Advanced Computational Econometrics: Machine Learning

Chapter 6: Kernel-based classification and regression

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Support Vector classification and regression

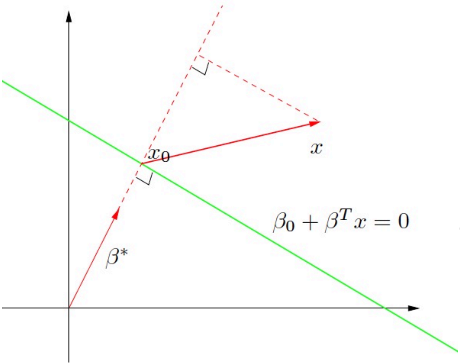
- In this chapter we describe new methods for linear and nonlinear classification and regression.
- Optimal separating hyperplanes are first introduced for the case when two classes are linearly separable. Then we cover extensions to the nonseparable case, where the classes overlap.
- These techniques are then generalized to the support vector machine (SVM), which produces nonlinear boundaries by constructing a linear boundary in a large, transformed version of the predictor space.
- Finally, we will transpose these ideas to regression, and introduce support vector regression (SVR).

Overview

Overview

Hyperplane

In $\mathbb{R}^p$, a hyperplane H is defined by the equation $g(x) = 0$ with $g(x) = \beta_0 + \beta^T x$. We have $g(x) > 0$ on one side of H and $g(x) < 0$ on the other side.

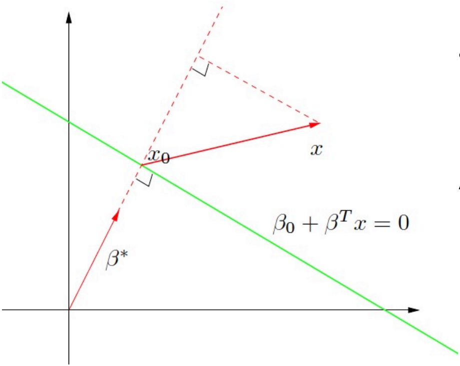


For any two points x_1 and x_2 lying in H, we have

$$\beta_0 + \beta^T x_1 = 0$$
$$\beta_0 + \beta^T x_2 = 0.$$

Consequently, $\beta^T(x_1 - x_2) = 0$, hence $\beta^* = \beta/\|\beta\|$ is the vector normal to the surface of H.

Hyperplane (continued)



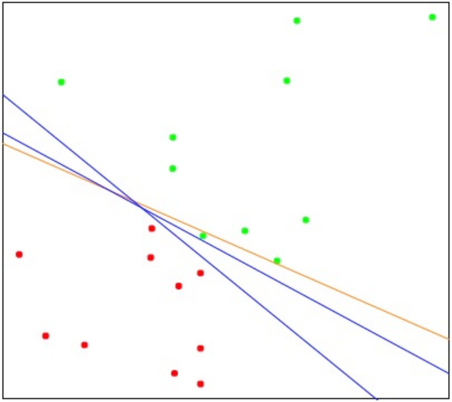
Let $x_0 \in H$. The signed distance of any point x to H is

$$d_s(x, H) = {\beta^*}^T (x - x_0)$$

As $\beta_0 = -\beta^T x_0$, we have

$$\begin{aligned} d_s(x, H) &= \frac{\beta^T x - \beta^T x_0}{\|\beta\|} \\ &= \frac{\beta^T x + \beta_0}{\|\beta\|} \\ &= \frac{g(x)}{\|\beta\|} \end{aligned}$$

Linearly separable data



- Consider a two-class data set $\{(x_i, y_i)\}_{i=1}^n$ with $y_i \in \{-1, 1\}$.
- It is said to be linearly separable if there exists a hyperplane $H : g(x) = 0$ that separates the two classes, i.e., such that

$$g(x_i)y_i > 0, \quad \forall i.$$

Optimal separating hyperplane

Let $H : g(x) = 0$ be a separating hyperplane. The distance between H and a learning vector x_i is

$$d(x_i, H) = \frac{g(x_i)y_i}{\|\beta\|}$$

Definition (Margin)

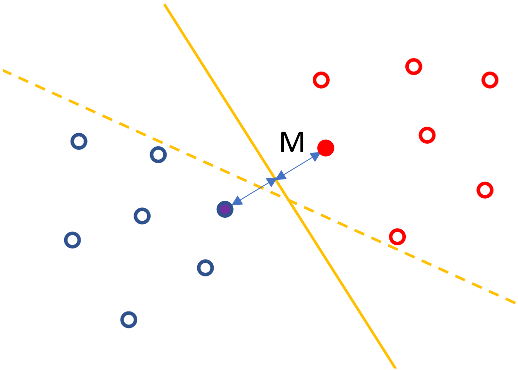
The margin *of H is the smallest distance between H and a learning vector x_i:*

$$M = \min_i d(x_i, H).$$

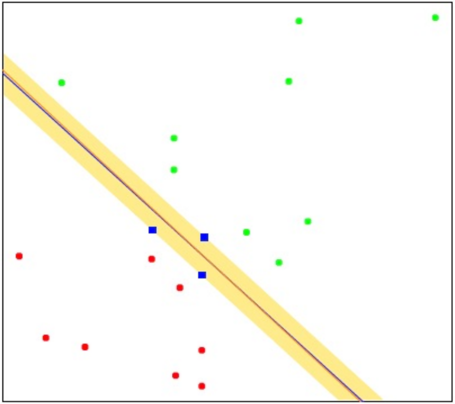
Definition (Optimal separating hyperplane, support vectors)

The optimal separating hyperplane *(OSH) is the hyperplane with the largest margin. The learning vectors x_i such that $d(x_i, H) = M$ are called the* support vectors *(SVs) of H.*

Example 1

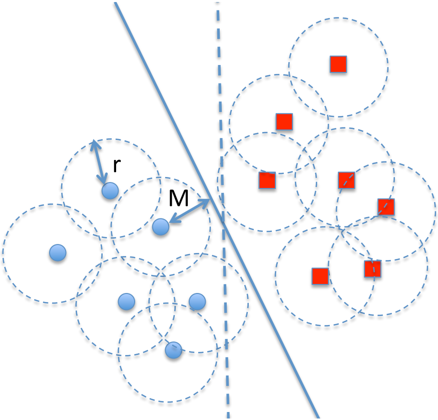


Example 2



The shaded region delineates the maximum margin separating the two classes. There are 3 SVs, and the OSH is the blue line. The boundary found using logistic regression is the red line. In this case, it is very close to the OSH.

