APA-L7

September 6, 2018

1 APA Laboratori 7 - SVMs

```
In [1]: # uncomment to install missing libraries
        # install.packages('e1071')
```

```
In [2]: options(repr.plot.width=6, repr.plot.height=6)
```

1.1 Modelling artificial 2D sinusoidal data for two-class problems

The SVM is located in two different packages: one of them is 'e1071'

```
In [3]: library(e1071)
```

First we create a simple two-class data set:

```
In [4]: N <- 200

        make.sinusoidals <- function(m,noise=0.2)
        {
          x1 <- c(1:2*m)
          x2 <- c(1:2*m)

          for (i in 1:m) {
            x1[i] <- (i/m) * pi
            x2[i] <- sin(x1[i]) + rnorm(1,0,noise)
          }

          for (j in 1:m) {
            x1[m+j] <- (j/m + 1/2) * pi
            x2[m+j] <- cos(x1[m+j]) + rnorm(1,0,noise)
          }

          target <- as.factor(c(rep(+1,m),rep(-1,m)))

          return(data.frame(x1,x2,target))
        }
```

let's generate the data

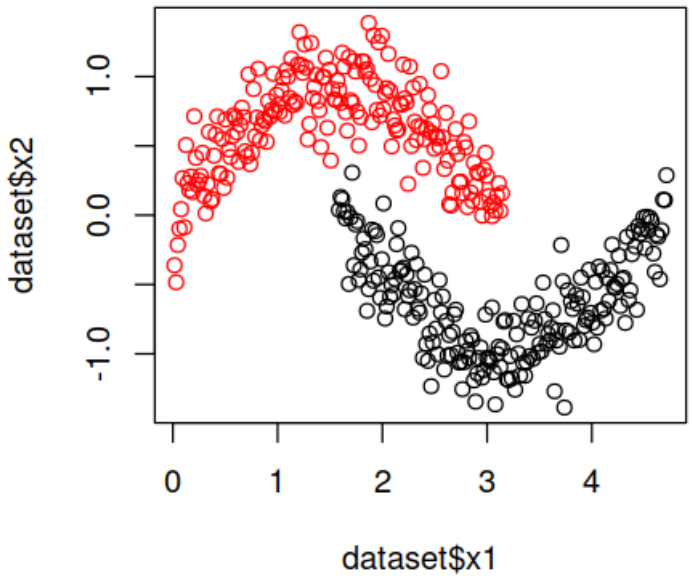
```
In [5]: dataset <- make.sinusoidals (N)
```

and have a look at it

```
In [6]: summary(dataset)
```

```
       x1                 x2              target
 Min.   :0.01571   Min.   :-1.387200   -1:200
 1st Qu.:1.58258   1st Qu.:-0.668201   1 :200
 Median :2.36405   Median : 0.028719
 Mean   :2.36405   Mean   :-0.006386
 3rd Qu.:3.14552   3rd Qu.: 0.645680
 Max.   :4.71239   Max.   : 1.386127
```

```
In [7]: options(repr.plot.width=4, repr.plot.height=4)
        plot(dataset$x1,dataset$x2,col=dataset$target)
```



Now we wish to fit and visualize different SVM models

1.1.1 model 1: LINEAR kernel, C=1 (cost parameter)

```
In [8]: (model <- svm(dataset[,1:2],
                      dataset[,3],
```

```
                      type="C-classification",
                      cost=1, kernel="linear",
                      scale = FALSE))


Call:
svm.default(x = dataset[, 1:2], y = dataset[, 3], scale = FALSE,
    type = "C-classification", kernel = "linear", cost = 1)


Parameters:
   SVM-Type:  C-classification
 SVM-Kernel:  linear
       cost:  1
      gamma:  0.5

Number of Support Vectors:  61
```

