appears that we cannot separate correctly these points in \mathbb{R}^2 .

If we consider now,

$\phi : \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \longrightarrow \begin{pmatrix} \alpha \\ \beta \\ \alpha^2 + \beta^2 \end{pmatrix}$ then the points $(\phi(x_i), y_i)_{i \in \llbracket 1, n \rrbracket}$ can be

separated by the hyperplane H of \mathbb{R}^3 defined by:

$$H = \left\{ \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} \in \mathbb{R}^3, \gamma = 1 \right\}$$

The Kernel Trick

We now consider transformations $\phi: \mathbb{R}^d \rightarrow l_2(\mathbb{R})$ where $l_2(\mathbb{R})$ is the vector space of sequences $(z_i)_{i \in \mathbb{N}}$ such that $\sum_{i \in \mathbb{N}} z_i^2 < +\infty$ and $\langle \cdot, \cdot \rangle_{\mathbb{N}}$ is

defined by $\langle (z_i)_{i \in \mathbb{N}}, (t_j)_{j \in \mathbb{N}} \rangle_{\mathbb{N}} = \sum_{i \in \mathbb{N}} z_i t_i$

In the space $\text{Vect}\{\phi(x_i), i \in \mathbb{N}\}$ a C-SVM classifies a point y according to

the values of: $\sum_{i=1}^{i=n} \alpha_i^* y_i \langle \phi(x_i^*), y \rangle_{\mathbb{N}} + b^*$

and we will now classify a new observation x based on the values of:

$\sum_{i=1}^{i=n} \alpha_i^* y_i \langle \phi(x_i^*), \phi(x) \rangle_{\mathbb{N}} + b^*$ that we can write as $\sum_{i=1}^{i=n} \alpha_i^* y_i K_{\phi}(x_i^*, x) + b^*$

where $K_{\phi}: \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ is defined by $K_{\phi}(x, z) = \langle \phi(x), \phi(z) \rangle_{\mathbb{N}}$

To determine what flexibility we earn by using classifiers based on functions K_{ϕ} we are going to determine what the set of functions $\{K_{\phi}\}$ is. For this purpose we use Mercer's theorem.

Theorem and Definition : Mercer's Theorem

Let $K : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ be such that,

- $\forall x, y \in \mathbb{R}^d, K(x, y) = K(y, x)$
- $\forall f \in L^2(\mathbb{R}^d, \mathbb{R}), \int K(x, y)f(y)dy \in L^2(\mathbb{R}^d, \mathbb{R})$

If we define $\langle \cdot, \cdot \rangle_K : L^2(\mathbb{R}^d, \mathbb{R}) \times L^2(\mathbb{R}^d, \mathbb{R}) \rightarrow \mathbb{R}$ by,
 $\langle f, g \rangle_K = \int K(x, y)f(x)g(y)dxdy$

then the two following propositions are equivalent:

- (P1): $\exists \phi : \mathbb{R}^d \rightarrow l_2(\mathbb{R})$ such that $K(x, y) = \langle \phi(x), \phi(y) \rangle_{\mathbb{N}}$
- (P2): the bilinear symmetric form $\langle \cdot, \cdot \rangle_K$ is positive on $L^2(\mathbb{R}^d, \mathbb{R})$.

A function K satisfying these properties is called a Kernel.

Demonstration:

If we assume (P1), then $\forall f \in L^2(\mathbb{R}^d, \mathbb{R})$:

$$\langle f, f \rangle_K = \int \int K(x, y) f(x) f(y) dx dy = \int \int \langle \phi(x), \phi(y) \rangle_{\mathbb{N}} f(x) f(y) dx dy \\ = \langle \int \phi(x) f(x) dx, \int \phi(y) f(y) dy \rangle_{\mathbb{N}} = \left\| \int \phi(x) f(x) dx \right\|_{\mathbb{N}}^2.$$

So $\langle \cdot, \cdot \rangle_K$ is positive (and bilinear and symmetric as well)

If we assume (P2). As $\langle \cdot, \cdot \rangle_K$ is symmetric it can be diagonalised so $\exists (e_i)_{i \in \mathbb{N}} \in L^2(\mathbb{R}^d, \mathbb{R})$ and $(\lambda_i)_{i \in \mathbb{N}}$ elements of \mathbb{R} such that:

- $\langle e_i, e_j \rangle_{L^2} = \delta_{i,j}$
- $\forall f \in L^2(\mathbb{R}^d, \mathbb{R}), \langle f, e_i \rangle_K = \lambda_i \langle f, e_i \rangle_{L^2}$

So, if f and g are in $L^2(\mathbb{R}^d, \mathbb{R})$, after decomposing f and g on the orthonormal basis $(e_i)_{i \in \mathbb{N}}$ we get:

$$\langle f, g \rangle_K = \left\langle \sum_{i \in \mathbb{N}} \langle f, e_i \rangle_{L^2} e_i, \sum_{j \in \mathbb{N}} \langle g, e_j \rangle_{L^2} e_j \right\rangle_K = \sum_{i \in \mathbb{N}} \langle f, e_i \rangle_{L^2} \langle g, e_i \rangle_{L^2} \lambda_i.$$

The Kernel Trick

As $\langle \cdot, \cdot \rangle_K$ is assumed to be positive $\lambda_i \geq 0$. so:

$$\begin{aligned}\langle f, g \rangle_K &= \sum_{i \in \mathbb{N}} \lambda_i \left(\int f(x) e_i(x) dx \right) \left(\int g(y) e_i(y) dy \right) \text{ and by Fubini} \\ &= \sum_{i \in \mathbb{N}} \lambda_i \int \int f(x) e_i(x) g(y) e_i(y) dx dy \text{ and by inversions of the sums} \\ &= \int \int \sum_{i \in \mathbb{N}} \lambda_i e_i(x) e_i(y) f(x) g(y) dx dy\end{aligned}$$

as the equality holds for any function f and g we can identify K as:

$$K(x, y) = \sum_{i \in \mathbb{N}} \lambda_i e_i(x) e_i(y) = \langle \phi(x), \phi(y) \rangle_{\mathbb{N}} \text{ with}$$

$$\phi(x) = (\sqrt{\lambda_i} e_i(x))_{i \in \mathbb{N}} \text{ Q.E.D}$$

Remarks:

- $\|\phi(x)\|_{\mathbb{N}}^2 = \sum_{i \in \mathbb{N}} \lambda_i e_i^2(x)$
- $\int \|\phi(x)\|_{\mathbb{N}}^2 dx = \sum_{i \in \mathbb{N}} \lambda_i$

The Kernel Trick: Radial Basis Functions

Theorem: Example of Kernels in \mathbb{R}^d

- a) $\forall k \in \mathbb{N} : (x, y) \rightarrow \langle x, y \rangle_d^k$ is a kernel
- b) $(x, y) \rightarrow \exp(-\|x - y\|_d^2)$ is a kernel

Demonstration:

$$\begin{aligned} \int \int \langle x, y \rangle_d^k f(x) f(y) dx dy &= \int \int \left(\sum_{i=1}^{i=d} x^i y^i \right)^k f(x) f(y) dx dy \\ &= \int \int \sum_{i_1, i_2, \dots, i_k} x^{i_1} x^{i_2} \dots x^{i_k} y^{i_1} y^{i_2} \dots y^{i_k} f(x) f(y) dx dy \\ &= \sum_{i_1, i_2, \dots, i_k} \left(\int x^{i_1} x^{i_2} \dots x^{i_k} f(x) dx \right) \left(\int y^{i_1} y^{i_2} \dots y^{i_k} f(y) dy \right) \\ &= \sum_{i_1, i_2, \dots, i_k} \left(\int x^{i_1} x^{i_2} \dots x^{i_k} f(x) dx \right)^2 \geq 0 \end{aligned}$$

As the form is positive, according to Mercer's Theorem $\langle x, y \rangle_d^k$ is a kernel.