The OSH is more likely to separate future data



- Future data can be assumed to be "close" to past data.
- Assume they will lie with a distance r of a past data point.
- If $M > r$, the hyperplane will classify future data perfectly.

Overview

How to find the OSH?

- The OSH can be found by solving the following optimization problem:

$$\max_{\beta,\beta_0} M$$

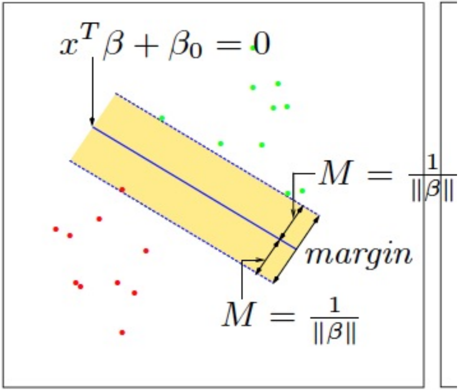
$$\text{subject to} \quad \frac{y_i(\beta^T x_i + \beta_0)}{\|\beta\|} \geq M, \quad i = 1, \ldots, n.$$

- If (β, β_0) is a solution, so is $(\lambda\beta, \lambda\beta_0)$ for any λ. Hence, we can fix $\|\beta\| = 1/M$ and reformulate the problem as

$$\min_{\beta,\beta_0} \frac{1}{2}\|\beta\|^2$$

$$\text{subject to} \quad y_i(\beta^T x_i + \beta_0) \geq 1, \quad i = 1, \ldots, n.$$

Interpretation



- The constraints define an empty band or margin around the linear decision boundary of thickness $1/\|\beta\|$.
- The vectors x_i such that

$$\frac{y_i(\beta^T x_i + \beta_0)}{\|\beta\|} = \frac{1}{\|\beta\|},$$

i.e., $y_i(\beta^T x_i + \beta_0) = 1$, are the SVs.

Reminder on constrained optimization

Lagrange function

Consider the following minimization problem:

$$\min_{\beta} f(\beta) \tag{1}$$

subject to the constraints $c_i(\beta) \geq 0$, $i = 1, \ldots, n$, where f and the c_i's are differentiable functions.

Definition (Lagrange function)

The Lagrange function is defined by

$$L(\beta, \alpha) = f(\beta) - \sum_{i=1}^{n} \alpha_i c_i(\beta),$$

where $\alpha = (\alpha_1, \ldots, \alpha_n)$ is the vector of Lagrange multipliers.

Reminder on constrained optimization

Karush-Kuhn-Tucker conditions

Theorem (Karush-Kuhn-Tucker)

If function f has a minimum for some value β^* in the feasibility region, the following Karush-Kuhn-Tucker (KKT) conditions are verified for some vector $\alpha^* = (\alpha_1^*, \ldots, \alpha_n^*)$:

$$
\begin{aligned}
\frac{\partial L}{\partial \beta}(\beta^*, \alpha^*) &= 0 && \text{(2a)}\\
c_i(\beta^*) &\geq 0, \quad i = 1, \ldots, n && \text{(2b)}\\
\alpha_i^* c_i(\beta^*) &= 0 \quad i = 1, \ldots, n && \text{(2c)}\\
\alpha_i^* &\geq 0 \quad i = 1, \ldots, n. && \text{(2d)}
\end{aligned}
$$

Remark: if $\alpha_i^* > 0$, then $c_i(\beta^*) = 0$: constraint i is active.

Reminder on constrained optimization

Wolfe dual

Theorem (Wolfe dual)

Problem (1) is equivalent to the following problem (Wolfe dual):

$$\max_{\beta,\alpha} L(\beta, \alpha) \tag{3}$$

subject to

$$\frac{\partial L}{\partial \beta} = 0 \tag{4}$$

$$\alpha_i \geq 0 \quad i = 1, \ldots, n. \tag{5}$$

Lagrange function

- Let us come back to the problem $\min_{\beta,\beta_0} \frac{1}{2}\|\beta\|^2$ subject to $y_i(\beta^T x_i + \beta_0) \geq 1$, $i = 1, \ldots, n$.
- This is a convex optimization problem (quadratic criterion with linear inequality constraints), so the solution exists and it is unique.
- The Lagrange function is

$$\boxed{L(\beta, \beta_0, \alpha) = \frac{1}{2}\|\beta\|^2 - \sum_{i=1}^{n} \alpha_i[y_i(\beta^T x_i + \beta_0) - 1]} \tag{6}$$

- Setting the derivatives to zero, we obtain:

$$\frac{\partial L}{\partial \beta} = \beta - \sum_{i=1}^{n} \alpha_i y_i x_i = 0 \Rightarrow \boxed{\beta = \sum_{i=1}^{n} \alpha_i y_i x_i} \tag{7}$$

$$\text{and} \quad \frac{\partial L}{\partial \beta_0} = \boxed{-\sum_{i=1}^{n} \alpha_i y_i = 0} \tag{8}$$

Lagrangian of the dual problem

Substituting (7) and (8) in (6), we get

$$L_D(\alpha) = \underbrace{\frac{1}{2}\left(\sum_{i=1}^n \alpha_i y_i x_i\right)^T \left(\sum_{j=1}^n \alpha_j y_j x_j\right)}_{\sum_{i,j} \alpha_i \alpha_j y_i y_j x_i^T x_j} -$$

$$\underbrace{\sum_i \alpha_i y_i \left(\sum_{j=1}^n \alpha_j y_j x_j\right)^T x_i}_{\sum_{i,j} \alpha_i \alpha_j y_i y_j x_i^T x_j} - \underbrace{\sum_i \alpha_i y_i \beta_0}_{0} + \sum_i \alpha_i$$

which can be written as

$$\boxed{L_D(\alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j x_i^T x_j}$$

Solving the dual problem

- The solution is obtained by maximizing $L_D(\alpha)$ subject to the constraints
$$\alpha_i \geq 0 \text{ and } \sum_{i=1}^{n} \alpha_i y_i = 0. \tag{9}$$
- This can be done using standard quadratic programming software. We will discuss a specialized optimization algorithm later.