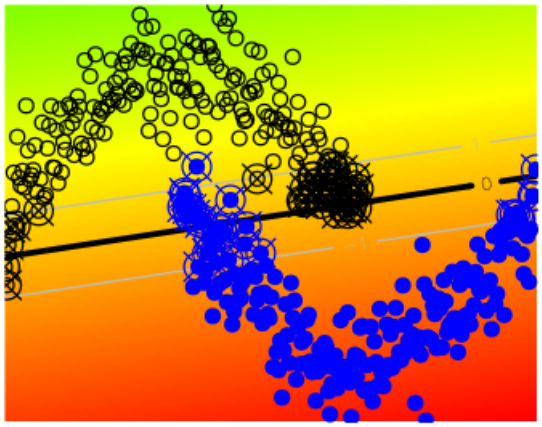
Now we are going to visualize what we have done; since we have artificial data, instead of creating a random test set, we can create a grid of points as test

```
In [9]: plot.prediction <- function (model, model.name, resol=200)
        # the grid has a (resol x resol) resolution
        {
          x <- cbind(dataset$x1,dataset$x2)
          rng <- apply(x,2,range);
          tx <- seq(rng[1,1],rng[2,1],length=resol);
          ty <- seq(rng[1,2],rng[2,2],length=resol);
          pnts <- matrix(nrow=length(tx)*length(ty),ncol=2);
          k <- 1
          for(j in 1:length(ty))
          {
            for(i in 1:length(tx))
            {
              pnts[k,] <- c(tx[i],ty[j])
              k <- k+1
            }
          }

        #  we calculate the predictions on the grid

        pred <- predict(model, pnts, decision.values = TRUE)

        z <- matrix(attr(pred,"decision.values"),
                    nrow=length(tx),ncol=length(ty))
```

```
    # and plot them


      image(tx,ty,z,xlab=model.name,ylab="",axes=FALSE,
            xlim=c(rng[1,1],rng[2,1]),ylim=c(rng[1,2],rng[2,2]),
            col = rainbow(200, start=0, end=.25))


      # then we draw the optimal separation and its margins


      contour(tx,ty,z,add=TRUE,
              drawlabels=TRUE,
              level=0, lwd=3)
      contour(tx,ty,z,add=TRUE,
              drawlabels=TRUE, level=1,
              lty=1, lwd=1, col="grey")
      contour(tx,ty,z,add=TRUE,
              drawlabels=TRUE, level=-1,
              lty=1, lwd=1, col="grey")

      # then we plot the input data from the two classes

      points(dataset[dataset$target==1,1:2],pch=21,col=1,cex=1)
      points(dataset[dataset$target==-1,1:2],pch=19,col=4,cex=1)

      # finally we add the SVs

      sv <- dataset[c(model$index),];
      sv1 <- sv[sv$target==1,];
      sv2 <- sv[sv$target==-1,];
      points(sv1[,1:2],pch=13,col=1,cex=2)
      points(sv2[,1:2],pch=13,col=4,cex=2)
    }
```

make sure you understand the following results (one by one and their differences) plot the data, the OSH with margins, the support vectors, ...

```
In [10]: plot.prediction (model, "linear, C=1")
```



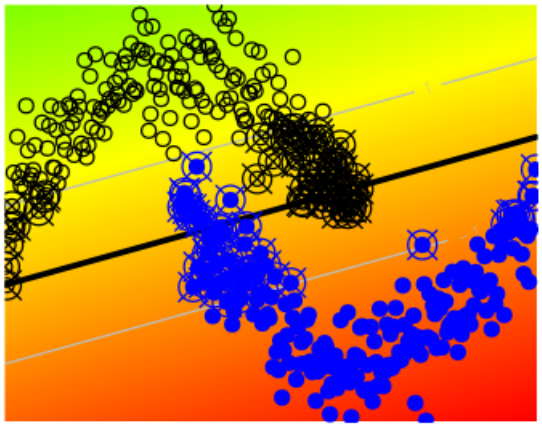
linear, C=1

model 2: linear kernel, C=0.1 (cost parameter)

```
In [11]: (model <- svm(dataset[,1:2],dataset[,3],
                       type="C-classification",
                       cost=0.1, kernel="linear",
                       scale = FALSE))
```

```
Call:
svm.default(x = dataset[, 1:2], y = dataset[, 3], scale = FALSE,
    type = "C-classification", kernel = "linear", cost = 0.1)


Parameters:
   SVM-Type:  C-classification
 SVM-Kernel:  linear
       cost:  0.1
      gamma:  0.5

Number of Support Vectors:  99
```

```
In [12]: plot.prediction (model, "linear, C=0.1")
```



linear, C=0.1

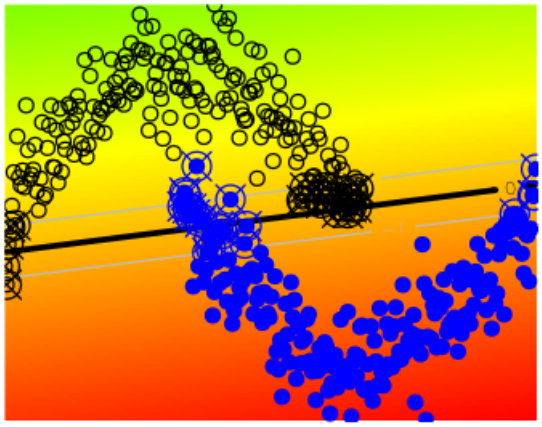
the margin is wider (lower VC dimension), number of support vectors is larger (more violations of the margin)

1.1.2 model 3: linear kernel, C=25 (cost parameter)

```
In [13]: (model <- svm(dataset[,1:2],dataset[,3],
                       type="C-classification",
                       cost=25, kernel="linear",
                       scale = FALSE))
```

```
Call:
svm.default(x = dataset[, 1:2], y = dataset[, 3], scale = FALSE,
    type = "C-classification", kernel = "linear", cost = 25)


Parameters:
   SVM-Type:  C-classification
 SVM-Kernel:  linear
       cost:  25
      gamma:  0.5

Number of Support Vectors:  45
```

