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Ruoqing Zhu

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Support Vector Machines

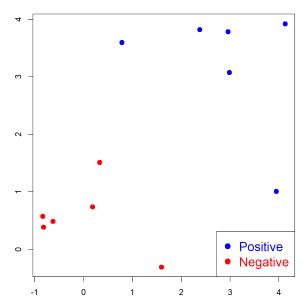
Support Vector Machine (SVM) is one of the most popular classification models. The original SVM was proposed by Vladimir Vapnik and Alexey Chervonenkis in 1963. Then two important improvements was developed in the 90's: the soft margin version Cortes and Vapnik (1995) and the nonlinear SVM using the kernel trick Boser, Guyon and Vapnik (1992). We will start with the hard margin version, and then introduce all other techniques.

Maximum-margin Classifier

This is the original SVM proposed in 1963. It shares similarities with the perception algorithm, but in certain sense is a stable version. We observe the training data $\Box_n = \{\mathbf{x}_i, y_i\}_{i=1}^n$, where we code y_i as a binary outcome from $\{-1, 1\}$. The advantages of using this coding instead of 0/1 will be seen later. The goal is to find a linear classification rule $f(\mathbf{x}) = \beta_0 + \mathbf{x}^T \boldsymbol{\beta}$ such that the classification rule is the sign of $f(\mathbf{x})$:

$$\hat{y} = \begin{cases} +1, & \text{if } f(\mathbf{x}) > 0 \\ -1, & \text{if } f(\mathbf{x}) < 0 \end{cases}$$

Hence, a correct classification would satisfy $y_i f(\mathbf{x}_i) > 0$. Let's look at the following example of data from two classes.



There are many linear lines that can perfectly separate the two classes. But which is better? The SVM defines this as the line that maximizes the margin, which can be seen in the following.

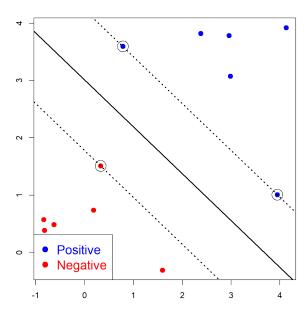
We use the e1071 package to fit the SVM. There is a cost parameter C, with default value 1. This parameter has a significant impact on non-separable problems. However, for this **separable case**, we should set this to be a very large value, meaning that the cost for having a wrong classification is very large. We also need to specify the linear kernel.

The following code can recover the fitted linear separation margin. Note here that the points on the margins are the ones with $\alpha_i > 0$ (details will be introduced later):

- index gives the index of all support vectors
- coefs provides the $y_i \alpha_i$ for the support vectors

- SV are the x_i values correspond to the support vectors
- rho is negative β_0

Hide



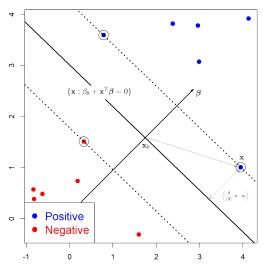
As we can see, the separation line is trying to have the maximum distance from both classes. This is why it is called the **Maximum-margin Classifier**.

Linearly Separable SVM

In linearly SVM, $f(\mathbf{x}) = \beta_0 + \mathbf{x}^T \boldsymbol{\beta}$. When $f(\mathbf{x}) = 0$, it corresponds to a hyperplane that separates the two classes:

$$\{\mathbf{x}: \boldsymbol{\beta}_0 + \mathbf{x}^{\mathrm{T}}\boldsymbol{\beta} = 0\}$$

Hence, for this separable case, all observations with $y_i = 1$ are on one side $f(\mathbf{x}) > 0$, and observations with $y_i = -1$ are on the other side.



First, let's calculate the **distance from any point** \mathbf{x} **to this hyperplane**. We can first find a point \mathbf{x}_0 on the hyperplane, such that $\mathbf{x}_0^T \boldsymbol{\beta} = -\beta_0$. By taking the difference between \mathbf{x} and \mathbf{x}_0 , and project this vector to the direction of $\boldsymbol{\beta}$, we have that the distance from \mathbf{x} to the hyperplane is the projection of $\mathbf{x} - \mathbf{x}_0$ onto the normed vector $\frac{\boldsymbol{\beta}}{\|\boldsymbol{\beta}\|}$:

$$\left\langle \frac{\beta}{\|\beta\|}, \mathbf{x} - \mathbf{x}_0 \right\rangle$$

$$= \frac{1}{\|\beta\|} (\mathbf{x} - \mathbf{x}_0)^{\mathrm{T}} \boldsymbol{\beta}$$

$$= \frac{1}{\|\beta\|} (\mathbf{x}^{\mathrm{T}} \boldsymbol{\beta} + \beta_0)$$

$$= \frac{1}{\|\beta\|} f(\mathbf{x})$$

Since the goal of SVM is to create the maximum margin, let's denote this as M. Then we want all observations to be lied on the correct side, with at least an margin M. This means $y_i(\mathbf{x}_i^T\boldsymbol{\beta}+\beta_0)\geq M$. But the scale of $\boldsymbol{\beta}$ is also playing a role in calculating the margin. Hence, we will use the normed version. Then, the linearly separable SVM is to solve this constrained optimization problem:

$$\label{eq:max_beta_0} \begin{aligned} & \max_{\pmb{\beta}, \beta_0} & M \\ & \text{subject to} & & \frac{1}{\|\pmb{\beta}\|} y_i(\mathbf{x}^\mathsf{T} \pmb{\beta} + \beta_0) \geq M, \ i = 1, \dots, n. \end{aligned}$$