Interpreting the solution

Support vectors

- The solution α^* must satisfy the KKT conditions, which include (7), (8), (9) and

$$\alpha_i^*[y_i({\beta^*}^T x_i + \beta_0^*) - 1] = 0, \quad i = 1, \ldots, n. \tag{10}$$

- From these we can see that, if $\alpha_i^* > 0$, then $y_i({\beta^*}^T x_i + \beta_0^*) = 1$, i.e., x_i is a SV.
- The SV's are the input vectors x_i such that $\alpha_i^* > 0$.

Interpreting the solution

Computing β^* and β_0^*

- From (7) we see that the solution vector β^* is defined in terms of a linear combination of the SVs:

$$\beta^* = \sum_{i=1}^{n} \alpha_i^* y_i x_i = \sum_{i \in \mathcal{S}} \alpha_i^* y_i x_i \tag{11}$$

  with $\mathcal{S} = \{i : \alpha_i^* > 0\}$.

- The intercept β_0^* can be found from (10): for any SV x_i, we have

$$y_i({\beta^*}^T x_i + \beta_0^*) = 1,$$

  from which we can get β_0^*.

SVM classifier

- The equation of the OSH is

$$g^*(x) = {\beta^*}^T x + \beta_0^* = \sum_{i \in S} \alpha_i^* y_i x_i^T x + \beta_0^* = 0$$

- The corresponding classifier is

$$D(x) = \text{sign } g^*(x).$$

- The classifier is based only on SVs, which are close to the boundary between classes.

Overview

Extension to non-separable data

- Until now, we have assumed that the data are linearly separable.
- This will generally not be the case with real data, so the technique derived so far is not really useful in practice.
- We need to propose an alternative formulation for the non-separable case.

Weakening the constraints

- Suppose that the classes overlap in predictor space.
- One way to deal with the overlap is to still maximize the margin M, but allow for some points to be on the wrong side of the margin.
- Define the slack variables $\xi = (\xi_1, \xi_2, \ldots, \xi_n)$ with $\xi_i \geq 0$. The constraints can be modified as

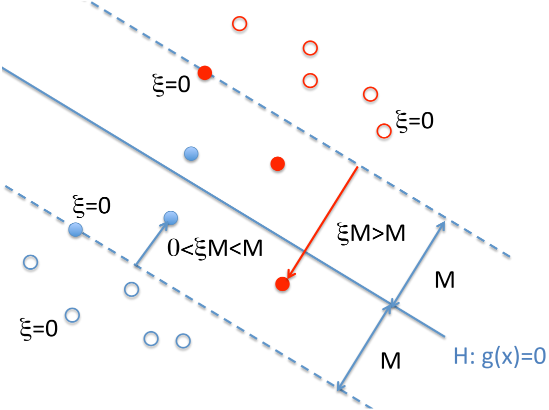
$$\frac{y_i(\beta^T x_i + \beta_0)}{\|\beta\|} \geq M(1 - \xi_i), \quad i = 1, \ldots, n.$$

- As before, fixing $\|\beta\| = 1/M$, this is equivalent to

$$y_i(\beta^T x_i + \beta_0) \geq 1 - \xi_i, \quad i = 1, \ldots, n.$$

- The value ξ_i is the proportional amount by which vector x_i is on the wrong side of its margin.

Interpretation



- The filled points are on the wrong side of their margin by an amount $M\xi_i$.
- Points on the correct side have $\xi_i = 0$.
- Misclassified points have $\xi_i > 1$.

Optimization problem

The optimization problem now becomes:

$$\boxed{\min_{\beta,\beta_0,\{\xi_i\}} \frac{1}{2}\|\beta\|^2 + \frac{C}{n}\sum_{i=1}^{n} \xi_i,} \tag{12}$$

subject to

$$\xi_i \geq 0, \quad i = 1, \ldots, n$$

$$y_i(\beta^T x_i + \beta_0) \geq 1 - \xi_i, \quad i = 1, \ldots, n$$

where C is a hyperparameter.

Lagrange function

- The Lagrange function is

$$L(\beta, \beta_0, \xi, \alpha, \mu) = \frac{1}{2}\|\beta\|^2 + \frac{C}{n}\sum_{i=1}^n \xi_i - \sum_{i=1}^n \alpha_i [y_i(\beta^T x_i + \beta_0) - (1 - \xi_i)] - \sum_{i=1}^n \mu_i \xi_i.$$

- Setting the derivatives w.r.t. β, β_0 and ξ to zero, we get, as before,

$$\beta = \sum_{i=1}^n \alpha_i y_i x_i, \quad \sum_{i=1}^n \alpha_i y_i = 0, \tag{13}$$

and

$$\frac{C}{n} - \alpha_i - \mu_i = 0 \Rightarrow \alpha_i = \frac{C}{n} - \mu_i \tag{14}$$

Dual formulation

- By substituting (13), we obtain the Lagrangian dual objective function

$$L_D(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j x_i^T x_j + \sum_{i=1}^{n} \underbrace{\left(\frac{C}{n} - \alpha_i - \mu_i \right)}_{0} \xi_i, \quad (15)$$

which has exactly the same form as in the previous problem.
- We maximize L_D subject to $0 \leq \alpha_i \leq \frac{C}{n}$ and $\sum_{i=1}^{n} \alpha_i y_i = 0$.
- The sequential minimal optimization (SMO) algorithm gives an efficient way of solving this problem.

SMO algorithm

- The SMO algorithm is a grouped coordinate ascent procedure.
- Maximizing $L_D(\alpha)$ one α_i at a time does not work, because due to the constraint

$$\sum_{i=1}^{n} \alpha_i y_i = 0,$$

variable α_i is uniquely determined from the other α_j's through the equation

$$\alpha_i = -y_i \sum_{j \neq i} \alpha_j y_j.$$

- Instead, the SMO algorithm maximizes $L_D(\alpha)$ w.r.t. to each pair of variables (α_i, α_j) sequentially.

SMO algorithm (continued)

`Repeat until convergence {`

1. `Select some pair` α_i `and` α_j `to update next (using a heuristic that tries to pick the two that will allow us to make the biggest progress towards the global maximum).`
2. `Reoptimize` $L_D(\alpha)$ `with respect to` α_i `and` α_j`, while holding all the other` α_k`'s (`$k \neq i, j$`) fixed.`

`}`

To test for convergence of this algorithm, we can check whether the KKT conditions are satisfied to within some tolerance (see next slide).