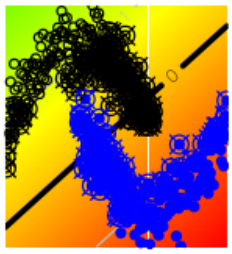
```
In [14]: plot.prediction (model, "linear, C=25")
```



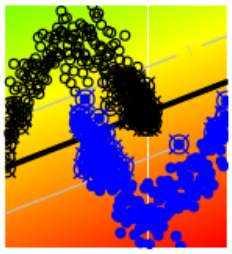
the margin is narrower (higher VC dimension), number of support vectors is smaller (less violations of the margin)

Let's put it together, for 6 values of C:

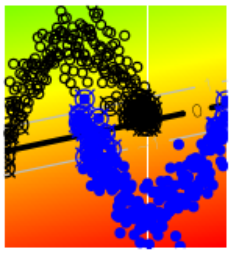
```
In [15]: options(repr.plot.width=6, repr.plot.height=5)
         par(mfrow=c(2,3))

         for (C in 10^seq(-2,3))
         {
           model <- svm(dataset[,1:2],dataset[,3],
                        type="C-classification",
                        cost=C, kernel="linear",
                        scale = FALSE)
           plot.prediction (model, paste ("linear (C=", C, ") ",
                                          model$tot.nSV, " Support Vectors",
                                          sep=""))
         }
```



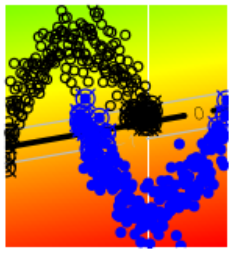
linear (C=0.01) 196 Support Vectors



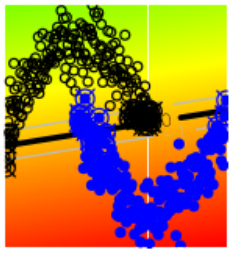
linear (C=0.1) 99 Support Vectors



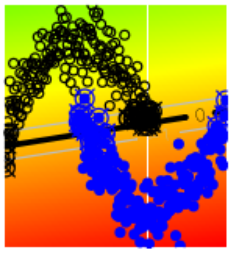
linear (C=1) 61 Support Vectors



linear (C=10) 46 Support Vectors



linear (C=100) 44 Support Vectors



linear (C=1000) 43 Support Vectors

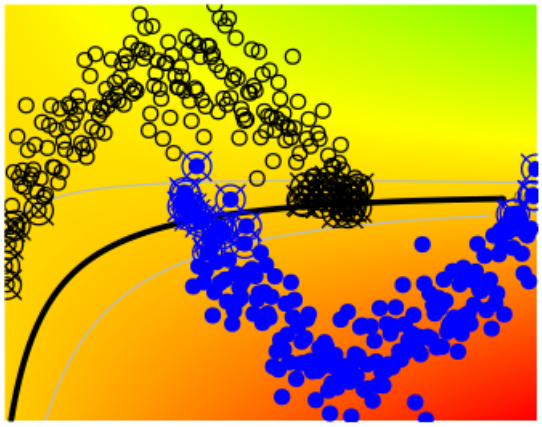
Now we move to a QUADRATIC kernel (polynomial of degree 2); the kernel has the form: $k(x,y) = (< x,y > +coef0)^{degree}$
quadratic kernel, C=1 (cost parameter)

```
In [16]: (model <- svm(dataset[,1:2],dataset[,3],
                      type="C-classification",
                      cost=1, kernel="polynomial",
                      degree=2, coef0=1,
                      scale = FALSE))
```

```
Call:
svm.default(x = dataset[, 1:2], y = dataset[, 3], scale = FALSE,
    type = "C-classification", kernel = "polynomial", degree = 2,
    coef0 = 1, cost = 1)


Parameters:
   SVM-Type:  C-classification
```

```
 SVM-Kernel:  polynomial
       cost:  1
     degree:  2
      gamma:  0.5
     coef.0:  1

Number of Support Vectors:  48
```

```
In [17]: options(repr.plot.width=4, repr.plot.height=4)
         par(mfrow=c(1,1))

         plot.prediction (model, "quadratic, C=1")
```



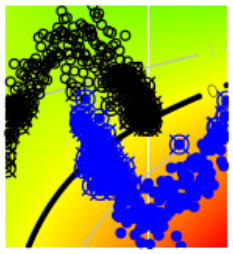
quadratic, C=1

notice that neither the OSH or the margins are linear (they are quadratic); they are linear in the feature space in the previous linear kernel, both spaces coincide

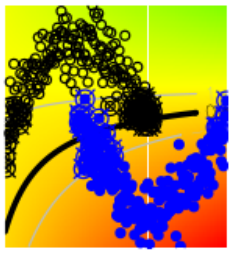
Let's put it together directly, for 6 values of C:

```
In [18]: options(repr.plot.width=6, repr.plot.height=5)
         par(mfrow=c(2,3))

         for (C in 10^seq(-2,3))
         {
```

