

Data Science for Actuaries (ACT6100)

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Supervisé # 2 (régularisation - 3)

automne 2020

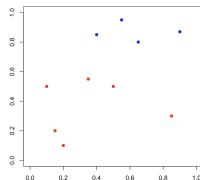
 <https://github.com/freakonometrics/ACT6100/>

SVM : Support Vector Machine

Linearly Separable sample [regression notations]

Data $(y_1, \mathbf{x}_1), \dots, (y_n, \mathbf{x}_n)$ - with $y \in \{0, 1\}$ - are linearly separable if there are $(\beta_0, \boldsymbol{\beta})$ such that

- $y_i = 1$ if $\beta_0 + \mathbf{x}_i^\top \boldsymbol{\beta} > 0$
- $y_i = 0$ if $\beta_0 + \mathbf{x}_i^\top \boldsymbol{\beta} < 0$

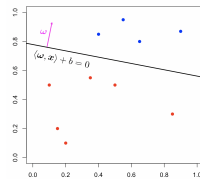


Linearly Separable sample [ML notations]

Data $(y_1, \mathbf{x}_1), \dots, (y_n, \mathbf{x}_n)$ - with $y \in \{-1, +1\}$ - are linearly separable if there are $(b, \boldsymbol{\omega})$ such that

- $y_i = +1$ if $b + \langle \mathbf{x}_i, \boldsymbol{\omega} \rangle > 0$
- $y_i = -1$ if $b + \langle \mathbf{x}_i, \boldsymbol{\omega} \rangle < 0$

or equivalently $y_i \cdot (b + \langle \mathbf{x}_i, \boldsymbol{\omega} \rangle) > 0, \forall i.$



SVM : Support Vector Machine

$$(b + \langle \mathbf{x}, \boldsymbol{\omega} \rangle) = b + \mathbf{x}^\top \boldsymbol{\omega} = 0$$

is an hyperplane (in \mathbb{R}^p) orthogonal with $\boldsymbol{\omega}$
Use $m(\mathbf{x}) = \mathbf{1}_{b + \langle \mathbf{x}, \boldsymbol{\omega} \rangle \geq 0} - \mathbf{1}_{b + \langle \mathbf{x}, \boldsymbol{\omega} \rangle < 0}$ as classifier

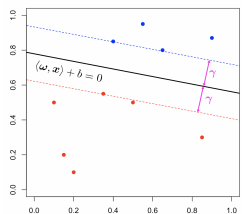
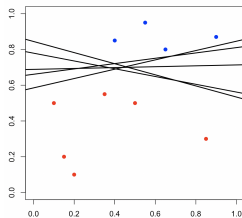
Problem : equation (i.e. $(b, \boldsymbol{\omega})$) is not unique !

Canonical form : $\min_{i=1, \dots, n} \{ |b + \langle \mathbf{x}_i, \boldsymbol{\omega} \rangle| \} = 1$

Problem : solution here is not unique !

Idea : use the widest (safety) margin γ

Vapnik & Lerner (1963) and or Cover (1965).



The distance from point \mathbf{x}_i to Δ is $d(\mathbf{x}_i, \Delta) = \frac{\boldsymbol{\omega}^\top \mathbf{x}_i + b}{\|\boldsymbol{\omega}\|}$. Consider

$$\max_{\boldsymbol{\omega}, b} \left\{ \min_{i=1, \dots, n} \{ d(\mathbf{x}_i, \Delta) \} \right\}$$

SVM : Support Vector Machine

Consider two points, \mathbf{x}_{-1} and \mathbf{x}_{+1}

$$\gamma = \frac{1}{2} \frac{\langle \omega, \mathbf{x}_{+1} - \mathbf{x}_{-1} \rangle}{\|\omega\|}$$