Interpretation of the solution

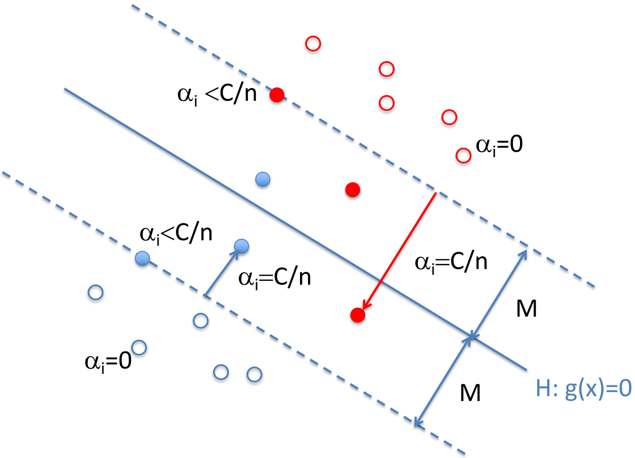
- The solution verifies the KKT conditions (13)-(14) and

$$\alpha_i^*[y_i(\beta^{*T} x_i + \beta_0^*) - (1 - \xi_i^*)] = 0, \quad i = 1, \ldots, n \tag{16}$$

$$\mu_i^* \xi_i^* = 0, \quad i = 1, \ldots, n \tag{17}$$

- As before, the SVs are defined as the points such that $\alpha_i^* > 0$.
- From (14) and (17), the SVs such that $\alpha_i^* < C/n$ verify $\mu_i^* > 0$ and $\xi_i^* = 0$: they lie on the edge of the margin ("in-bound SVs"). The remainder ($\xi_i^* > 0$) have $\alpha_i^* = C/n$ and usually lie inside the margin ("margin errors").
- The SVs such that $\xi_i^* > 1$ are misclassified.
- From (16) we can see that any of the in-bound SVs ($\alpha_i^* > 0$, $\xi_i^* = 0$) can be used to solve for β_0^*, and we typically use an average of all the solutions for numerical stability.

Interpretation



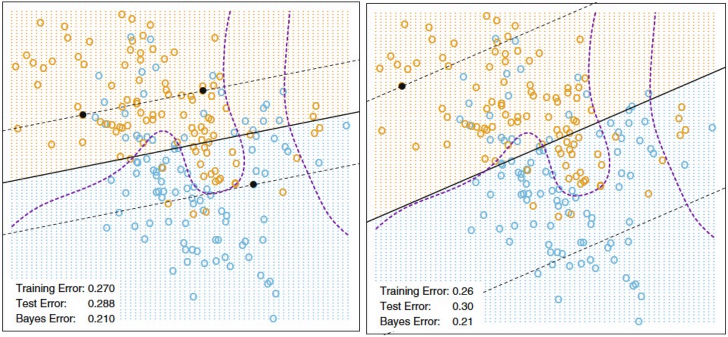
Tuning C

- The tuning parameter of this procedure is the cost parameter C.
- The optimal value for C can be estimated by cross-validation.
- From (12), the margin is smaller for larger C. Hence larger values of C focus attention more on points near the decision boundary, while smaller values involve data further away.

Bound on the LOO error

- The LOO cross-validation error can be bounded above by the proportion of SVs in the data.
- The reason is that leaving out an observation that is not a SV will not change the solution. Hence these observations, being classified correctly by the original boundary, will be classified correctly in the cross-validation process.
- However this bound tends to be too high, and not generally useful for choosing C.

Example



$C = 10000$ $\qquad$ $C = 0.01$

The SVs ($\alpha_i^* > 0$) are all the points on the wrong side of their margin. The black solid dots are in-bound SVs ($\alpha_i^* < C/n$). In the left (resp., right) panel 62% (resp., 85%) of the observations are SVs.

Application in R

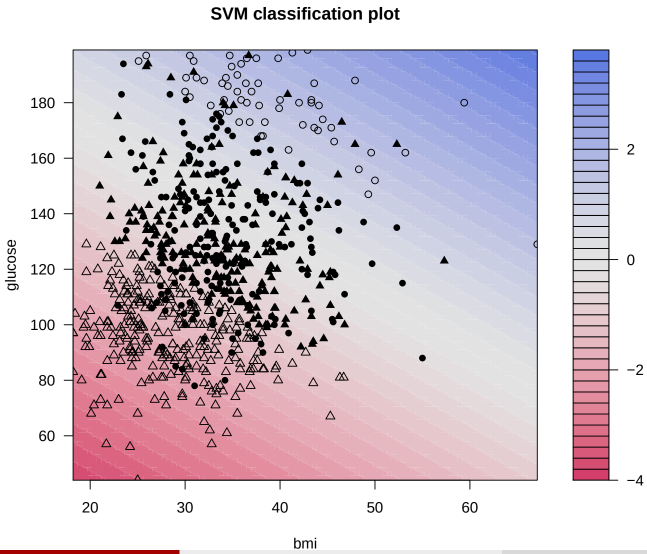
```
library("kernlab")

ii<-which((pima$glucose>0) & (pima$bmi>0))

svmfit<-ksvm(as.factor(class)~ glucose+bmi,data=pima[ii,],
            type="C-svc",kernel="vanilladot",C=10)

plot(svmfit,data=pima[ii,],grid=100)
```

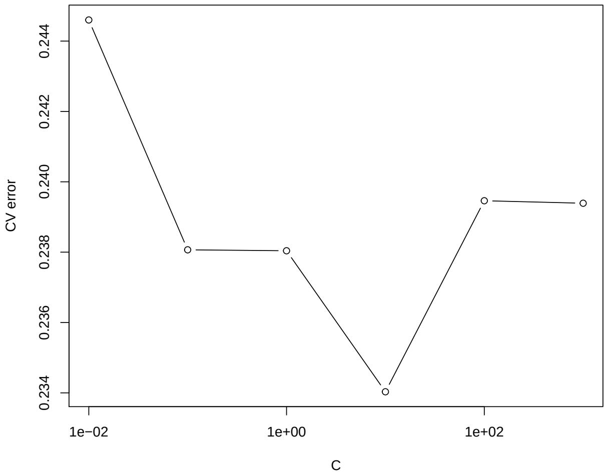
Result


SVM classification plot
glucose
bmi
180
160
140
120
100
80
60
20
30
40
50
60
2
0
−2
−4

Selection of C by cross-validation

```
CC<-c(0.01,0.1,1,10,100,1000)
N<-length(CC)
err<-rep(0,N)
for(i in 1:N){
err[i]<-cross(ksvm(as.factor(class)~glucose+bmi,data=pima[ii,],
            type="C-svc",kernel="vanilladot",C=CC[i],cross=5))
}
plot(CC,err,type="b",log="x",xlab="C",ylab="CV error")
```

Cross-validation result



Overview

Overview

Extension to non-linear classification

- The support vector classifier described so far finds linear boundaries in the predictor space.
- As with other linear methods, we could make the procedure more flexible by enlarging the predictor space using basis expansions such as, e.g., polynomials or splines.
- Linear boundaries in the enlarged space generally achieve better training-class separation, and translate to nonlinear boundaries in the original space.