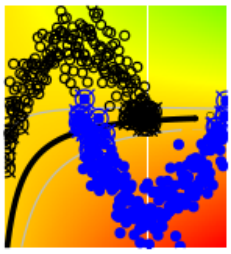
```
  model <- svm(dataset[,1:2],dataset[,3],
               type="C-classification",
               cost=C, kernel="polynomial",
               degree=2, coef0=1,
               scale = FALSE)
  plot.prediction (model,
                   paste ("quadratic (C=", C, ") ",
                          model$tot.nSV, " Support Vectors",
                          sep=""))
}
```



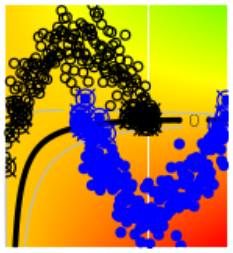
quadratic (C=0.01) 131 Support Vecto



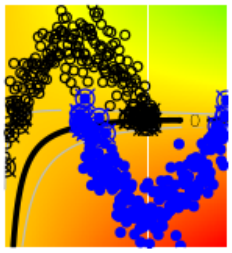
quadratic (C=0.1) 72 Support Vectors



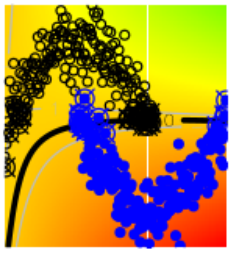
quadratic (C=1) 48 Support Vectors



quadratic (C=10) 39 Support Vectors



quadratic (C=100) 38 Support Vectors



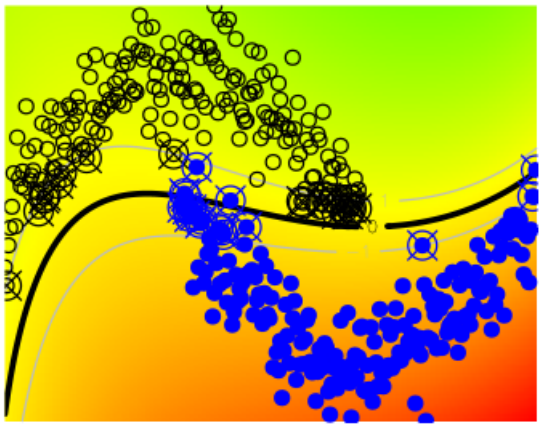
quadratic (C=1000) 38 Support Vecto

Now we move to a CUBIC kernel (polynomial of degree 3); the kernel has the form:
$k(x,y) = (< x,y > +coef0)^{degree}$
cubic kernel, C=1 (cost parameter)

In [19]:
```
(model <- svm(dataset[,1:2],dataset[,3],
              type="C-classification",
              cost=1, kernel="polynomial",
              degree=3, coef0=1,
              scale = FALSE))
```

```
Call:
svm.default(x = dataset[, 1:2], y = dataset[, 3], scale = FALSE,
    type = "C-classification", kernel = "polynomial", degree = 3,
    coef0 = 1, cost = 1)


Parameters:
   SVM-Type:  C-classification
 SVM-Kernel:  polynomial
       cost:  1
     degree:  3
      gamma:  0.5
     coef.0:  1

Number of Support Vectors:  37
```

```
In [20]: options(repr.plot.width=4, repr.plot.height=4)
         par(mfrow=c(1,1))

         plot.prediction (model, "cubic, C=1")
```

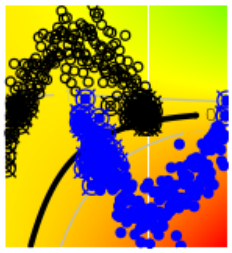


cubic, C=1

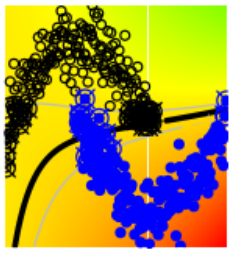
notice that neither the OSH or the margins are linear (they are now cubic); they are linear in the feature space this choice seems much better, given the structure of the classes

Let's put it together directly, for 6 values of C:

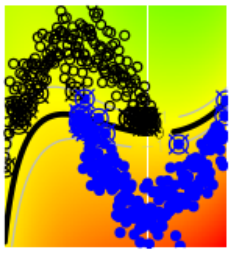
```
In [21]: options(repr.plot.width=6, repr.plot.height=5)
         par(mfrow=c(2,3))

         for (C in 10^seq(-2,3))
         {
           model <- svm(dataset[,1:2],dataset[,3],
                        type="C-classification",
                        cost=C, kernel="polynomial",
                        degree=3, coef0=1,
                        scale = FALSE)
           plot.prediction (model, paste ("cubic (C=", C, ") ",
                                          model$tot.nSV,
                                          " Support Vectors",
                                          sep=""))
         }
```