Q.E.D

The Kernel Trick: Radial Basis Functions

$$\begin{aligned} & \int \int \exp(-\|x - y\|_d^2) f(x) f(y) dx dy \\ &= \int \int \exp(2\langle x, y \rangle_d) \exp(-\|x\|_d^2) \exp(-\|y\|_d^2) f(x) f(y) dx dy \\ &= \sum_{k \in \mathbb{N}} \int \int 2^k \frac{\langle x, y \rangle_d^k}{k!} [\exp(-\|x\|_d^2) f(x)] [\exp(-\|y\|_d^2) f(y)] dx dy \end{aligned}$$

as $\langle x, y \rangle_d^k$ is a kernel, each of the terms are positive, so the sum is positive, so $\exp(-\|x - y\|_d^2)$ is a kernel. Q.E.D

Remarks:

- $\forall \sigma \in \mathbb{R}, \exp(-\frac{\|x-y\|_d^2}{2\sigma^2})$ is a kernel, called the "Gaussian Kernel"
- $h(x, y)$ is called radial basis function i.i.f we can find ψ such that $h(x, y) = \psi(\|x - y\|_d)$
- the Gaussian kernel is a radial basis function

The Kernel Trick: Radial Basis Functions

Theorem and Definition

For any $(z_j)_{j \in \llbracket 1, l \rrbracket}$ of \mathbb{R}^d it is equivalent to classify a point x :

- in $\phi(\mathbb{R}^d)$ based on the sign of $\langle \sum_{j=1}^l \beta_j \phi(z_j), \phi(x) \rangle + b$
- in \mathbb{R}^d based on the sign of $\sum_{j=1}^l \beta_j K_\phi(z_j, x) + b$

These classifiers parametrized by z_j, β_j, b, l are called classifiers of Kernel K and form a set (machine) noted \mathcal{F}^K

When classifying $(\phi(x_j), y_j)_{j \in \llbracket 1, n \rrbracket}$ in $\text{Vect}\{\phi(x_i), i \in \llbracket 1, n \rrbracket\}$ (or $\text{Vect}\{\phi(\mathbb{R}^d)\}$) the maximum margin classifier corresponds to the classifier of \mathcal{F}^{K_ϕ} defined by $l = n, z_j = x_j, \beta_j = \alpha_j^* y_j, b = b^*$

It is equivalent to do SVM classification in $\text{Vect}\{\phi(\mathbb{R}^d)\}$ or classification of Kernel K_ϕ in \mathbb{R}^d

Demonstration: simple

The Kernel Trick: Radial Basis Functions

Remark 1: for a C-SVM the margin of the hyperplane in $\phi(\mathbb{R}^d)$ is defined by $\frac{2}{\|\omega^*\|_{\mathbb{N}}}$ where $\omega^* = \sum_{i=1}^{i=n} \alpha_i^* y_i \phi(x_i)$. This quantity can be calculated from

the kernel K as $\|\sum_{i=1}^{i=n} \alpha_i^* y_i \phi(x_i)\|_{\mathbb{N}}^2 = \beta^{*'} [K(x_i, x_j)] \beta^*$ where $[K(x_i, x_j)]$ is the matrix of $\mathbb{R}^n \times \mathbb{R}^n$ formed by the $\{K(x_i, x_j)\}_{i,j \in \llbracket 1, n \rrbracket}$ and β^* is the vector of components $\alpha_i^* y_i$.

Remark 2: in $\mathbb{R}^{\mathbb{N}}$ the hyperplanes $\langle \omega, x \rangle_{\mathbb{N}} + b = 0$ have an infinite VC dimension therefore we may wonder if the Kernel method is going to lead to some over-fitting. For a Gaussian Kernel $K_{\sigma}(x, z) = \exp(-\frac{\|x-z\|}{2\sigma^2})$ we can make the following remarks:

- $\forall x \in \mathbb{R}^d$, $\|\phi(x)\|_{\mathbb{N}} = 1$ because $\|\phi(x)\|_{\mathbb{N}}^2 = K(x, x) = \exp(-\frac{\|0\|}{2\sigma^2}) = 1$ so the transformed points to classify are localized on the surface of the sphere centred on zero and of radius 1 of $\mathbb{R}^{\mathbb{N}}$ (which is an important restriction).

The Kernel Trick: Radial Basis Functions

- $\forall x, z \in \mathbb{R}^d$, $\langle \phi(x), \phi(z) \rangle_{\mathbb{N}} \geq 0$ because $K_{\sigma}(x, z) \geq 0$. so, all the points to classify are situated in the same orthant of $\text{Vect}\{\phi(x_i), i \in \llbracket 1, n \rrbracket\}$ (which restricts further where the points can lay).
- all the points $\phi(x_i)$ to classify can be separated from 0 as for all the points $\langle \sum_{j=1}^{j=n} \phi(x_j), \phi(x_i) \rangle \geq \langle \phi(x_j), \phi(x_i) \rangle \geq 1$
- when using a kernel K we can restrict the set \mathcal{F}^K to the set of classifiers \mathcal{F}_{Δ}^K for which $\frac{2}{\sqrt{\beta' [K(z_i, z_j)]^{\beta}}} \geq \Delta$ by doing so we know that the corresponding classifiers in $\text{Vect}\{\phi(\mathbb{R}^d)\}$ are Δ -GAP-tolerant classifiers of radius 1 and margin at least Δ . From this we deduct that $VC(\mathcal{F}_{\Delta}^K) \leq 1 + \frac{4}{\Delta^2}$.

The Kernel Trick: Radial Basis Functions

Exercise:

$$\text{Let } \mathcal{F}_\sigma^n = \left\{ \begin{array}{l} h : \mathbb{R}^d \longrightarrow \{-1, 1\}, h(x) = \Theta \left(\sum_{i=1}^{i=n} \mu_i K_\sigma(x, z_i) + b \right), \\ z_i \in \mathbb{R}^d, \mu_i \in \mathbb{R}, b \in \mathbb{R}, \end{array} \right\}$$

where, $\Theta(u) = 1$ if $u \geq 0$ and otherwise $\Theta(u) = -1$ be a machine of $\{-1, 1\}$ -classifiers and let $(x_i)_{i \in \llbracket 1, n \rrbracket}$ be n distinct points of \mathbb{R}^d , and d be the minimum distance between the points i.e $d = \min_{i \neq j} \|x_i - x_j\|_d$.

Let σ be such that $(n-1)\exp(-\frac{d}{2\sigma^2}) < 1$.

Let $(y_i)_{i \in \llbracket 1, n \rrbracket}$ be a $\{-1, 1\}$ labelling of the $(x_i)_{i \in \llbracket 1, n \rrbracket}$.

a) show that $\Theta \left(\sum_{i=1}^{i=n} y_i K_\sigma(x, x_i) \right)$ classifies correctly the $(x_i, y_i)_{i \in \llbracket 1, n \rrbracket}$

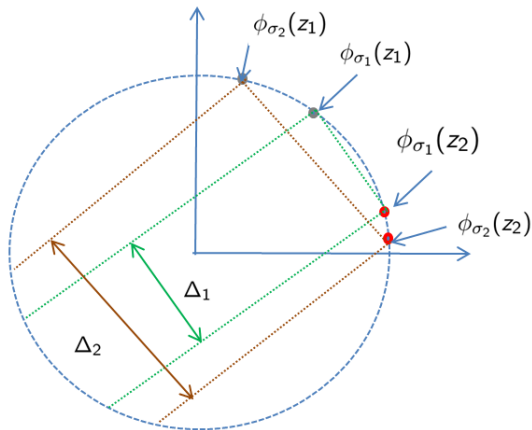
b) deduct from a) that $VC(\mathcal{F}_\sigma^n) \geq n$

The Kernel Trick: Radial Basis Functions

Remarks:

- Let $(x_i)_{i \in \llbracket 1, n \rrbracket}$ be n distinct points of \mathbb{R}^d , then $\forall i \neq j$
 $\langle \phi_\sigma(x_i), \phi_\sigma(x_j) \rangle_{\mathbb{N}} \xrightarrow{\sigma \rightarrow 0} 0$ so in the limit the $(\phi_\sigma(x_i))_{i \in \llbracket 1, n \rrbracket}$ are orthonormal in $\mathbb{R}^{\mathbb{N}}$ and thus independent and therefore separable by an hyperplane of the vector space they generate in $\mathbb{R}^{\mathbb{N}}$. So if σ is small enough the $(x_i)_{i \in \llbracket 1, n \rrbracket}$ can be labelled as desired in \mathbb{R}^d .
- as we will see later if n^+ points are labelled 1 and n^- are labelled -1 on a sphere of radius 1 and are orthogonal they can be separated by an hyperplane of margin $\sqrt{\frac{1}{n^+} + \frac{1}{n^-}}$. So if σ is very small it is easy to separate the points with such a margin as random orthogonal points on the sphere with random labelling could be classified with this margin.
- If there is a real structure the classes should be separable without having to totally "orthogonalize" the observations
- In general cross-validation will be used to justify that the model is adequate.