Extension to non-linear classification (continued)

- Once the basis functions $\Phi_j(x)$, $j = 1, \ldots, J$ are selected, the procedure is the same as before:
  - We fit the SV classifier using predictors

    $$\Phi(x_i) = (\Phi_1(x_i), \Phi_2(x_i), \ldots, \Phi_J(x_i)), \quad i = 1, \ldots, n,$$

    and produce the (nonlinear) function $g^*(x) = \Phi(x)^T\beta^* + \beta_0$.
  - The classifier is $D^*(x) = \text{sign}(g^*(x))$ as before.
- In SVM, the mapping $x \rightarrow \Phi(x)$ will be defined implicitly, and J will be potentially very large (even infinite!).

The OSH depends only on dot-products

A key feature of the OSH is that it depends only on the dot products between input vectors:

- The solution is found by maximizing

$$L_D(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j x_i^T x_j, \tag{18}$$

  subject to $0 \leq \alpha_i \leq C/n$ and $\sum_{i=1}^{n} \alpha_i y_i = 0$.

- The optimal discriminant function is

$$g^*(x) = \sum_{i \in \mathcal{S}} \alpha_i^* y_i x_i^T x + \beta_0^* = 0,$$

  where β_0^* also depends only on the dot products $x_i^T x_j$.

Dot-products in the transformed input space

- Assume that the input vector x is replaced by $\Phi(x)$ for some transformation $\Phi : \mathbb{R}^p \to \mathcal{H}$.
- The objective function will become

$$L_D(\alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j \langle \Phi(x_i), \Phi(x_j) \rangle \tag{19}$$

  and the optimal discriminant function will be

$$g^*(x) = \sum_{i \in \mathcal{S}} \alpha_i^* y_i \langle \Phi(x_i), \Phi(x) \rangle + \beta_0^* = 0,$$

  where $\langle \cdot, \cdot \rangle$ denotes the dot-product in $\mathcal{H}$.
- All we need is a method to compute dot-products in $\mathcal{H}$.

The "kernel trick"

- If there exists a kernel function $\mathcal{K} : \mathbb{R}^p \times \mathbb{R}^p \rightarrow \mathbb{R}_+$ such that

$$\mathcal{K}(x, x') = \langle \Phi(x), \Phi(x') \rangle,$$

  then the transformation Φ will be defined implicitly.
- This is the "kernel trick".

Example

- Assume $p = 2$ and $\mathcal{K}(x, x') = (x^T x')^2$.
- We have

$$\begin{aligned}
\mathcal{K}(x, x') &= (x_1 x_1' + x_2 x_2')^2 \\
&= x_1^2 (x_1')^2 + 2 x_1 x_2 x_1' x_2' + x_2^2 (x_2')^2 \\
&= \Phi(x)^T \Phi(x')
\end{aligned}$$

with

$$\Phi : x \longrightarrow \begin{pmatrix} x_1^2 \\ \sqrt{2} x_1 x_2 \\ x_2^2 \end{pmatrix}$$

- Function Φ is defined implicitly by the kernel function $\mathcal{K}$.

Overview

Mercer condition

Theorem

A kernel function $\mathcal{K}$ corresponds to a dot-product in some space $\mathcal{H}$ iff it verifies the following Mercer condition:

$$\forall f : \mathbb{R}^p \to \mathbb{R} \ s.t. \int f(x)^2 dx < \infty, \quad \int \mathcal{K}(x, x')f(x)f(x')dxdx' \geq 0.$$

- If the Mercer condition is not verified, the Wolf dual problem may not have a solution.
- In practice, the method may still work most of the time with a kernel function that does not meet this condition.

Popular kernel functions

- Three popular choices for $\mathcal{K}$ in the SVM literature are

$$
\begin{array}{rll}
\mathcal{K}(x,x') = & (a + b\cdot x^T x')^d, \quad d>0 & \text{(polynomial kernel)}\\
\mathcal{K}(x,x') = & \exp\left[-\sigma\|x-x'\|^2\right], \quad \sigma>0 & \text{(RBF or Gaussian kernel)}\\
\mathcal{K}(x,x') = & \tanh(a + b\cdot x^T x') & \text{(MLP kernel).}
\end{array}
$$

- The polynomial and Gaussian verify the Mercer condition, but the MLP kernel does not.
- With the MLP kernel, the discriminant function is

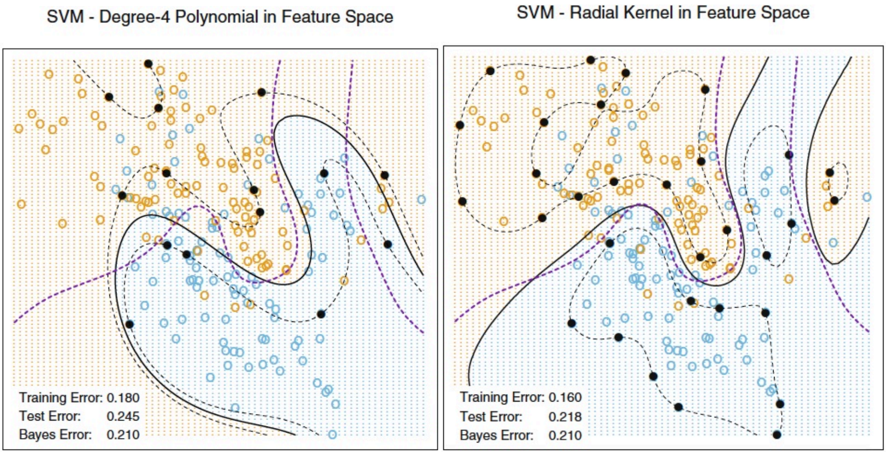
$$g(x) = \sum_{i\in\mathcal{S}} \alpha_i^* y_i \tanh(a + b\cdot x_i^T x) + \beta_0^*.$$

  It is the transfer function of a neural network with $n_S = \text{card}(\mathcal{S})$ hidden units (see chapter on neural networks).