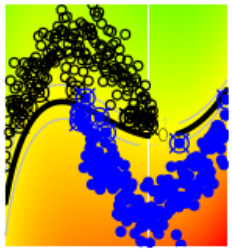
cubic (C=0.01) 88 Support Vectors



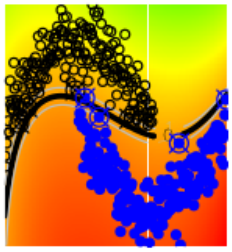
cubic (C=0.1) 54 Support Vectors



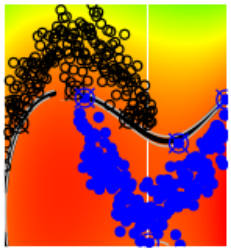
cubic (C=1) 37 Support Vectors



cubic (C=10) 16 Support Vectors



cubic (C=100) 8 Support Vectors



cubic (C=1000) 7 Support Vectors

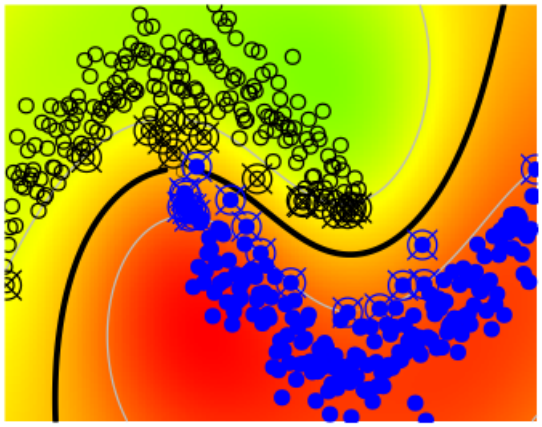
Finally we use the Gaussian RBF kernel (polynomial of infinite degree; the kernel has the form: $k(x,y) = exp(-gamma||x-y||^2)$
RBF kernel, C=1 (cost parameter)

```
In [22]: (model <- svm(dataset[,1:2],dataset[,3],
                       type="C-classification",
                       cost=1, kernel="radial",
                       scale = FALSE))
```

```
Call:
svm.default(x = dataset[, 1:2], y = dataset[, 3], scale = FALSE,
    type = "C-classification", kernel = "radial", cost = 1)


Parameters:
   SVM-Type:  C-classification
 SVM-Kernel:  radial
       cost:  1
      gamma:  0.5

Number of Support Vectors:  34
```

the default value for gamma is 0.5

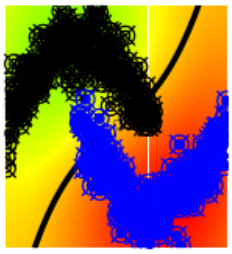
```
In [23]: options(repr.plot.width=4, repr.plot.height=4)
         par(mfrow=c(1,1))

         plot.prediction (model, "radial, C=1, gamma=0.5")
```



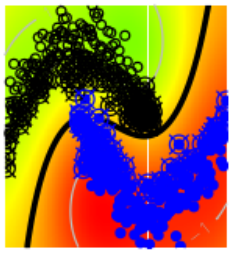
radial, C=1, gamma=0.5

Let's put it together directly, for 6 values of C, holding gamma constant = 0.5:

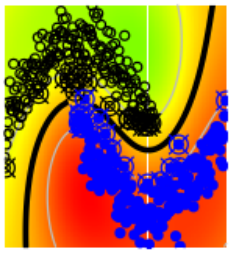
```
In [24]: options(repr.plot.width=6, repr.plot.height=5)
         par(mfrow=c(2,3))

         for (C in 10^seq(-2,3))
         {
           model <- svm(dataset[,1:2],dataset[,3],
                        type="C-classification",
                        cost=C, kernel="radial",
                        scale = FALSE)
           plot.prediction (model, paste ("RBF (C=", C, ") ",
                                          model$tot.nSV,
                                          " Support Vectors",
                                          sep=""))
         }
```