It is minimal when

$$b + \langle \omega_i, \mathbf{x}_{-1} \rangle = -1 \text{ and}$$

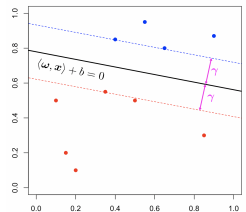
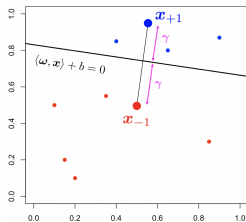
$$b + \langle \omega_i, \mathbf{x}_{+1} \rangle = +1, \text{ and therefore}$$

$$\gamma^* = \frac{1}{\|\omega\|}$$

Optimization problem $\max\{\gamma\}$ becomes

$$\min_{(b, \omega)} \left\{ \frac{1}{2} \|\omega\|_{\ell_2}^2 \right\} \text{ s.t. } y_i \cdot (b + \langle \mathbf{x}, \omega \rangle) > 0, \forall i.$$

convex optimization problem with linear constraints



SVM : Support Vector Machine

Here, $L(b, \omega, \alpha) = \frac{1}{2} \|\omega\|^2 - \sum_{i=1}^n \alpha_i \cdot (y_i \cdot (b + \langle \mathbf{x}_i, \omega \rangle) - 1)$

From the first order conditions,

$$\frac{\partial L(b, \omega, \alpha)}{\partial \omega} = \omega - \sum_{i=1}^n \alpha_i \cdot y_i \mathbf{x}_i = \mathbf{0}, \text{ i.e. } \omega^* = \sum_{i=1}^n \alpha_i^* y_i \mathbf{x}_i$$

$$\frac{\partial L(b, \omega, \alpha)}{\partial b} = - \sum_{i=1}^n \alpha_i \cdot y_i = 0, \text{ i.e. } \sum_{i=1}^n \alpha_i^* \cdot y_i = 0$$

and

$$\Lambda(\alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n \alpha_i \alpha_j y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle$$

$$\text{i.e. } \Lambda(\alpha) = \mathbf{1}^\top \alpha - \frac{1}{2} \alpha^\top \mathbf{Q} \alpha$$

SVM : Support Vector Machine

The dual problem is

$$\min_{\alpha} \left\{ \frac{1}{2} \alpha^{\top} \mathbf{Q} \alpha - \mathbf{1}^{\top} \alpha \right\} \text{ s.t. } \begin{cases} \alpha_i \geq 0, \forall i \\ \mathbf{y}^{\top} \alpha = 0 \end{cases}$$

where $\mathbf{Q} = [\mathbf{Q}_{i,j}]$ and $\mathbf{Q}_{i,j} = y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle$, and then

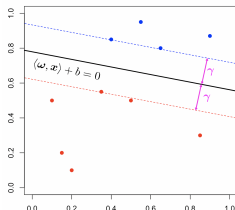
$$\omega^* = \sum_{i=1}^n \alpha_i^* y_i \mathbf{x}_i \text{ and } b^* = -\frac{1}{2} \left[\min_{i:y_i=+1} \{ \langle \mathbf{x}_i, \omega^* \rangle \} + \min_{i:y_i=-1} \{ \langle \mathbf{x}_i, \omega^* \rangle \} \right]$$

Points \mathbf{x}_i such that $\alpha_i^* > 0$ are called support

$$y_i \cdot (b^* + \langle \mathbf{x}_i, \omega^* \rangle) = 1$$

Classifier $m^*(\mathbf{x}) = \mathbf{1}_{b^* + \langle \mathbf{x}, \omega^* \rangle \geq 0} - \mathbf{1}_{b^* + \langle \mathbf{x}, \omega^* \rangle < 0}$

Observe that $\gamma^* = \left(\sum_{i=1}^n \alpha_i^{*2} \right)^{-1/2}$



SVM : Support Vector Machine

Consider here the more general case where the space is not linearly separable

$$(\langle \omega, \mathbf{x}_i \rangle + b)y_i \geq 1$$

becomes

$$(\langle \omega, \mathbf{x}_i \rangle + b)y_i \geq 1 - \xi_i$$

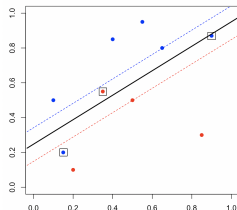
for some slack variables ξ_i 's.

and penalize large slack variables ξ_i (when > 0) by solving (for some cost C)

$$\min_{\omega, b} \left\{ \frac{1}{2} \omega^\top \omega + C \sum_{i=1}^n \xi_i \right\}$$

subject to $\forall i, \xi_i \geq 0$ and $(\mathbf{x}_i^\top \omega + b)y_i \geq 1 - \xi_i$.