Influence of C

- The role of parameter C is clearer in an enlarged predictor space, since perfect separation is often achievable there. (The dimension of $\mathcal{H}$ may be very large and even infinite.)
- A small value of C will encourage a small value of $\|\beta\|$, which in turn causes $g(x)$ and hence the boundary to be smoother.
- Both C and the kernel parameters (a, b, d, σ, etc.) are usually tuned by cross-validation.

Example

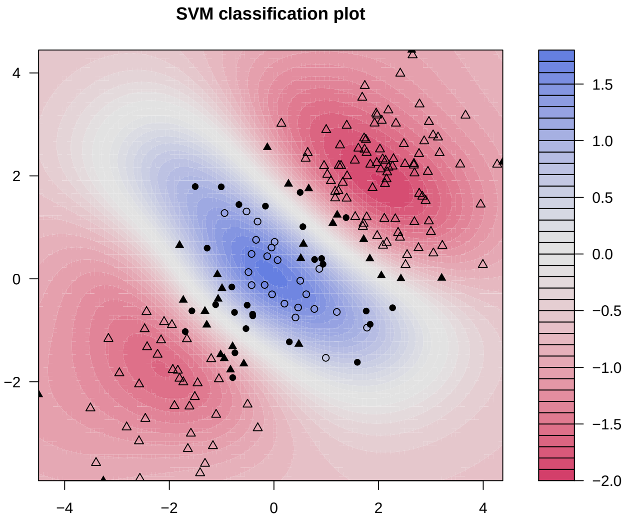

SVM - Degree-4 Polynomial in Feature Space
Training Error: 0.180
Test Error: 0.245
Bayes Error: 0.210
SVM - Radial Kernel in Feature Space
Training Error: 0.160
Test Error: 0.218
Bayes Error: 0.210

Application in R

```
x<-matrix(rnorm(200*2),ncol=2)
y<-as.factor(c(rep(-1,150),rep(1,50)))
x[1:100,]<- x[1:100,]+2
x[101:150,]<- x[101:150,]-2

svmfit<-ksvm(x,y,type="C-svc",kernel="rbfdot",
           kpar=list(sigma=1),C=1)
plot(svmfit,data=x,grid=100)
```

Result



Estimation of posterior probabilities

- The SVM classifier gives us a decision function, but it does not provide estimates of conditional class probabilities $P(x) = \mathbb{P}(Y = +1 \mid X = x)$.
- One approach to estimate these probabilities is to use logistic regression, with the output $g(x)$ of the SVM classifier as the predictor. We then have
$$\widehat{P}(x) = \frac{1}{1 + \exp[-(a + b \cdot g(x))]}$$
- To avoid overfitting, it is preferable to estimate the additional parameters a and b from a validation dataset or using cross-validation.

Overview

Unconstrained formulation

- Let $g(x_i) = \langle \beta, \Phi(x_i) \rangle + \beta_0$. The problem

$$\min_{\beta,\beta_0,\{\xi_i\}} \frac{1}{2}\|\beta\|^2 + \frac{C}{n}\sum_{i=1}^n \xi_i,$$

subject to $\xi_i \geq 0$ and $y_i g(x_i) \geq 1 - \xi_i$, $i = 1, \ldots, n$ is equivalent to the unconstrained optimization problem:

$$\boxed{\min_{\beta,\beta_0} \sum_{i=1}^n \underbrace{[1 - y_i g(x_i)]_+}_{\text{``hinge'' loss}} + \underbrace{\frac{\lambda}{2}\|\beta\|^2}_{\text{penalty}},}$$

where $[\cdot]_+$ denotes the positive part, with $\lambda = n/C$.

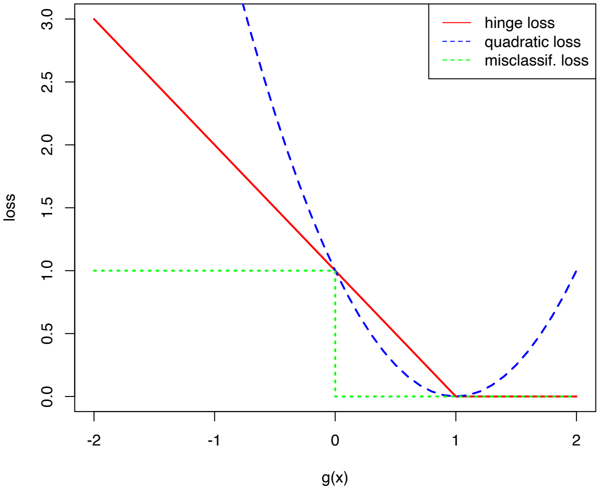
- Proof: see next slide.

Hinge loss

- Proof: from $\xi_i \geq 0$ and $\xi_i \geq 1 - y_i g(x_i)$, we get equivalently $\xi_i \geq \max(0, 1 - y_i g(x_i)) = [1 - y_i g(x_i)]_+$. Since we minimize ξ_i, we set $\xi_i = [1 - y_i g(x_i)]_+$.
- The hinge loss can be compared to other loss functions such as:
  - Misclassification: $I(\text{sign}(g(x)) \neq y)$
  - Squared error loss: $(y - g(x))^2$

(see next slide)

Hinge loss (case $y = +1$)



Overview

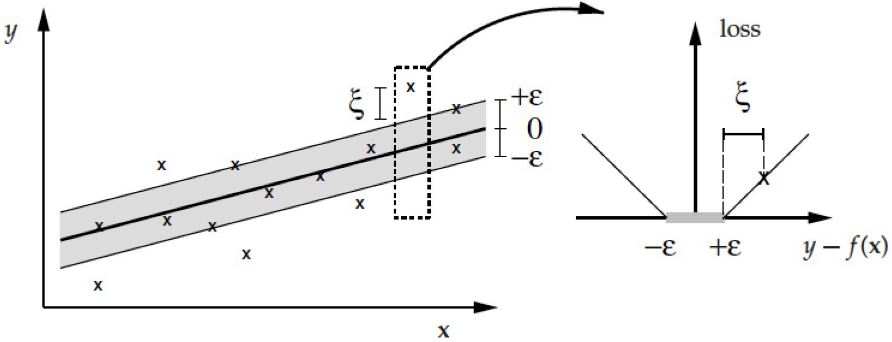
Overview

From classification to regression

- SVMs were first developed for classification.
- As described in the previous chapter, they represent the decision boundary in terms of a typically small subset of all training examples – the Support Vectors.
- To generalize the SV algorithm to regression, we need to find a way of retaining this feature. This can be achieved using the ϵ-insensitive loss function

$$
\begin{aligned}
|f(x)-y|_\epsilon &= \begin{cases} 0 & \text{if } |f(x)-y| \leq \epsilon, \\ |f(x)-y|-\epsilon & \text{otherwise.} \end{cases} \\
&= [|f(x)-y|-\epsilon]_+
\end{aligned}
$$

ϵ-insensitive loss function



The ϵ-insensitive loss function does not penalize errors below some ϵ, chosen a priori. The ϵ-insensitive zone is sometimes referred to as the ϵ-tube.