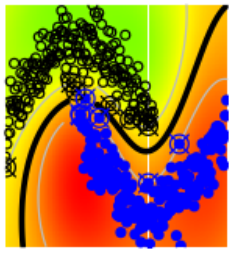
RBF (C=0.01) 390 Support Vectors



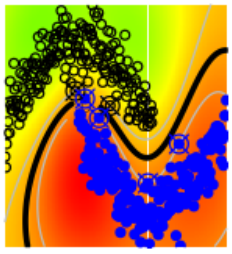
RBF (C=0.1) 123 Support Vectors



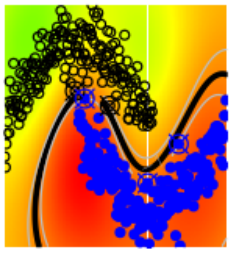
RBF (C=1) 34 Support Vectors



RBF (C=10) 12 Support Vectors



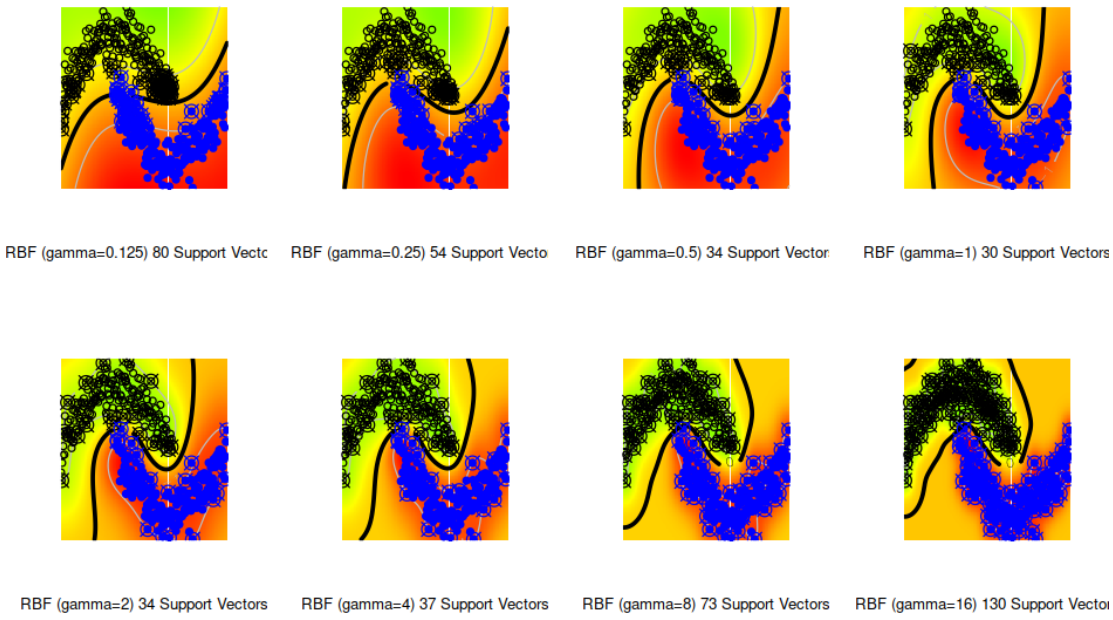
RBF (C=100) 6 Support Vectors



RBF (C=1000) 5 Support Vectors

Now for 8 values of gamma, holding C constant = 1:

In [25]:
```
options(repr.plot.width=8, repr.plot.height=5)
par(mfrow=c(2,4))

for (g in 2^seq(-3,4))
{
  model <- svm(dataset[,1:2],dataset[,3],
               type="C-classification",
               cost=1, kernel="radial",
               gamma=g, scale = FALSE)
  plot.prediction (model, paste ("RBF (gamma=", g, ") ",
                                 model$tot.nSV,
                                 " Support Vectors",
                                 sep=""))
}
```



In practice we should optimize both (C,gamma) at the same time
How? Using cross-validation or trying to get "good" estimates analyzing the data
Now we define a utility function for performing k-fold CV: a typical choice is k=10

```
In [26]: k <- 10
         folds <- sample(rep(1:k, length=N), N, replace=FALSE)

         valid.error <- rep(0,k)
```

this function is not intended to be useful for general training purposes but it is useful for illustration in particular, it does not optimize the value of C (it requires it as parameter)

```
In [27]: train.svm.kCV <- function (which.kernel, myC, kCV=10)
         {
           for (i in 1:kCV)
           {
             train <- dataset[folds!=i,] # for building the model (training)
             valid <- dataset[folds==i,] # for prediction (validation)

             x_train <- train[,1:2]
             t_train <- train[,3]

             switch(which.kernel,
                    linear={model <- svm(x_train, t_train,
                                         type="C-classification",
                                         cost=myC, kernel="linear",
```

```
                                scale = FALSE)},
                poly.2={model <- svm(x_train, t_train,
                                type="C-classification",
                                cost=myC, kernel="polynomial",
                                degree=2, coef0=1,
                                scale = FALSE)},
                poly.3={model <- svm(x_train, t_train,
                                type="C-classification",
                                cost=myC,
                                kernel="polynomial",
                                degree=3, coef0=1,
                                scale = FALSE)},
                RBF={model <- svm(x_train, t_train,
                                  type="C-classification",
                                  cost=myC, kernel="radial",
                                  scale = FALSE)},
                stop("Enter one of 'linear', 'poly.2', 'poly.3', 'radial'"))

      x_valid <- valid[,1:2]
      pred <- predict(model,x_valid)
      t_true <- valid[,3]

      # compute validation error for part 'i'
      valid.error[i] <- sum(pred != t_true)/length(t_true)
    }
    # return average validation error
    100*sum(valid.error)/length(valid.error)
  }
```

Fit an SVM with linear kernel

In [28]:
```
C <- 1000

(VA.error.linear <- train.svm.kCV ("linear", myC=C))
```

4

The procedure is to choose the model with the lowest CV error and then refit it with the whole learning data, then use it to predict the test set; we will do this at the end

Fit an SVM with quadratic kernel

In [29]:
```
(VA.error.poly.2 <- train.svm.kCV ("poly.2", myC=C))
```

4

Fit an SVM with cubic kernel

In [30]:
```
(VA.error.poly.3 <- train.svm.kCV ("poly.3", myC=C))
```

1

we get a series of decreasing CV errors ...

