

svm() internals

Some technical notes about the `svm()` in package `e1071`

by David Meyer
FH Technikum Wien, Austria
<mailto:David.Meyer@R-Project.org>

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This document explains how to use the parameters in an object returned by `svm()` for own prediction functions.

1 Binary Classifier

For class prediction in the binary case, the class of a new data vector n is usually given by *the sign* of

$$\sum_i a_i y_i K(x_i, n) + \rho \quad (1)$$

where x_i is the i -th support vector, y_i the corresponding label, a_i the corresponding coefficient, and K is the kernel (for example the linear one, i.e. $K(u, v) = u^\top v$).

Now, the `libsvm` library interfaced by the `svm()` function actually returns $a_i y_i$ as i -th coefficient and the *negative* ρ , so in fact uses the formula:

$$\sum_i \text{coef}_i K(x_i, n) - \rho$$

where the training examples (=training data) are labeled $\{1, -1\}$ (!). A simplified R function for prediction with linear kernel would be:

```
svmpred <- function (m, newdata, K=crossprod)
{
  ## this guy does the computation:
  pred.one <- function (x)
    sign(sum(sapply(1:m$tot.nSV, function (j)
      K(m$SV[j,], x) * m$coefs[j]
    ) - m$rho
  )

  ## this is just for convenience:
  if (is.vector(newdata))
    newdata <- t(as.matrix(x))
  sapply (1:nrow(newdata),
    function (i) pred.one(newdata[i,]))
}
```

where `pred.one()` does the actual prediction for one new data vector, the remainder is just a convenience for prediction of multiple new examples. It is easy to extend this to other kernels, just replace `K()` with the appropriate function (see the help page for the formulas used) and supply the additional constants.

As we will see in the next section, the multi-class prediction is more complicated, because the coefficients of the diverse binary SVMs are stored in a compressed format.

2 Multiclass-classifier

To handle k classes, $k > 2$, `svm()` trains all binary subclassifiers (one-against-one-method) and then uses a voting mechanism to determine the actual class. Now, this means $k(k-1)/2$ classifiers, hence in principle $k(k-1)/2$ sets of SVs, coefficients and rhos. These are stored in a compressed format:

1. Only one SV is stored in case it were used by several classifiers. The `model$SV-matrix` is ordered by classes, and you find the starting indices by using `nSV` (number of SVs):

```
start <- c(1, cumsum(model$nSV))
start <- start[-length(start)]
```

`sum(nSV)` equals the total number of (distinct) SVs.

2. The coefficients of the SVs are stored in the `model$coefs`-matrix, grouped by classes. Because the separating hyperplanes found by the SVM algorithm has SVs on both sides, you will have two sets of coefficients per binary classifier, and e.g., for 3 classes, you could build a *block*-matrix like this for the classifiers (i, j) (i, j =class numbers):

$i \setminus j$	0	1	2
0	X	set (0, 1)	set (0, 2)
1	set (1, 0)	X	set (1, 2)
2	set (2, 0)	set (2, 1)	X

where `set(i, j)` are the coefficients for the classifier (i, j) , lying on the side of class j . Because there are no entries for (i, i) , we can save the diagonal and shift up the lower triangular matrix to get

$i \setminus j$	0	1	2
0	set (1,0)	set (0,1)	set (0,2)
1	set (2,0)	set (2,1)	set (1,2)

Each `set(., j)` has length `nSV[j]`, so of course, there will be some filling 0s in some sets.

`model$coefs` is the *transposed* of such a matrix, therefore for a data set with, say, 6 classes, you get $6-1=5$ columns.

The coefficients of (i, j) start at `model$coefs[start[i],j]` and those of (j, i) at `model$coefs[start[j],i-1]`.

3. The $k(k-1)/2$ rhos are just linearly stored in the vector `model$rho`.

The following code shows how to use this for prediction:

```
## Linear Kernel function
K <- function(i,j) crossprod(i,j)

predsvm <- function(object, newdata)
{
  ## compute start-index
  start <- c(1, cumsum(object$nSV)+1)
  start <- start[-length(start)]

  ## compute kernel values
  kernel <- sapply (1:object$tot.nSV,
                    function (x) K(object$SV[x,], newdata))

  ## compute raw prediction for classifier (i,j)
  predone <- function (i,j)
  {
    ## ranges for class i and j:
    ri <- start[i] : (start[i] + object$nSV[i] - 1)
    rj <- start[j] : (start[j] + object$nSV[j] - 1)

    ## coefs for (i,j):
    coef1 <- object$coefs[ri, j-1]
    coef2 <- object$coefs[rj, i]

    ## return raw values:
    crossprod(coef1, kernel[ri]) + crossprod(coef2, kernel[rj])
  }

  ## compute votes for all classifiers
  votes <- rep(0,object$nclasses)
  c <- 0 # rho counter
  for (i in 1 : (object$nclasses - 1))
    for (j in (i + 1) : object$nclasses)
      if (predone(i,j) > object$rho[c <- c + 1])
        votes[i] <- votes[i] + 1
      else
        votes[j] <- votes[j] + 1

  ## return winner (index with max. votes)
  object$levels[which(votes %in% max(votes))[1]]
}
```

In case data were scaled prior fitting the model (note that this is the default for `svm()`), the new data needs to be scaled as well before applying the prediction functions, for example using the following code snippet (object is an object returned by `svm()`, `newdata` a data frame):

```
if (any(object$scaled))
  newdata[,object$scaled] <-
    scale(newdata[,object$scaled, drop = FALSE],
          center = object$x.scale$"scaled:center",
          scale = object$x.scale$"scaled:scale"
    )
```

For regression, the response needs to be scaled as well before training, and the predictions need to be scaled back accordingly.