Basic approach

- The regression algorithm is then developed in close analogy to the case of classification.
- Again, we estimate linear functions, use a $\|\beta\|^2$ regularizer, and rewrite everything in terms of dot products to generalize to the nonlinear case.

Overview

Problem formulation

- We search for the linear function $f(x) = \beta^T x + \beta_0$ minimizing the following criterion:

$$\underbrace{\frac{1}{2}\|\beta\|^2}_{\text{regularization}} + \frac{C}{n} \underbrace{\sum_{i=1}^{n} |f(x_i) - y_i|_\epsilon}_{\text{loss function}}.$$

- C is a hyperparameter, which balances training error and model complexity.
- To solve this problem, we transform it into an equivalent constrained optimization problem.

Reformulation as a constrained optimization problem

- We have

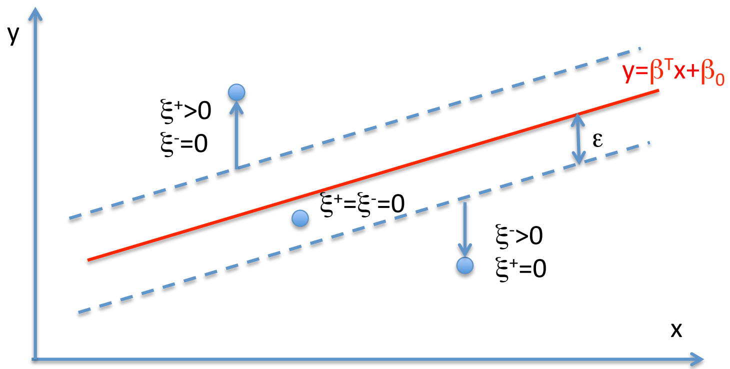
$$\begin{aligned}|f(x_i) - y_i|_\epsilon &= [|f(x_i) - y_i| - \epsilon]_+ \\ &= \begin{cases} [f(x_i) - y_i - \epsilon]_+ = \xi_i^- & \text{if } f(x_i) \geq y_i \\ [y_i - f(x_i) - \epsilon]_+ = \xi_i^+ & \text{if } f(x_i) < y_i \end{cases}\end{aligned}$$

- Furthermore, $\xi_i^- = 0$ if $f(x_i) < y_i$, and $\xi_i^+ = 0$ if $f(x_i) \geq y_i$. We can thus write

$$|f(x_i) - y_i|_\epsilon = \xi_i^+ + \xi_i^-$$

- The quantities ξ_i^+ and ξ_i^- are called "slack variables" (they will become slack variables in the constrained optimization formulation of the problem)

Representation of the slack variables



Primal objective function

Using the slack variables, the previous problem can be reformulated as a quadratic optimization problem:

$$\min_{\beta,\beta_0,\xi^-,\xi^+} \frac{1}{2}\|\beta\|^2 + \frac{C}{n}\sum_{i=1}^{n}(\xi_i^- + \xi_i^+)$$

subject to:

$$\begin{aligned}
\xi_i^+ &\geq y_i - \beta^T x_i - \beta_0 - \epsilon \\
\xi_i^+ &\geq 0 \\
\xi_i^- &\geq \beta^T x_i + \beta_0 - y_i - \epsilon \\
\xi_i^- &\geq 0
\end{aligned}$$

for $i = 1, \ldots, n$.

Lagrange function

The Lagrange function is

$$
\begin{aligned}
L(\beta, \beta_0, \alpha_i^-, \alpha_i^+, \eta_i^-, \eta_i^+) = \frac{1}{2}\|\beta\|^2 + \frac{C}{n}\sum_{i=1}^{n}(\xi_i^- + \xi_i^+) \\
- \sum_{i=1}^{n}(\eta_i^-\xi_i^- + \eta_i^+\xi_i^+) - \sum_{i=1}^{n}\alpha_i^-(\epsilon + \xi_i^- + y_i - \beta^T x_i - \beta_0) \\
- \sum_{i=1}^{n}\alpha_i^+(\epsilon + \xi_i^+ - y_i + \beta^T x_i + \beta_0),
\end{aligned}
$$

where α_i^-, α_i^+, η_i^-, η_i^+ are Lagrange multipliers.

Derivatives of the Lagrange function

- Setting the derivatives to zero, we obtain:

$$
\begin{aligned}
\frac{\partial L}{\partial \beta} &= \beta - \sum_{i=1}^{n} (\alpha_i^+ - \alpha_i^-) x_i = 0, \\
\frac{\partial L}{\partial \beta_0} &= \sum_{i=1}^{n} (\alpha_i^- - \alpha_i^+) = 0, \\
\frac{\partial L}{\partial \xi_i^-} &= \frac{C}{n} - \alpha_i^- - \eta_i^- = 0, \quad i = 1, \ldots, n \\
\frac{\partial L}{\partial \xi_i^+} &= \frac{C}{n} - \alpha_i^+ - \eta_i^+ = 0, \quad i = 1, \ldots, n.
\end{aligned}
$$

- We use these relations to simplify the expression of the Lagrange function (see next slide).