and finally an RBF Gaussian kernel

```
In [31]: (VA.error.RBF <- train.svm.kCV ("RBF", myC=C))
```

0.75

Now in a real scenario we should choose the model with the lowest CV error which in this case is the RBF (we get a very low CV error because this problem is easy for a SVM)

so we choose RBF and C=1 and refit the model in the whole training set (no CV)

```
In [32]: model <- svm(dataset[,1:2],dataset[,3], type="C-classification", cost=C, kernel="radial
```

and make it predict a test set:

let's generate the test data

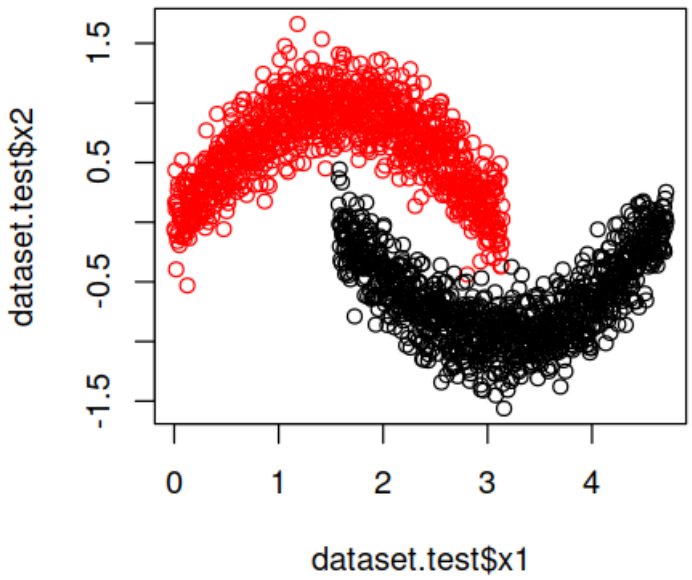
```
In [33]: dataset.test <- make.sinusoidals (1000)
```

and have a look at it

```
In [34]: summary(dataset.test)
```

```
       x1                  x2             target
 Min.   :0.003142   Min.   :-1.561915   -1:1000
 1st Qu.:1.573153   1st Qu.:-0.683925   1 :1000
 Median :2.357765   Median :-0.013291
 Mean   :2.357765   Mean   :-0.008065
 3rd Qu.:3.142378   3rd Qu.: 0.669875
 Max.   :4.712389   Max.   : 1.661682
```

```
In [35]: options(repr.plot.width=4, repr.plot.height=4)
         par(mfrow=c(1,1))
         plot(dataset.test$x1,dataset.test$x2,col=dataset.test$target)
```



```
In [36]: pred <- predict(model,dataset.test[,1:2])
         t_true <- dataset.test[,3]

         table(pred,t_true)
```

```
    t_true
pred   -1    1
  -1  996    0
  1     4 1000
```

compute testing error (in %)

```
In [37]: (sum(pred != t_true)/length(t_true))
```

0.002

In a real setting we should also optimize the value of C, again with CV; all this can be done very conveniently using tune() to do automatic grid-search (very much as we did in the last laboratory for nnet())

other packages provide with heuristic methods to estimate the gamma in the RBF kernel (see below)

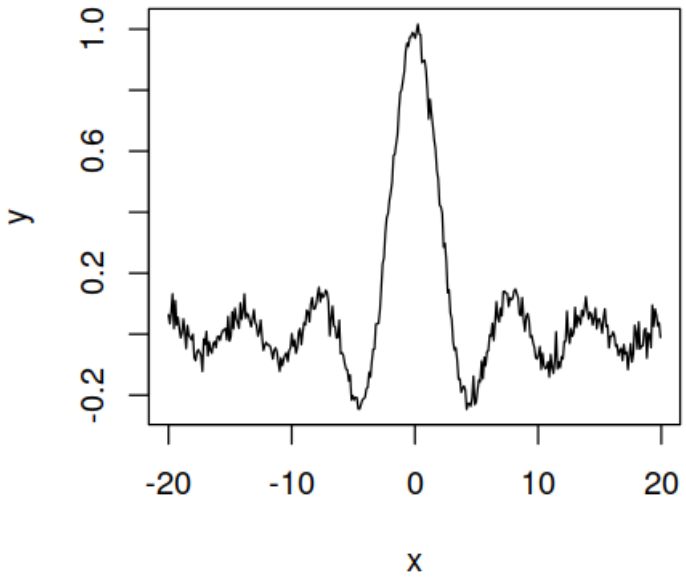
1.2 Playing with the SVM for regression and 1D data

Now we do regression; we have an extra parameter: the 'epsilon', which controls the width of the epsilon-insensitive tube (in feature space)

```
In [38]: A <- 20
```