The Kernel Trick: classifications for various parameters



The margin increases as σ decreases ($\sigma_2 < \sigma_1$) and the points on the sphere are "orthogonalized"

The Kernel Trick: Radial Basis Functions

Example:

We consider the Δ -classifier h in \mathbb{R}^2 defined by:

$$h(x) = 1 \Leftrightarrow \sum_{i=1}^{i=4} \alpha_i y_i K_\sigma(x, z_i) + b_1 \geq 0$$

$$h(x) = -1 \Leftrightarrow \sum_{i=1}^{i=4} \alpha_i y_i K_\sigma(x, z_i) + b_2 \leq 0 \text{ with}$$

$$z_1 = \begin{pmatrix} 0.2 \\ 0.2 \end{pmatrix} \quad z_2 = \begin{pmatrix} 0.2 \\ 0.8 \end{pmatrix} \quad z_3 = \begin{pmatrix} 0.8 \\ 0.2 \end{pmatrix} \quad z_4 = \begin{pmatrix} 0.8 \\ 0.8 \end{pmatrix}$$

$$\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = 1 \text{ and } y_1 = 1, y_2 = -1, y_3 = -1, y_4 = 1$$

We colour in green the region classified $\{-1\}$, in blue the region classified $\{1\}$ and leave in white the rest of the space.

The Kernel Trick: Radial Basis Functions

- in all the examples here the 4 points z_i are classified correctly but with different margins
- to understand how $\phi_\sigma(\cdot)$ spreads apart the points z_i , on the sphere of radius 1, we calculate: $\min_{i \neq j} d(\phi_\sigma(z_i), \phi_\sigma(z_j)) = \min_{i \neq j} K_\sigma(z_i, z_j)$.

For $\sigma = 0.1$ we have $\min_{i \neq j} d(\phi_\sigma(z_i), \phi_\sigma(z_j)) = 1.414$, which means that the $\phi_\sigma(z_i)$ are "almost" orthogonal (they would be orthogonal for the value $\sqrt{1^2 + 1^2} = \sqrt{2}$ which is their maximum value).

For $\sigma = 1$ we have $\min_{i \neq j} d(\phi_\sigma(z_i), \phi_\sigma(z_j)) = 0.574$, and the points are not "orthogonalized" as previously.

- in terms of the margins at which we separate the (transformed) points we first calculate for $\omega = \sum_{i=1}^{i=4} \phi_\sigma(z_i)$ the quantity

$$\|\omega\|_{\mathbb{N}} = \sqrt{\mathbf{1}'_4 [\mathcal{K}(z_i, z_j)] \mathbf{1}_4} = 2 \text{ then:}$$

The Kernel Trick: Radial Basis Functions

for $\sigma = 1$, $b_1 = -0.00164$, $b_2 = 0.00164$ we get $\Delta = \frac{|b_2 - b_1|}{\|\omega\|_N} = 0.1$

for $\sigma = 0.1$, $b_1 = -0.80$, $b_2 = 0.80$ we get $\Delta = \frac{|b_2 - b_1|}{\|\omega\|_N} = 0.8$

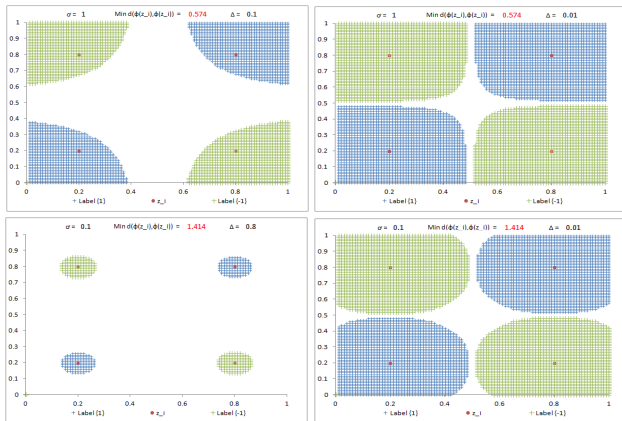
as we will see later, the maximum margin at which we can separate 2 group of two points all orthogonal and on a sphere of radius 1 is $\frac{1}{\sqrt{\frac{1}{2} + \frac{1}{2}}} = 1$

and in the two numerical examples here:

for $\sigma = 0.1$ (where the points have almost been orthogonalized) we can come close to this limit while

for $\sigma = 1$ even with a margin at only around 0.1 it is starting to become challenging to classify the points

The Kernel Trick: classifications for various parameters

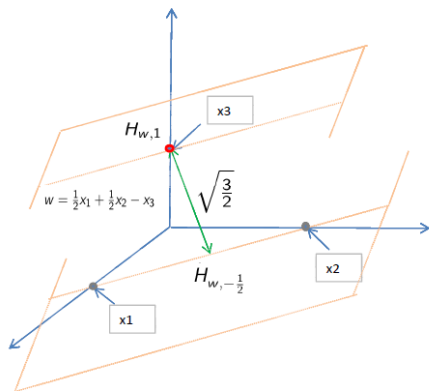
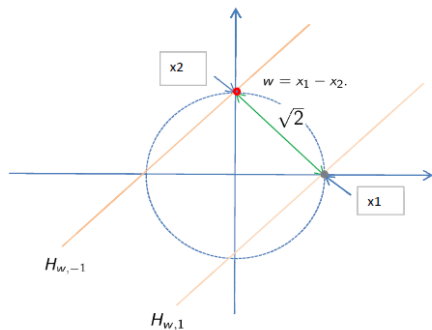


various classifications



Shattering Orthogonal Vectors

Shattering Orthogonal Vectors



Maximum margin for separation of orthogonal points of $S_{\mathbb{N}}^1$

Shattering Orthogonal Vectors

Remarks:

- For two vectors x_1, x_2 of $S_{\mathbb{N}}^1$ orthogonal and classified 1 and -1 , the maximum margin of an hyperplane separating them is $\sqrt{2}$. The hyperplanes forming the borders of the separation set are: $H_{w,-1}$ and $H_{w,1}$ with $w = x_1 - x_2$.
- For three vectors x_1, x_2, x_3 of $S_{\mathbb{N}}^1$ orthogonal and classified -1 for x_3 and 1 for the others, the maximum margin of an hyperplane separating them is $\sqrt{\frac{3}{2}}$. The hyperplanes forming the borders are: $H_{w,-\frac{1}{2}}$ and $H_{w,1}$ with $w = \frac{1}{2}x_1 + \frac{1}{2}x_2 - x_3$

Shattering Orthogonal Vectors

Proposition: Maximum Margin on $S_{\mathbb{N}}^1$

Let $\{x_i\}_{i \in \llbracket 1, n^+ \rrbracket}$ be n^+ vectors of $S_{\mathbb{N}}^1$ labelled 1 and $\{z_j\}_{j \in \llbracket 1, n^- \rrbracket}$ be n^- vectors of $S_{\mathbb{N}}^1$ labelled -1 . If we assume that the $\{x_i, z_j\}$ form a family of

orthogonal vectors and define $w = \frac{1}{n^+} \sum_{i=1}^{i=n^+} x_i - \frac{1}{n^-} \sum_{j=1}^{j=n^-} z_j$ then :

- Any hyperplane of margin Δ which separates the $\{x_i\}$ from the $\{z_j\}$ satisfies $\Delta \leq \sqrt{\frac{1}{n^-} + \frac{1}{n^+}}$
- $H_{w, \frac{1}{n^+}}$ and $H_{w, -\frac{1}{n^-}}$ are the borders of the maximum margin hyperplane classifier which separates the $\{x_i\}$ from the $\{z_j\}$ and $d(H_{w, \frac{1}{n^+}}, H_{w, -\frac{1}{n^-}}) = \sqrt{\frac{1}{n^-} + \frac{1}{n^+}}$

Shattering Orthogonal Vectors

Demonstration:

$w^+ = \frac{1}{n^+} \sum_{i=1}^{i=n^+} x_i$ belongs to the convex envelope of the $\{x_i\}$ and

$w^- = \frac{1}{n^-} \sum_{j=1}^{j=n^-} z_j$ belongs to the convex envelope of the $\{z_j\}$.

As the maximum margin is the distance between the two convex envelopes we have: $\Delta \leq \text{MaxMargin} = d(\mathcal{C}_x, \mathcal{C}_z) \leq d(w^+, w^-)$ and

$d(w^+, w^-) = \sqrt{\frac{1}{n^-} + \frac{1}{n^+}}$ which proves the first bullet point.

