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

\[
\sum_i a_i y_i K(x_i, n) + \rho
\]

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. \( K(u,v) = u^T v \)).

Now, the \texttt{libsvm} library interfaced by the \texttt{svm()} function actually returns \( a_i y_i \) as \( i \)-th coefficiant and the negative \( \rho \), 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 \texttt{R} function for prediction with linear kernel would be:

```r
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 \texttt{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 \texttt{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, $k > 2$, \texttt{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 \texttt{model$SV-matrix} is ordered by classes, and you find the starting indices by using \texttt{nSV} (number of SVs):

\begin{verbatim}
start <- c(1, cumsum(model$nSV))
start <- start[-length(start)]
\end{verbatim}

\texttt{sum(nSV)} equals the total number of (distinct) SVs.

2. The coefficients of the SVs are stored in the \texttt{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 $(i,j)$ ($i,j=\text{class numbers}$):

\begin{verbatim}
1 \ 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
\end{verbatim}

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

\begin{verbatim}
1 \ j  0 1 2
0 set (1,0) set (0,1) set (0,2)
1 set (2,0) set (2,1) set (1,2)
\end{verbatim}

Each set $(., j)$ has length \texttt{nSV}[j], so of course, there will be some filling 0s in some sets. \texttt{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 \texttt{model$coefs[start[i],j]} and those of $(j, i)$ at \texttt{model$coefs[start[j],i-1]}.

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

2
The following code shows how to use this for prediction:

```r
## Linear Kernel function
K <- function(i,j) crossprod(i,j)
preds <- function(object, newdata)
{
  ## compute start-index
  start <- c(1, cumsum(object$nSV)+1)
  start <- start[-length(start)]
  
  ## compute kernel values
  kernel <- sapply (1:object$tot.nSV,
    function (i) K(object$SV[,i], 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$nSVM)
  c <- 0 # rho counter
  for (i in 1 : (object$nSVM - 1))
    for (j in (i + 1) : object$nSVM)
      if (predone(i,j) > object$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):

```r
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.