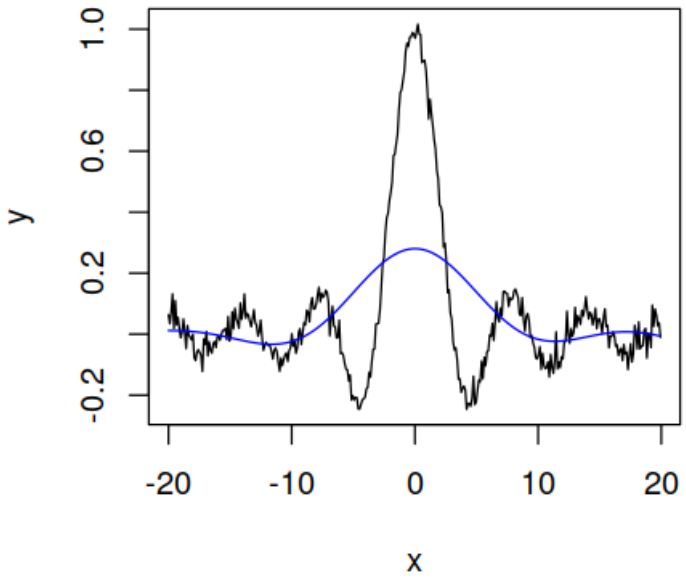
a really nice-looking function

```
In [39]: x <- seq(-A,A,by=0.11)
         y <- sin(x)/x + rnorm(x,sd=0.03)

         plot(x,y,type="l")
```



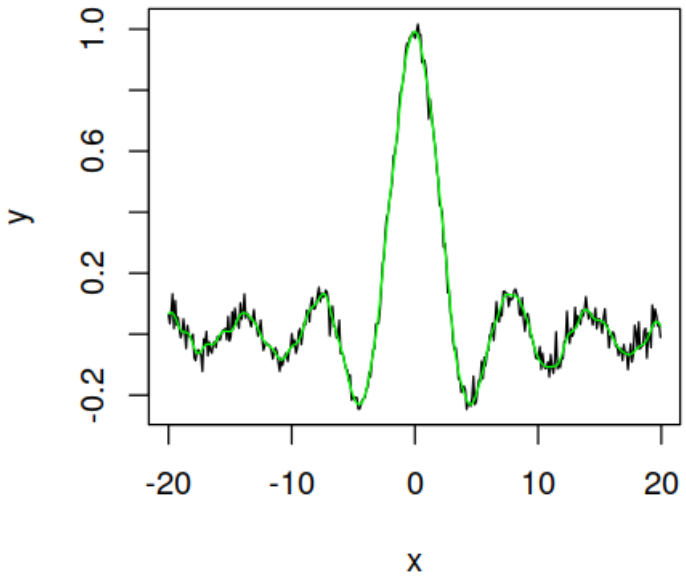
With this choice of the 'epsilon', 'gamma' and C parameters, the SVM underfits the data (blue line)

```
In [40]: model1 <- svm (x,y,epsilon=0.01)
         plot(x,y,type="l")
         lines(x,predict(model1,x),col="blue")
```



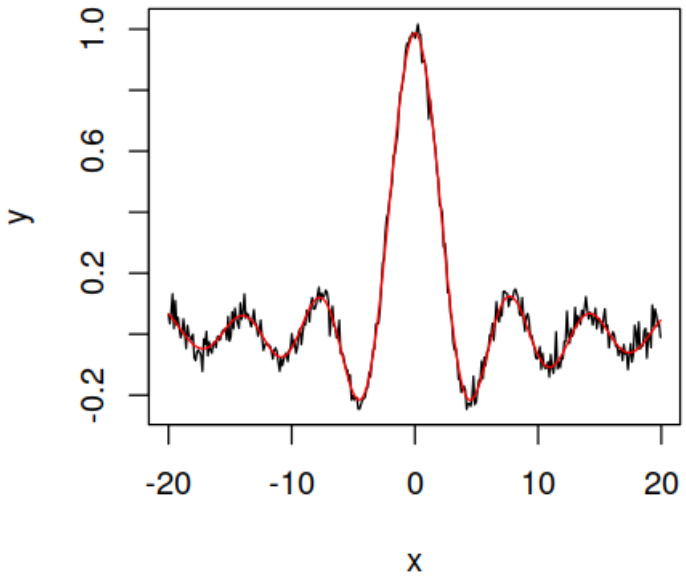
With this choice of the 'epsilon', 'gamma' and C parameters, the SVM overfits the data (green line)

```
In [41]: model2 <- svm (x,y,epsilon=0.01,gamma=200, C=100)
         plot(x,y,type="l")
         lines(x,predict(model2,x),col="green")
```



With this choice of the 'epsilon', 'gamma' and C parameters, the SVM has a very decent fit (red line)

```
In [42]: model3 <- svm (x,y,epsilon=0.01,gamma=10)
         plot(x,y,type="l")
         lines(x,predict(model3,x),col="red")
```



the other nice package where the SVM is located is {kernlab}

```
In [43]: library(kernlab)
```

the ksvm() method has some nice features, as creation of user-defined kernels (not seen in this course) and automatic cross-validation (via the 'cross' parameter)