As the vectors are orthogonal we have:

$\forall x_i, \langle w, x_i \rangle = \frac{1}{n^+}$ and $\forall z_j, \langle w, z_j \rangle = -\frac{1}{n^-}$ so $H_{w, -\frac{1}{n^-}}$ and $H_{w, \frac{1}{n^+}}$ separate the points. We also have:

$d(H_{w, -\frac{1}{n^-}}, H_{w, \frac{1}{n^+}}) = \frac{|-\frac{1}{n^-} - \frac{1}{n^+}|}{\|w\|} = \sqrt{\frac{1}{n^-} + \frac{1}{n^+}}$ which means that the maximum margin is reached for $H_{w, -\frac{1}{n^-}}$ and $H_{w, \frac{1}{n^+}}$ which therefore constitute the borders of the maximum margin hyperplane classifier.

Shattering Orthogonal Vectors

Remarks:

If we note $k + 1 = n^+ + n^-$, $\{p_i\}_{i \in \llbracket 1, 1+k \rrbracket} = \{x_i\}_{i \in \llbracket 1, n^+ \rrbracket} \cup \{z_j\}_{j \in \llbracket 1, n^- \rrbracket}$ and

$$p = \frac{1}{k+1} \sum_{i=1}^{i=1+k} p_i \text{ then:}$$

- $\forall i \in \llbracket 1, 1+k \rrbracket$, $d(p, p_i) = \sqrt{\frac{k}{k+1}}$ so p and the $k + 1$ points p_i are in an affine space of dimension k and the p_i 's are on the sphere of center p and radius $\sqrt{\frac{k}{k+1}}$ of this affine space
- $\min_{i \in \llbracket 0, k+1 \rrbracket} \sqrt{\frac{1}{i} + \frac{1}{k+1-i}} = \sqrt{\frac{1}{\lfloor \frac{k+1}{2} \rfloor} + \frac{1}{k+1 - \lfloor \frac{k+1}{2} \rfloor}}$
- the $k + 1$ points $q_i = \sqrt{\frac{k+1}{k}} p_i$ are orthogonal on a sphere of radius 1 and according to the previous proposition can always be classified (whatever there label is) with a margin equal to:

$$\sqrt{\frac{k+1}{k}} \sqrt{\frac{1}{\lfloor \frac{k+1}{2} \rfloor} + \frac{1}{k+1 - \lfloor \frac{k+1}{2} \rfloor}}$$

Shattering Orthogonal Vectors

Corollary: Maximum Margin on $S_{\mathbb{N}}^1$

The maximum margin for a Gap tolerant classifier of radius 1 for $k + 1$ points is attained by taking $k + 1$ points p_i forming an orthogonal family with norms $\sqrt{\frac{k+1}{k}}$ of \mathbb{R}^{k+1} . Seen from the affine space of dimension k they generate these points lay on a sphere of radius 1 and can be separated with the maximum possible margin.

Demonstration:

According to the previous remarks the points q_i can be classified with Gap classifiers reaching the maximum margin according the admitted theorem in the section on Gap classifiers

Remarks:

The $k + 1$ points q_i form a simplex in the affine space of dimension k that they generate as $\forall i \neq j, d(q_i, q_j) = \sqrt{2}$

Shattering Orthogonal Vectors

Example:

Let z_1, z_2, z_3 be three orthogonal vectors of norms 1. We note $w = \frac{1}{3}(z_1 + z_2 + z_3)$ and $H_{w,-1}$ the hyperplane of the vector space $\text{Vect}(z_1, z_2, z_3)$ defined by $H_{w,-1} = \{x \in \text{Vect}(z_1, z_2, z_3), \langle w, x \rangle = \frac{1}{3}\}$ then:

- z_1, z_2, z_3 and w belongs to $H_{w,-1}$ as they all verify $\langle w, x \rangle = \frac{1}{3}$
- z_1, z_2, z_3 lay on a circle of center w and radius $\sqrt{\frac{2}{3}}$ as they all verify
$$d(z_i, w) = \sqrt{\left(\frac{2}{3}\right)^2 + \left(\frac{1}{3}\right)^2 + \left(\frac{1}{3}\right)^2}$$
- z_1, z_2, z_3 form a simplex / equilateral triangle as for all $i \neq j$,
$$d(z_i, z_j) = \sqrt{2}$$
- the distance between the segment (convex envelope) formed by any 2 points z_i, z_j and the third one z_k , which is also the maximum margin of an hyperplane classifier separating the points, equal:

$$d\left(\frac{1}{2}(z_i + z_j), z_k\right) = \sqrt{\frac{1}{4} + \frac{1}{4} + 1} = \sqrt{\frac{3}{2}}$$

ν -SVM

Definition: ν -SVM

For any learning sample $\{(x_i, y_i)\}_{i \in \llbracket 1, n \rrbracket}$ and $\nu > 0$ we call ν -SVM the

solution of: $(P_\nu) \begin{cases} \min_{w, b, \rho, \xi_i} \frac{1}{2} \|w\|^2 - 2\rho + \frac{\nu}{n} \sum_{i=1}^n \xi_i \\ y_i (\langle w, x_i \rangle + b) \geq \rho - \xi_i \\ \xi_i \geq 0 \end{cases}$

Remark 1:

The definition is similar to the definition of a C -SVM but the new parameter ρ is introduced to enable a better geometric interpretation of the problem and to have an upper bound on the fraction of misclassified points ($\xi_i > 0$) and a lower bound on the fraction of support vectors ($\alpha_i > 0$). We did not put the condition $\rho \geq 0$ which is automatically verified for a solution of this problem.

Remark 2:

In (P_ν) the two hyperplanes which classify the points -1 and 1 are $H_{w,b-\rho}$ and $H_{-w,-b+\rho}$ and the distance between them (which represents the margin of the classifier) is $\frac{2\rho}{\|w\|_d}$. In the minimization the quantity $\frac{\|w\|_d}{\rho}$ does not appear but instead the quantity $\|w\|_d - \rho$ which leads to simpler numerical implementations and geometric interpretations of the results.

Proposition: Dual Problem for ν -SVM

$$(P_\nu) \Leftrightarrow (D_\nu) \text{ where } (D_\nu) \left\{ \begin{array}{l} \min_{\alpha_i} \frac{1}{2} \left\| \sum_{i=1}^{i=n} \alpha_i y_i x_i \right\|_d^2 \\ \sum_{i=1}^{i=n} \alpha_i y_i = 0 \\ \sum_{i=1}^{i=n} \alpha_i = 2 \\ 0 \leq \alpha_i \leq \frac{\nu}{n} \end{array} \right. \quad \text{and } w^* = \sum_{i=1}^{i=n} \alpha_i^* y_i x_i$$

Demonstration (hint):

The Lagrangian $L(w, b, \rho, \xi, \alpha, \beta)$ of P_ν is:

$$\frac{1}{2} \|w\|^2 - 2\rho + \frac{\nu}{n} \sum_{i=1}^{i=n} \xi_i - \sum_{i=1}^{i=n} \alpha_i [y_i (\langle w, x_i \rangle + b) - \rho + \xi_i] - \sum_{i=1}^{i=n} \beta_i \xi_i.$$

so we get: $\frac{\partial L}{\partial w} = w' - \sum_{i=1}^{i=n} \alpha_i y_i x_i' = 0$ ($C_\nu 1$)

$$\frac{\partial L}{\partial b} = - \sum_{i=1}^{i=n} \alpha_i y_i = 0$$
 ($C_\nu 2$)

$$\frac{\partial L}{\partial \rho} = -2 + \sum_{i=1}^{i=n} \alpha_i = 0$$
 ($C_\nu 3$)

$$\frac{\partial L}{\partial \xi_i} = \frac{\nu}{n} - \alpha_i - \beta_i = 0 \implies 0 \leq \alpha_i \leq \frac{\nu}{n}$$
 ($C_\nu 4$)

From these equations we see that (D_ν) is the dual of (P_ν) and that consequently (due to the form of the problem) the solutions will be the same each time (D_ν) has a finite solution. We note also that for (D_ν) to have a finite solution we need $\nu \geq 2$ otherwise the last two constraints of (D_ν) cannot be satisfied simultaneously.

Theorem and Definition : Reduced Convex Envelope

Let $\{(x_i, y_i)\}_{i \in \llbracket 1, n \rrbracket}$ be a sample. We assume that the two classes $\{-1, 1\}$ are represented in this sample (i.e $\mathcal{X}_{-1} \neq \emptyset$ and $\mathcal{X}_1 \neq \emptyset$).