Simplification of the Lagrange function

$$
\begin{aligned}
L = \frac{1}{2} &\left(\sum_i (\alpha_i^+ - \alpha_i^-) x_i\right)^T \left(\sum_j (\alpha_j^+ - \alpha_j^-) x_j\right) \\
&+ \sum_{i=1}^n \xi_i^- \underbrace{\left(\frac{C}{n} - \eta_i^- - \alpha_i^-\right)}_{0} + \sum_{i=1}^n \xi_i^+ \underbrace{\left(\frac{C}{n} - \eta_i^+ - \alpha_i^+\right)}_{0} \\
&- \epsilon \sum_i (\alpha_i^+ + \alpha_i^-) - \beta_0 \underbrace{\sum_i (\alpha_i^+ - \alpha_i^-)}_{0} + \sum_i y_i (\alpha_i^+ - \alpha_i^-) \\
&- \sum_{i=1}^n (\alpha_i^+ - \alpha_i^-) \left(\sum_j (\alpha_j^+ - \alpha_j^-) x_j\right)^T x_i
\end{aligned}
$$

Dual problem

$$L_D(\alpha_i^-, \alpha_i^+) = -\frac{1}{2}\sum_{i,j}(\alpha_i^+ - \alpha_i^-)(\alpha_j^+ - \alpha_j^-)x_i^T x_j$$
$$- \epsilon \sum_{i=1}^n (\alpha_i^+ + \alpha_i^-) + \sum_{i=1}^n y_i(\alpha_i^+ - \alpha_i^-),$$

to be maximized subject to

$$\sum_{i=1}^n (\alpha_i^+ - \alpha_i^-) = 0$$

$$0 \leq \alpha_i^- \leq \frac{C}{n}, \quad i = 1, \ldots, n,$$

$$0 \leq \alpha_i^+ \leq \frac{C}{n}, \quad i = 1, \ldots, n.$$

Overview

Support vectors

- As in the case of SVMs, the dual problem can be solved using any quadratic programming solver.
- Let $\alpha_i^{-*}, \alpha_i^{+*}$, $i = 1, \ldots, n$ be the solution.
- The learning vectors x_i such that $\alpha_i^{-*} > 0$ or $\alpha_i^{+*} > 0$ are called the support vectors. They lie outside the tube (or at the border).
- Let $\mathcal{S}$ be the set of support vectors. We have

$$\beta^* = \sum_{i \in \mathcal{S}} (\alpha_i^{+*} - \alpha_i^{-*}) x_i$$

and

$$f^*(x) = \sum_{i \in \mathcal{S}} (\alpha_i^{+*} - \alpha_i^{-*}) x_i^T x + \beta_0^*$$

Sparsity of the SV expansion

- We thus have a sparse expansion of β in terms of x_i (we do not need all x_i to compute β^*).
- The points inside the tube (i.e., which are not support vectors) do not contribute to the solution: we could remove any one of them, and still obtain the same solution.

Karush-Kuhn-Tucker conditions

- The solution $\alpha_i^{-*}, \alpha_i^{+*}$, $i = 1, \ldots, n$ must satisfy the KKT conditions

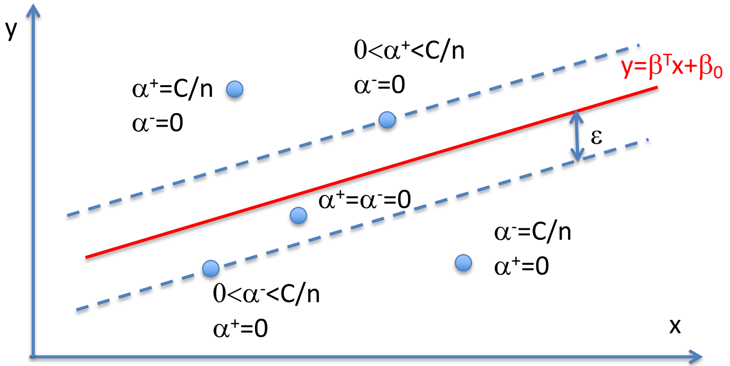
$$\alpha_i^{-*}(\epsilon + \xi_i^{-*} + y_i - {\beta^*}^T x_i - \beta_0^*) = 0 \tag{20a}$$

$$\alpha_i^{+*}(\epsilon + \xi_i^{+*} - y_i + {\beta^*}^T x_i + \beta_0^*) = 0 \tag{20b}$$

$$\left(\frac{C}{n} - \alpha_i^{-*}\right)\xi_i^{-*} = 0, \quad \left(\frac{C}{n} - \alpha_i^{+*}\right)\xi_i^{+*} = 0 \tag{20c}$$

- Consequences:
  - Only examples (x_i, y_i) with corresponding $\alpha_i^{-*} = C/n$ or $\alpha_i^{+*} = C/n$ can lie outside the tube (i.e., $\xi_i^{-*} > 0$ or $\xi_i^{+*} > 0$).
  - When $\alpha_i^{+*} \in (0, C/n)$ or $\alpha_i^{-*} \in (0, C/n)$, we have $\xi_i^{+*} = \xi_i^{-*} = 0$. The corresponding SVs lie at the border of the tube (see next slide).

Interpretation of α_i^+ and α_i^-



Calculation of β_0

- β_0^* can be calculated from (20a) or (20b) for SVs at the border of the tube as

$$\beta_0^* = \begin{cases} \epsilon + y_i - {\beta^*}^T x_i & \text{for } \alpha_i^{-*} \in (0, C/n) \\ y_i - {\beta^*}^T x_i - \epsilon & \text{for } \alpha_i^{+*} \in (0, C/n) \end{cases}$$

- Theoretically, it suffices to use any Lagrange multiplier in $(0, C/n)$.
- If given the choice between several such multipliers in $(0, C/n)$, it is safer to use one that is not too close to 0 or C/n.

Parameter tuning

The solution depends on two parameters, ϵ and C. These play different roles:

- Parameter ϵ in the loss function specifies the desired accuracy of the approximation. If we scale our response, then we might consider using preset values for ϵ.
- The quantity C is a more traditional regularization parameter. It can be estimated, for example, by cross-validation.

Nonlinear extension

- As in the classification case, the complete algorithm can be described in terms of dot products between the data.
- This makes it possible to formulate a nonlinear extension using kernels, replacing dot products ${x_i}^T x_j$ in $\mathcal{X}$ with dot products

$$\langle \Phi(x_i), \Phi(x_j) \rangle = \mathcal{K}(x_i, x_j)$$

  in $\mathcal{H}$.
- Additional kernel parameters may be determined by cross-validation.

Application in R

```
library('kernlab')
library('MASS')
mcycle.data<-data.frame(mcycle)
mcycle.data$accel<-scale(mcycle.data$accel)
t<- seq(min(mcycle.data$times),max(mcycle.data$times),0.5)
testdat<-data.frame(times=t)

svmfit<-ksvm(accel~.,data=mcycle.data,scaled=TRUE,type="eps-svr",
            kernel="rbfdot",C=100,epsilon=0.1,kpar=list(sigma=1))

yhat<-predict(svmfit,newdata=testdat)
plot(mcycle.data$times,mcycle.data$accel)
lines(t,yhat)
```

Result