This is the soft-margin extension, see



```
1 > e1071::svm()  
2 > kernlab::ksvm()
```

SVM : Support Vector Machine

The dual optimization problem is now

$$\min_{\alpha} \left\{ \frac{1}{2} \alpha^{\top} \mathbf{Q} \alpha - \mathbf{1}^{\top} \alpha \right\} \text{ s.t. } \begin{cases} 0 \leq \alpha_i \leq C, \forall i \\ \mathbf{y}^{\top} \mathbf{1} = 0 \end{cases}$$

where $\mathbf{Q} = [\mathbf{Q}_{i,j}]$ and $\mathbf{Q}_{i,j} = y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle$, and then

$$\omega^* = \sum_{i=1}^n \alpha_i^* y_i \mathbf{x}_i \text{ and } b^* = -\frac{1}{2} \left[\min_{i:y_i=+1} \{ \langle \mathbf{x}_i, \omega^* \rangle \} + \min_{i:y_i=-1} \{ \langle \mathbf{x}_i, \omega^* \rangle \} \right]$$

Note further that the (primal) optimization problem can be written

$$\min_{(b, \omega)} \left\{ \frac{1}{2} \|\omega\|_{\ell_2}^2 + \sum_{i=1}^n (1 - y_i \cdot (b + \langle \mathbf{x}_i, \omega \rangle))_+ \right\},$$

where $(1 - z)_+$ is a convex upper bound for empirical error $\mathbf{1}_{z \leq 0}$

SVM : Support Vector Machine, with R

The dual optimization problem is now

$$\min_{\alpha} \left\{ \frac{1}{2} \alpha^{\top} \mathbf{Q} \alpha - \mathbf{1}^{\top} \alpha \right\} \text{ s.t. } \begin{cases} 0 \leq \alpha_i \leq C, \forall i \\ \mathbf{y}^{\top} \alpha = 0 \end{cases}$$

where $\mathbf{Q} = [\mathbf{Q}_{i,j}]$ and $\mathbf{Q}_{i,j} = y_i y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle$

```
1 > library(quadprog)
2 > C = .5
3 > y = (myocarde[, "PRONO"] == "SURVIE") * 2 - 1
4 > X = as.matrix(cbind(1, myocarde[, 1:7]))
5 > n = length(y)
6 > Q = sapply(1:n, function(i) y[i] * t(X)[, i])
7 > D = t(Q) %*% Q
8 > d = matrix(1, nrow=n)
9 > A = rbind(y, diag(n), -diag(n))
10 > b = c(0, rep(0, n), rep(-C, n))
```

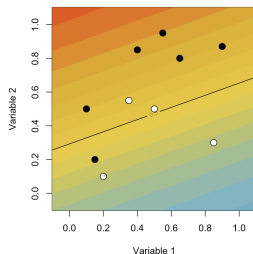
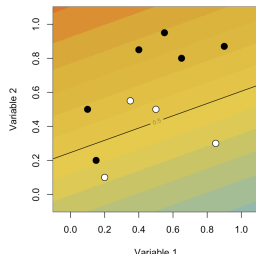
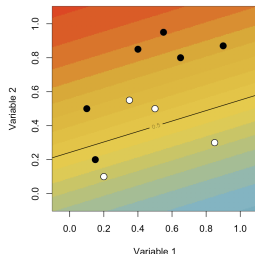
SVM : Support Vector Machine, with R

```
1 > eps = 5e-4
2 > sol = solve.QP(D+eps*diag(n), d, t(A),b, meq=1,
  factorized=FALSE)
3 > qpsol = sol$solution
4 > omega = apply(qpsol*y*X,2,sum)
5 > omega
6      1   FRCAR   INCAR   INSYS   PRDIA   PAPUL   PVENT   REPUL
7 0.000  0.055 -0.092  0.361 -0.109 -0.049 -0.066  0.001
```

$$\text{car } \omega^* = \sum_{i=1}^n \alpha_i^* y_i \mathbf{x}_i$$

SVM : Support Vector Machine, with R

```
1 x1 = c(.4,.55,.65,.9,.1,.35,.5,.15,.2,.85)
2 x2 = c(.85,.95,.8,.87,.5,.55,.5,.2,.1,.3)
3 y = c(1,1,1,1,1,0,0,1,0,0)
4 df = data.frame(x1=x1,x2=x2,y=2*y-1)
5 library(kernlab)
6 SVM2 = ksvm(y ~ x1 + x2, data = df, C=2.5, kernel = "
  vanilladot" , prob.model=TRUE, type="C-svc")
```