Let $\mathcal{E}_\nu(\mathcal{X}_1) = \left\{ \sum_{\{i, y_i=1\}} \alpha_i x_i / \sum_{\{i, y_i=1\}} \alpha_i = 1 \text{ and } 0 \leq \alpha_i \leq \frac{\nu}{n} \right\}$ and

$\mathcal{E}_\nu(\mathcal{X}_{-1}) = \left\{ \sum_{\{i, y_i=-1\}} \alpha_i x_i / \sum_{\{i, y_i=-1\}} \alpha_i = 1 \text{ and } 0 \leq \alpha_i \leq \frac{\nu}{n} \right\}$ then:

- $\mathcal{E}_\nu(\mathcal{X}_1)$ and $\mathcal{E}_\nu(\mathcal{X}_{-1})$ are convex sets and are called reduced convex envelopes of \mathcal{X}_{-1} and \mathcal{X}_1
- finding $d(\mathcal{E}_\nu(\mathcal{X}_1), \mathcal{E}_\nu(\mathcal{X}_{-1}))$ and solving (D_ν) is the same problem

Demonstration (hint):

Demonstrating the convexity of $\mathcal{E}_\nu(\mathcal{X}_1)$ and $\mathcal{E}_\nu(\mathcal{X}_{-1})$ is straightforward.

The points on which $d(\mathcal{E}_\nu(\mathcal{X}_1), \mathcal{E}_\nu(\mathcal{X}_{-1}))$ is attained are the solutions of:

$$\left\{ \begin{array}{l} \min_{\alpha_i \geq 0} \left\| \sum_{\{i, y_i=1\}} \alpha_i x_i - \sum_{\{i, y_i=-1\}} \alpha_i x_i \right\|_d^2 \\ \sum_{\{i, y_i=1\}} \alpha_i = 1 \\ \sum_{\{i, y_i=-1\}} \alpha_i = 1 \\ 0 \leq \alpha_i \leq \frac{\nu}{n} \end{array} \right. \Leftrightarrow \left\{ \begin{array}{l} \min_{\alpha_i} \left\| \sum_{i=1}^{i=n} \alpha_i x_i y_i \right\|_d^2 \\ \sum_{i=1}^{i=n} \alpha_i y_i = 0 \\ \sum_{i=1}^{i=n} \alpha_i = 2 \\ 0 \leq \alpha_i \leq \frac{\nu}{n} \end{array} \right. \quad \text{Q.E.D}$$

Corollary: Geometric Interpretation

If we note $z_1 = \sum_{\{i, y_i=1\}} \alpha_i^* x_i$ and $z_2 = \sum_{\{i, y_i=-1\}} \alpha_i^* x_i$ then:

- $\|z_1 - z_2\|_d = d(\mathcal{E}_\nu(\mathcal{X}_1), \mathcal{E}_\nu(\mathcal{X}_{-1}))$
- $H_{w^*, b^* - \rho^*}$ and $H_{-w^*, -b^* - \rho^*}$ derived from (P_ν) are both orthogonal to $z_1 - z_2$

Demonstration :

$z_1 - z_2 = \sum_{i=1}^{i=n} \alpha_i^* y_i x_i$ which is the expression of w^* for (P_ν) . Q.E.D

Corollary: Number of Support Vectors, Number of Errors for (P_ν)

For the classification problem (P_ν) ($\nu \geq 2$):

- $\frac{1}{n} \#\{i, \xi_i \neq 0\} \leq \frac{2}{\nu}$ (majoration of the proportion of points from the sample misclassified)
- $\frac{1}{n} \#\{i, \alpha_i \neq 0\} \geq \frac{2}{\nu}$ (minoration of the proportion of points from the sample used as support vectors)

Demonstration : The KKT conditions for (P_ν) are:

$$(KKT_\nu 1) : \alpha_i [y_i (\langle w, x_i \rangle + b) - \rho + \xi_i] = 0$$

$$(KKT_\nu 2) : \beta_i \xi_i = 0$$

$$(KKT_\nu 2) \text{ and } (C_\nu 4) \Rightarrow \left(\frac{\nu}{n} - \alpha_i\right) \xi_i = 0 \text{ so } \xi_i \neq 0 \Rightarrow \alpha_i = \frac{\nu}{n}$$

$$\text{using } (C_\nu 3) : \sum_{i=1}^{i=n} \alpha_i = 2 \Rightarrow \sum_{i, \xi_i \neq 0} \alpha_i \leq 2 \Rightarrow \#\{i, \xi_i \neq 0\} \frac{\nu}{n} \leq 2$$

so $\frac{1}{n} \#\{i, \xi_i \neq 0\} \leq \frac{2}{\nu}$ which shows the first point.

According to $(C_\nu 4)$ $0 \leq \alpha_i \leq \frac{\nu}{n}$

using $(C_\nu 3)$: $\sum_{i=1}^n \alpha_i = 2 \Rightarrow \sum_{i, \alpha_i \neq 0} \frac{\nu}{n} \geq 2 \Rightarrow \frac{1}{n} \#\{i, \alpha_i \neq 0\} \geq \frac{2}{\nu}$ Q.E.D

Remark: The ν -SVM enables to control the number of errors committed by the classifier through the parameter ν .

Theorem (admitted): B Schoelkopf, A Smola, R Williamson, P Bartlett

Under certain conditions of continuity on $P_{(X, Y)}$

- $\frac{1}{n} \#\{i, \xi_i \neq 0\} \rightarrow \frac{2}{\nu}$ (convergence in probability)
- $\frac{1}{n} \#\{i, \alpha_i \neq 0\} \rightarrow \frac{2}{\nu}$ (convergence in probability)

Proposition: Relationship between $C - SVM$ and $\nu - SVM$

Let $w(\nu)$, $b(\nu)$, $\rho(\nu)$, $\xi(\nu)$ be the solutions of the ν -SVM (P_ν) with $\rho(\nu) \neq 0$, then:

$\frac{w(\nu)}{\rho(\nu)}$, $\frac{b(\nu)}{\rho(\nu)}$, $\frac{\xi(\nu)}{\rho(\nu)}$ are the solutions of the C -SVM (P_C) with $C = \frac{2\nu}{n\rho(\nu)}$.
As a consequence these two classifiers have the same decision boundaries.

Demonstration :

$$(P_\nu) \Leftrightarrow \begin{cases} \min_{w, b, \rho, \xi_i} \frac{1}{2} \|w\|^2 - 2\rho + \frac{\nu}{n} \sum_{i=1}^{i=n} \xi_i \\ y_i(\langle w, x_i \rangle + b) \geq \rho - \xi_i \\ \xi_i \geq 0 \end{cases}$$

First note that $\rho(\nu) = 0$ would correspond to a trivial solution for (P_ν) because in this case the function to minimize would always be positive and would then reach its minimum value of zero for the trivial solution $w = 0, b = 0, \xi = 0$. So we consider here $\nu - SVM$ for which $\rho(\nu) \neq 0$.

If we assume now that (P_ν) has a non trivial solution (i.e $\rho(\nu) \neq 0$) then $w(\rho(\nu)), b(\rho(\nu)), \xi(\rho(\nu))$ are solutions of

$$\begin{cases} \min_{w, b, \xi_i} \frac{1}{2} \|w\|^2 - 2\rho(\nu) + \frac{\nu}{n} \sum_{i=1}^{i=n} \xi_i \\ y_i(\langle w, x_i \rangle + b) \geq \rho(\nu) - \xi_i \\ \xi_i \geq 0 \end{cases}$$

$$\Leftrightarrow \begin{cases} \min_{w, b, \xi_i} \frac{1}{2} \left\| \frac{w}{\rho(\nu)} \right\|^2 - \frac{2}{\rho(\nu)} + \frac{\nu}{n\rho(\nu)} \sum_{i=1}^{i=n} \frac{\xi_i}{\rho(\nu)} \\ y_i(\langle \frac{w}{\rho(\nu)}, x_i \rangle + \frac{b}{\rho(\nu)}) \geq 1 - \frac{\xi_i}{\rho(\nu)} \\ \frac{\xi_i}{\rho(\nu)} \geq 0 \end{cases}$$

So the arguments are the solutions of:

$$\left\{ \begin{array}{l} \min_{w, b, \xi_i} \left\| \frac{w}{\rho(\nu)} \right\|^2 + \frac{2\nu}{n\rho(\nu)} \sum_{i=1}^{i=n} \frac{\xi_i}{\rho(\nu)} \\ y_i \left(\left\langle \frac{w}{\rho(\nu)}, x_i \right\rangle + \frac{b}{\rho(\nu)} \right) \geq 1 - \frac{\xi_i}{\rho(\nu)} \\ \frac{\xi_i}{\rho(\nu)} \geq 0 \end{array} \right. \text{ which is a } C\text{-SVM with } C = \frac{2\nu}{n\rho(\nu)}$$

Q.E.D.

The hyperplane borders for the ν - classifier (P_ν problem) are:

$H_{w(\nu), b(\nu) - \rho(\nu)}$ and $H_{-w(\nu), -b(\nu) - \rho(\nu)}$ and

the hyperplane borders for the C - classifier (P_C problem) are:

$H_{\frac{w(\nu)}{\rho(\nu)}, \frac{b(\nu)}{\rho(\nu)} - 1}$ and $H_{-\frac{w(\nu)}{\rho(\nu)}, -\frac{b(\nu)}{\rho(\nu)} - 1}$ which are the same hyperplanes. Q.E.D

Single Class SVM, Unsupervised Learning

Background :

- For a learning sample $(x_i)_{i \in \llbracket 1, n \rrbracket}$ issued from a probability P_X we search a subset of \mathbb{R}^d as "simple" and "small" as possible containing the $(x_i)_{i \in \llbracket 1, n \rrbracket}$.
- The embedding is done after an immersion into \mathbb{R}^N via a function ϕ based on a Kernel K . Some points may be allowed to be misclassified (i.e left outside the domain) in \mathbb{R}^N but at a cost. In this case a trade-off is made between the size and complexity of the domain chosen to embed the x_i and the measure of the errors of classification made.
- For a new observation z in \mathbb{R}^d the hypothesis that z is issued from the probability distribution P_X will be accepted (with a certain confidence level) if $\phi(z)$ is in \mathcal{D} .

Remarks:

- $\mathcal{D}_K = \{x \in \mathbb{R}^d, \phi(x) \in \mathcal{D}\}$ may appear as a single or several clusters of \mathbb{R}^d .
- As the sample $(x_i)_{i \in \llbracket 1, n \rrbracket}$ consists here of unlabelled data, the problem of determining \mathcal{D}_K is called unsupervised learning
- From now on we will use the Kernel $K_\sigma(x, y) = \exp\left(-\frac{\|x-y\|_d^2}{2\sigma^2}\right)$ and note ϕ_σ the associated transformation.

Single Class SVM: Clusterization without errors

We consider first for the sample $(x_i)_{i \in \llbracket 1, n \rrbracket}$ of \mathbb{R}^d the problem:

$$(U_\sigma) \Leftrightarrow \begin{cases} \min_{w \in \mathbb{R}^N} \frac{1}{2} \|w\|^2 \\ \forall i \in \llbracket 1, n \rrbracket, \langle w, \phi_\sigma(x_i) \rangle \geq 1 \end{cases}$$

Remarks:

- As mentioned previously, $\forall x \in \mathbb{R}^d, \phi_\sigma(x) \in S_{\mathbb{N}}^1$ (the sphere of center 0 and radius 1 of $\mathbb{R}^{\mathbb{N}}$)

- (U_σ) has a domain of definition which is not empty because

$$w = \sum_{j=1}^{j=n} \phi_\sigma(x_j) \text{ verifies}$$

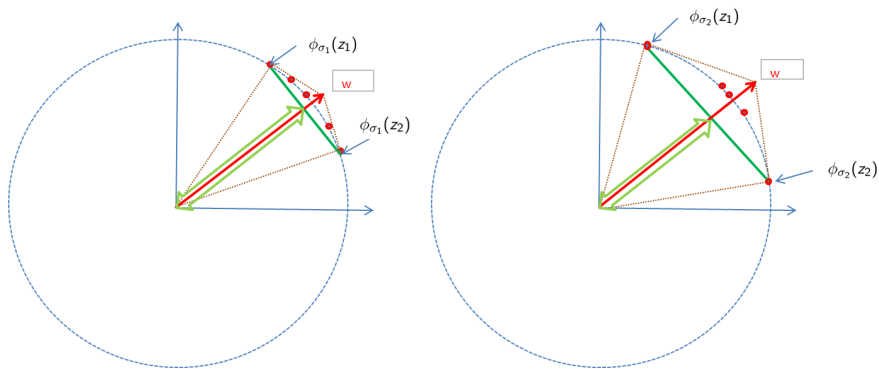
$$\langle w, \phi_\sigma(x_i) \rangle = \sum_{j=1}^{j=n} K_\sigma(x_j, x_i) = 1 + \sum_{j \neq i} K_\sigma(x_j, x_i) \geq 1$$

- We admit that the min for (U_σ) is attained. We note w_σ such a solution for (U_σ)

Single Class SVM: Clusterization without errors

- $\|w_\sigma\|_{\mathbb{N}} \geq 1$ because $1 \leq \langle w_\sigma, \phi_\sigma(x_i) \rangle \leq \|w_\sigma\|_{\mathbb{N}} \|\phi_\sigma(x_i)\|_{\mathbb{N}} = \|w_\sigma\|_{\mathbb{N}}$
- $\{\phi_\sigma(x), x \in \mathbb{R}^d, \langle w, \phi_\sigma(x_i) \rangle \geq 1\}$ are the points in the portion of the sphere delimited by $H_{w, -1}$
- The distance between the center of the sphere $S_{\mathbb{N}}^1$ and $H_{w_\sigma, -1}$ is $\frac{1}{\|w_\sigma\|_{\mathbb{N}}}$. By minimizing $\|w_\sigma\|_{\mathbb{N}}$ we minimize the portion of $S_{\mathbb{N}}^1$ delimited by $H_{w_\sigma, -1}$ which defines \mathcal{D}_{K_σ}
- σ defines the complexity of the model used and thus the complexity of the separation domain \mathcal{D}_{K_σ} . At σ fixed $\|w_\sigma\|_{\mathbb{N}}$ defines the size of the domain
- in the graph below we see w_σ and \mathcal{D}_{K_σ} for various values of σ . Note that despite the fact that \mathcal{D} (the slice of the sphere) increases when σ decreases, \mathcal{D}_{K_σ} decreases as σ decreases.

Single Class SVM: Clusterization without errors



Hyperplane separating the points with maximum distance to the origin (delimiting the smallest portion of the sphere)

Single Class SVM: Clusterization without errors

Example: we consider the points:

$x_1 = \begin{pmatrix} 0.327 \\ 0.3 \end{pmatrix}$ $x_2 = \begin{pmatrix} 0.673 \\ 0.3 \end{pmatrix}$ $x_3 = \begin{pmatrix} 0.5 \\ 0.6 \end{pmatrix}$ which form an equilateral triangle in \mathbb{R}^2 (with sides of lengths $d = 0.346$).

The problem is symmetric in \mathbb{R}^N as $\forall i \neq j, \langle \phi_\sigma(x_i), \phi_\sigma(x_j) \rangle = \exp(\frac{-d}{2\sigma^2})$ and the solution w_σ of (U_σ) will be a linear combination of the $\phi_\sigma(x_i)$ with equal coefficients $\alpha(\sigma)$ and the three $\phi_\sigma(x_i)$ will be on the hyperplane.

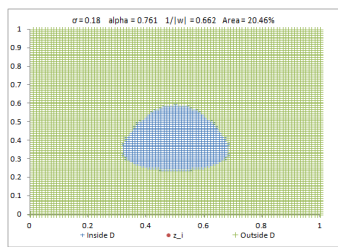
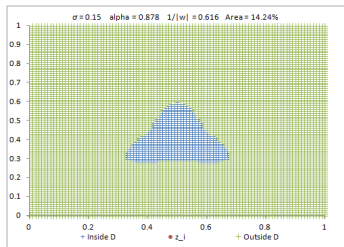
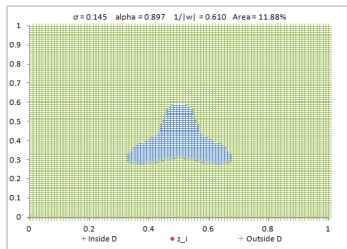
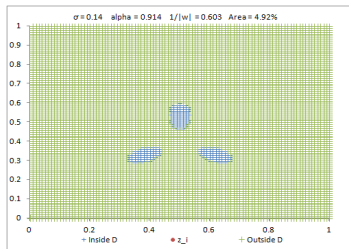
We determine $\alpha(\sigma)$ such that $\sum_{j=1}^{j=3} \alpha(\sigma) K_\sigma(x_j, x_i) = 1$

so, $\alpha(\sigma) = [1 + 2\exp(\frac{-d}{2\sigma^2})]^{-1}$ and $\mathcal{D}_{K_\sigma} = \{x \in \mathbb{R}^2, \sum_{i=1}^{i=3} \alpha(\sigma) K_\sigma(x_i, x) \geq 1\}$

We plot below \mathcal{D}_{K_σ} for various values of σ .