SVM : Support Vector Machine

One can also consider the **kernel trick** : $\mathbf{x}_i^\top \mathbf{x}_j$ is replaced by $\varphi(\mathbf{x}_i)^\top \varphi(\mathbf{x}_j)$ for some mapping φ ,

$$K(\mathbf{x}_i, \mathbf{x}_j) = \varphi(\mathbf{x}_i)^\top \varphi(\mathbf{x}_j)$$

For instance $K(\mathbf{a}, \mathbf{b}) = (\mathbf{a}^\top \mathbf{b})^3 = \varphi(\mathbf{a})^\top \varphi(\mathbf{b})$
where $\varphi(a_1, a_2) = (a_1^3, \sqrt{3}a_1^2a_2, \sqrt{3}a_1a_2^2, a_2^3)$
Consider polynomial kernels

$$K(\mathbf{a}, \mathbf{b}) = (1 + \mathbf{a}^\top \mathbf{b})^p$$

or a Gaussian kernel

$$K(\mathbf{a}, \mathbf{b}) = \exp(-(\mathbf{a} - \mathbf{b})^\top (\mathbf{a} - \mathbf{b}))$$

and solve $\max_{\alpha_i \geq 0} \left\{ \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n y_i y_j \alpha_i \alpha_j K(\mathbf{x}_i, \mathbf{x}_j) \right\}$

SVM : Support Vector Machine

The radial kernel is formed by taking an infinite sum over polynomial kernels...

$$K(\mathbf{x}, \mathbf{y}) = \exp(-\gamma \|\mathbf{x} - \mathbf{y}\|^2) = \langle \psi(\mathbf{x}), \psi(\mathbf{y}) \rangle$$

where ψ is some $\mathbb{R}^n \rightarrow \mathbb{R}^\infty$ function, since

$$K(\mathbf{x}, \mathbf{y}) = \exp(-\gamma \|\mathbf{x} - \mathbf{y}\|^2) = \underbrace{\exp(-\gamma \|\mathbf{x}\|^2 - \gamma \|\mathbf{y}\|^2)}_{=\text{constant}} \cdot \exp(2\gamma \langle \mathbf{x}, \mathbf{y} \rangle)$$

i.e.

$$K(\mathbf{x}, \mathbf{y}) \propto \exp(2\gamma \langle \mathbf{x}, \mathbf{y} \rangle) = \sum_{k=0}^{\infty} 2\gamma \frac{\langle \mathbf{x}, \mathbf{y} \rangle^k}{k!} = \sum_{k=0}^{\infty} 2\gamma K_k(\mathbf{x}, \mathbf{y})$$

where K_k is the polynomial kernel of degree k .

If $K = K_1 + K_2$ with $\psi_j : \mathbb{R}^n \rightarrow \mathbb{R}^{d_j}$ then $\psi : \mathbb{R}^n \rightarrow \mathbb{R}^d$ with
 $d \sim d_1 + d_2$

SVM : Support Vector Machine

A kernel is a measure of similarity between vectors.

The smaller the value of γ the narrower the vectors should be to have a small measure

Is there a probabilistic interpretation ?

Platt (2000, [Probabilities for SVM](#)) suggested to use a logistic function over the SVM scores,

$$p(\mathbf{x}) = \frac{\exp[b + \langle \mathbf{x}, \boldsymbol{\omega} \rangle]}{1 + \exp[b + \langle \mathbf{x}, \boldsymbol{\omega} \rangle]}$$

SVM : Support Vector Machine, with R

```
1 x1 = c(.4,.55,.65,.9,.1,.35,.5,.15,.2,.85)
2 x2 = c(.85,.95,.8,.87,.5,.55,.5,.2,.1,.3)
3 y = c(1,1,1,1,1,0,0,1,0,0)
4 df = data.frame(x1=x1,x2=x2,y=2*y-1)
5 library(kernlab)
6 SVM2 = ksvm(y ~ x1 + x2, data = df, C=1, kernel = "
  rbfdot" , prob.model=TRUE, type="C-svc")
```