The parameter σ defines the complexity of the domain and $\alpha(\sigma)$ defines the domain of minimum size that contains the $\{x_i\}_{i \in [1,3]}$.

Single Class SVM: Clusterization without errors



Single Class SVM: Clusterization without errors

Table: Size of the domain \mathcal{D}_{K_σ} for various levels of complexity

σ (complexity)	$\alpha(\sigma)$	$\frac{1}{\ w\ _N}$	$\lambda(\mathcal{D}_{K_\sigma})$ (size of the domain)
0.140	0.914	0.603	4.92%
0.145	0.897	0.610	11.88%
0.150	0.878	0.616	14.24%
0.180	0.761	0.662	20.46%

Remarks: Generally

- as $\sigma \rightarrow 0$, the domain \mathcal{D}_{K_σ} in \mathbb{R}^d "converges" to the set formed by the sample points only, while the $\phi_\sigma(x)$ for all points of \mathbb{R}^d get "orthogonalized" i.e verify $\forall x \neq y, \langle \phi_\sigma(x) \phi_\sigma(y) \rangle \rightarrow 0$

Single Class SVM: Clusterization without errors

- as $\sigma \rightarrow 0$, $w_\sigma \sim \sum_{i=1}^{i=n} \phi_\sigma(x_i)$ as all points from $\phi_\sigma(\mathbb{R}^d)$ becomes orthogonal on $S_{\mathbb{N}}^1$ resulting in all points z_j from the sample to verify $\langle w_\sigma, \phi_\sigma(x_j) \rangle \sim 1$ while any other point x in \mathbb{R}^d satisfies $\langle w_\sigma, \phi_\sigma(x) \rangle \sim 0$
- as $\sigma \rightarrow 0$, $d(H_{w_\sigma, -1}, 0) \sim \frac{1}{\sqrt{n}}$ so it is not an achievement to be able to separate the $\phi_\sigma(x_i)$ by an hyperplane of distance only $\frac{1}{\sqrt{n}}$ because any random set of n points "sufficiently orthogonalized" could have been separated with the same distance to the origin
- generally the adequation of the model chosen will be tested by cross validation.

Single Class SVM: Clusterization with errors

We consider now the problem:

$$(U_{\sigma,\nu}) \begin{cases} \min_{w \in \mathbb{R}^N, \rho, \xi_i} \frac{1}{2} \|w\|^2 - 2\rho + \frac{\nu}{n} \sum_{i=1}^{i=n} \xi_i \\ \langle w, \phi_{\sigma}(x_i) \rangle \geq \rho - \xi_i \\ \xi_i \geq 0 \end{cases}$$

which is the extension of the previous clustering problem but this time with some errors ξ_i allowed in the classification. A ν formulation has been chosen instead of a C -formulation in order to have a better-interpretability of the parameters.

This problem is the same as the problem (P_{ν}) studied previously but this time without the variable b and with all the y_i equal to 1 so the dual problem here is the same as the dual of (P_{ν}) but without the condition related to b (which was $\sum_{i=1}^{i=n} \alpha_i y_i = 0$) and with all the y_i taken equal to 1 in the equations

Single Class SVM: Clusterization with errors

So we obtain,

Proposition: Dual Problem for ν -SVM

$$(U_{\sigma,\nu}) \Leftrightarrow (U_{\sigma,\nu}^*) \text{ where } (U_{\sigma,\nu}^*) \left\{ \begin{array}{l} \min_{\alpha_i} \frac{1}{2} \sum_{i=1}^{i=n} \sum_{j=1}^{j=n} \alpha_i \alpha_j k(x_i, x_j) \\ \sum_{i=1}^{i=n} \alpha_i = 2 \\ 0 \leq \alpha_i \leq \frac{\nu}{n} \end{array} \right.$$

$$\text{with: } w^* = \sum_{i=1}^{i=n} \alpha_i^* \phi_{\sigma}(x_i)$$

Single Class SVM: Alternative Geometric Approach

Consider the problem

$$(B_{\sigma, \nu}) \left\{ \begin{array}{l} \min_{R \in \mathbb{R}, c \in \mathbb{R}^N, \xi \in \mathbb{R}^n} 2R^2 + \frac{\nu}{n} \sum_{i=1}^n \xi_i \\ \|\phi(x_i) - c\|_{\mathbb{N}}^2 \leq R^2 + \xi_i \\ \xi_i \geq 0 \end{array} \right.$$

where we search the ball of $R^{\mathbb{N}}$ of minimum radius which contains the $\phi(x_i)$. The cluster in \mathbb{R}^d will be defined as the points whose images $\phi(x)$ belongs to this ball. Some errors are permitted (some points from the sample are left outside the domain) in order to minimize the radius.

Proposition

When applied to the same vectors $\phi(x_i)$, $(B_{\sigma, \nu})$ and $(U_{\sigma, \nu})$ are two formulations of the same problem and $c^* = \frac{w^*}{2}$

Single Class SVM: Alternative Geometric Approach

Demonstration: we consider the Lagrangian

$$L(R, c, \xi, \alpha, \beta) = 2R^2 + \frac{\nu}{n} \sum_{i=1}^{i=n} \xi_i - \sum_{i=1}^{i=n} \alpha_i (R^2 + \xi_i - \|\phi(x_i) - c\|_{\mathbb{N}}^2) - \sum_{i=1}^{i=n} \beta_i \xi_i$$

so we get:

$$\frac{\partial L}{\partial R} = 4R - 2R \sum_{i=1}^{i=n} \alpha_i = 0 \implies \sum_{i=1}^{i=n} \alpha_i = 2$$

$$\frac{\partial L}{\partial c} = -2 \sum_{i=1}^{i=n} \alpha_i (\phi(x_i) - c)' = 0 \implies \left(\sum_{i=1}^{i=n} \alpha_i \right) c = \sum_{i=1}^{i=n} \alpha_i \phi(x_i)$$

and so from the previous equation $c = \frac{1}{2} \sum_{i=1}^{i=n} \alpha_i \phi(x_i)$

$$\frac{\partial L}{\partial \xi_i} = \frac{\nu}{n} - \alpha_i - \beta_i = 0 \implies 0 \leq \alpha_i \leq \frac{\nu}{n}$$

We can now rewrite $L(R, c, \xi, \alpha, \beta)$ as:

$$\left(2R^2 - \sum_{i=1}^{i=n} \alpha_i R^2 \right) + \sum_{i=1}^{i=n} \xi_i \left(\frac{\nu}{n} - \alpha_i - \beta_i \right) + \sum_{i=1}^{i=n} \alpha_i \|\phi(x_i) - c\|_{\mathbb{N}}^2$$

and the first two terms are zero when the conditions are satisfied

Single Class SVM: Alternative Geometric Approach

replacing c by its expression we get: $\sum_{i=1}^{i=n} \alpha_i \|\phi(x_i) - c\|_{\mathbb{N}}^2$

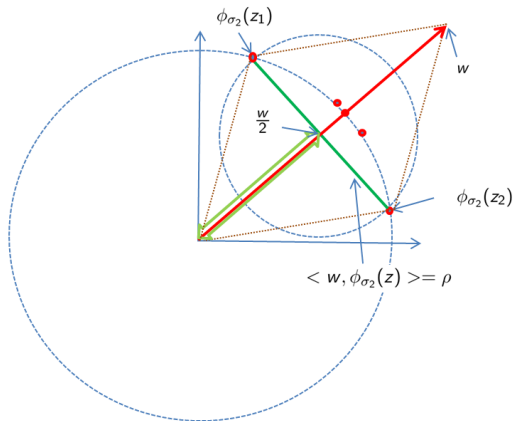
$$= \sum_{i=1}^{i=n} \alpha_i \|\phi(x_i)\|_{\mathbb{N}}^2 + \left(\sum_{i=1}^{i=n} \alpha_i \right) \|c\|_{\mathbb{N}}^2 - 2 \left\langle \sum_{i=1}^{i=n} \alpha_i \phi(x_i), c \right\rangle$$
$$= 2 + 2\|c\|_{\mathbb{N}}^2 - 4\|c\|_{\mathbb{N}}^2 = 2 - \frac{1}{2} \sum_{i=1}^{i=n} \sum_{j=1}^{j=n} \alpha_i \alpha_j K(x_i, x_j)$$

so the dual problem is

$$(B_{\sigma, \nu}^*) \left\{ \begin{array}{l} \max_{\alpha_i} 2 - \frac{1}{2} \sum_{i=1}^{i=n} \sum_{j=1}^{j=n} \alpha_i \alpha_j K(x_i, x_j) \\ \sum_{i=1}^{i=n} \alpha_i = 2 \\ 0 \leq \alpha_i \leq \frac{\nu}{n} \end{array} \right.$$

with $c^* = \frac{1}{2} \sum_{i=1}^{i=n} \alpha_i \phi(x_i)$ Q.E.D

Single Class SVM: Alternative Geometric Approach



Equivalent geometric approaches for clusterization (here for symmetry reasons $\alpha_1 = \alpha_2 = 1$)

Trees and Ensemble Methods

Background:

Let (X, Y) be a random variable of (Ω, \mathcal{F}, P) with Y taking its values in \mathbb{R}^d and being in $L^2(\Omega, \mathbb{R}^d, P)$

Let \mathcal{F} be a set of measurable functions such that

$$\forall f \in \mathcal{F}, \int \|f[X(w)]\|^2 dP(w) < +\infty$$

We note $g(X) = E[Y/X]$ and $\epsilon = Y - g(X)$

We are going to study how an estimator calibrated on a sample of (X, Y) depends on the sample and the uncertainty this creates in terms of the prediction function

We note $Z(n) = \{(X_i, Y_i)\}_{j \in [1, n]}$ a n -sample of (X, Y) and $f_{Z(n)}$ the estimator calibrated with this sample. So $\forall \omega \in \Omega, f_{Z(n)}(\omega) \in \mathcal{F}$ and we study the quantity $E[\|Y_{n+1} - f_{Z(n)}(X_{n+1})\|^2]$.

Theorem and Definition

With the previous notations where:

$Z = (X, Y)$, $g(X) = E[Y/X]$, $\epsilon = Y - g(X)$ and $\bar{f}(x) = E[f_{Z(n)}(x)]$

we have:

$$\begin{aligned} E[\|Y_{n+1} - f_{Z(n)}(X_{n+1})\|^2 / X_{n+1} = x] \\ = E[\|\epsilon\|^2] + \|g(x) - \bar{f}(x)\|^2 + E[\|f_{Z(n)}(x) - \bar{f}(x)\|^2] \end{aligned}$$

We call:

- $E[\|\epsilon\|^2]$ the irreducible error
- $\|g(x) - \bar{f}(x)\|^2$ the (*biais*)² of the model when predicting in x
- $E[\|f_{Z(n)}(x) - \bar{f}(x)\|^2]$ the variance of the model when predicting in x

Demonstration:

$$\begin{aligned} & E[\|Y_{n+1} - f_{Z(n)}(X_{n+1})\|^2 / X_{n+1} = x] \\ &= E[\|g(x) + \epsilon_{n+1} - f_{Z(n)}(x)\|^2 / X_{n+1} = x] \\ &= E[\|g(x) - f_{Z(n)}(x)\|^2 + \|\epsilon_{n+1}\|^2] \text{ because } \epsilon_{n+1} \text{ is centred and} \\ & \text{independent from } Z(n) \\ &= E[\|\epsilon_{n+1}\|^2] + E[\|\bar{f}(x) - f_{Z(n)}(x)\|^2] + \|g(x) - \bar{f}(x)\|^2 \text{ because for any} \\ & \text{random vector } U \text{ and vector } b \\ & E[\|U - b\|^2] = E[\|U - E(U)\|^2] + \|E(U) - b\|^2 \text{ Q.E.D} \end{aligned}$$

Corollary

$$\begin{aligned} & \forall x \ E[\|Y_{n+1} - f_{Z(n)}(x)\|^2 / X_{n+1} = x] \\ & \geq E[\|Y_{n+1} - \bar{f}(x)\|^2 / X_{n+1} = x] \\ & \geq E[\|Y_{n+1} - g(x)\|^2 / X_{n+1} = x] \end{aligned}$$

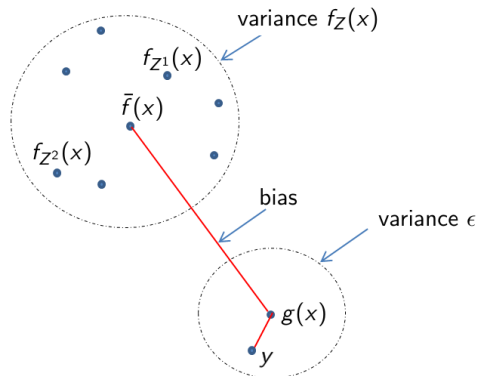
Remarks:

- the term $E[\|\bar{f}(x) - f_{Z(n)}(x)\|^2]$ reflects the variance of predictions resulting from the randomness of the calibration samples. As different learning samples produce different predictor functions we do not know which predictor will be the more accurate.
- the term $E[\|\bar{f}(x) - f_{Z(n)}(x)\|^2]$ shows that once we have defined the calibration process: $Z(n) \rightarrow f_{Z(n)}$ the "theoretical" estimator \bar{f} is better (from a quadratic error point of view) than using a "random" predictor $f_{Z(n)}$
- in practice it is usually not possible to calculate \bar{f} but if we have different learning samples $\{Z^j(n)\}_{j \in \llbracket 1, l \rrbracket}$ (or split one learning sample in l several learning samples) we can approximate \bar{f} by $\frac{1}{l} \sum_{i=1}^l f_{Z^i(n)}$

Remarks:(continued)

- in ensemble methods, the average predictor $\frac{1}{l} \sum_{j=1}^l f_{Z^j(n)}$ will be chosen instead of the single predictor $f_{Z^1(n), \dots, Z^l(n)}$ made on the aggregate of the l learning samples.
- in the bias-variance formula we see some analogy with the Vapnik's paradigm for estimation. Using a large/complex universe of estimators \mathcal{F} will make it more likely to find functions \bar{f} close to g (i.e verifying $\|\bar{f} - g\|$ small) but the complexity of \mathcal{F} may also have the effect of creating predictors exhibiting large variances to the calibrating parameters (i.e having large $E[\|\bar{f} - f_{Z(n)}\|^2]$. We will see later on how this principle is used for the construction of random forests...

Bias Variance Trade-off



Bias Variance illustrated

Boosting, Bagging

In ensemble methods, the average predictor $\frac{1}{T} \sum_{j=1}^{j=T} f_{Z^j(n)}$ in general is not built based on several distinct and independent training sets $Z^j(n)$ but on a single training set $Z(n)$ which is re-used several times according to the bootstrap method

Definition: bootstrap method

If $Z(n) = ((X_1, Y_1), (X_2, Y_2), \dots, (X_n, Y_n))$ is a learning set, the bootstrap method consists in building n new training sets $Z^i(n)$ by picking for each training set $Z^i(n)$ n samples (X_j, Y_j) from the original training set $Z(n)$ with replacements.

proposition

If we call $N(n)$ the number of distinct samples from the original training set $Z(n)$ that are picked at least once when building a new training set $Z^i(n)$ we have $E[\frac{N(n)}{n}] = 1 - (1 - \frac{1}{n})^n$ and so $E[\frac{N(n)}{n}] \underset{+\infty}{\sim} 1 - \frac{1}{e} = 0.6321\dots$

demonstration Let 1_i be the random variable which takes the value 1 if the sample (X_i, Y_i) is picked for the new training set $Z^j(n)$

$$P(1_i = 0) = \left(1 - \frac{1}{n}\right)^n.$$

The number of distinct samples picked to build (X_j, Y_j) is $N = \sum_{i=1}^{i=n} 1_i$

$$\text{so } E[N] = \sum_{i=1}^{i=n} E[1_i] = n\left[1 - \left(1 - \frac{1}{n}\right)^n\right] \text{ Q.E.D}$$

Remarks:

- Random Forests are built, by training trees on bootstrapped samples
- in case of a regression problem an average is made over all the random trees created. When averaging, the variance is reduced while the bias stays constant
- in case of a classification problem some majority decision rules or others will be taken depending on the classifications made by the various trees



Bernhard Schölkopf, Alex J.Smola, Robert C.Williamson, Peter L.Bartlett
New Support Vector Algorithms
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