Note that the scale of β can be arbitrary, let's set it as $\|\beta\| = 1/M$. The maximization becomes minimization, and its equivalent to minimizing $\frac{1}{2}\|\beta\|^2$. Then we have the **primal form** of the SVM optimization problem.

min
$$\frac{1}{2} \|\boldsymbol{\beta}\|^2$$

subject to $y_i(\mathbf{x}^T \boldsymbol{\beta} + \beta_0) \ge 1, \ i = 1, ..., n.$

From Primal to Dual

This is a general inequality constrained optimization problem.

min
$$g(\theta)$$

subject to $h(\theta) \le 0, i = 1, ..., n$.

We can consider the corresponding Lagrangian (with all α_i 's positive):

$$\Box(\boldsymbol{\theta}, \boldsymbol{\alpha}) = g(\boldsymbol{\theta}) + \sum_{i=1}^{n} \alpha_i h_i(\boldsymbol{\theta})$$

Then there can be two ways to optimize this. If we maximize α_i 's first, for any fixed θ , then for any θ that violates the constraint, i.e., $h_i(\theta) > 0$ for some i, we can always choose an extremely large α_i so that $\square(\theta, \alpha)$ is infinity. Hence the solution of this **primal form** must satisfy the constraint.

$$\min_{\theta} \max_{\alpha \geq 0} \Box(\theta, \alpha)$$

On the other hand, if we minimize θ first, then maximize for α , we have the **dual form**:

$$\max_{\alpha \geq 0} \min_{\theta} \Box(\theta, \alpha)$$

In general, the two are not the same:

$$\max_{\alpha \geq 0} \min_{\theta} \Box(\theta, \alpha) \leq \min_{\substack{\theta \quad \alpha \geq 0 \\ \text{duel}}} \max_{\theta \quad \alpha \geq 0} \Box(\theta, \alpha)$$

But a sufficient condition is that if both g and h_i 's are convex and also the constraints h_i 's are feasible. We will use this technique to solve the SVM problem.

First, rewrite the problem as

min
$$\frac{1}{2} \|\boldsymbol{\beta}\|^2$$

subject to $-\{y_i(\mathbf{x}^T\boldsymbol{\beta} + \beta_0) - 1\} \le 0, i = 1, \dots, n.$

Then the Lagrangian is

$$\square(\boldsymbol{\beta}, \beta_0, \boldsymbol{\alpha}) = \frac{1}{2} \|\boldsymbol{\beta}\|^2 - \sum_{i=1}^n \alpha_i \left\{ y_i(\mathbf{x}_i^{\mathsf{T}} \boldsymbol{\beta} + \beta_0) - 1 \right\}$$

To solve this using the dual form, we first find the optimizer of β and β_0 . We take derivatives with respect to them:

$$\boldsymbol{\beta} - \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i = 0 \quad (\nabla_{\boldsymbol{\beta}} \square = 0)$$
$$\sum_{i=1}^{n} \alpha_i y_i = 0 \quad (\nabla_{\beta_0} \square = 0)$$

Take these solution and plug them back into the Lagrangian, we have

$$\Box(\boldsymbol{\beta}, \beta_0, \boldsymbol{\alpha}) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n y_i y_j \alpha_i \alpha_j \mathbf{x}_i^{\mathrm{T}} \mathbf{x}_j$$

Hence, the dual optimization problem is

$$\max_{\alpha} \sum_{i=1}^{n} \alpha_{i} - \frac{1}{2} \sum_{i,j=1}^{n} y_{i} y_{j} \alpha_{i} \alpha_{j} \mathbf{x}_{i}^{\mathrm{T}} \mathbf{x}_{j}$$
subject to
$$\alpha_{i} \geq 0, \ i = 1, \dots, n.$$

$$\sum_{i=1}^{n} \alpha_{i} y_{i} = 0$$

Compared with the original primal form, this version has a trivial feasible solution with all α_i 's being 0. One can start from this solution to search for the optimizer while maintaining within the contained region. However, the primal form is difficult since there is no apparent way to satisfy the constraint.

After solving the dual form, we have all the α_i values. The ones with $\alpha_i > 0$ are called the support vectors. Based on our previous analysis, $\widehat{\beta} = \sum_{i=1}^n \alpha_i y_i x_i$, and we can also obtain β_0 by calculating the midpoint of two "closest" support vectors to the separating hyperplane:

$$\widehat{\boldsymbol{\beta}}_0 = - \frac{\max_{i:y_i = -1} \mathbf{x}_i^{\mathrm{T}} \widehat{\boldsymbol{\beta}} + \min_{i:y_i = 1} \mathbf{x}_i^{\mathrm{T}} \widehat{\boldsymbol{\beta}}}{2}$$

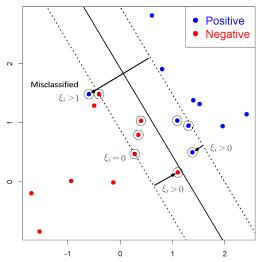
And the decision is $sign(\mathbf{x}^T \widehat{\boldsymbol{\beta}} + \widehat{\boldsymbol{\beta}}_0)$. An example has been demonstrated previously with the e1071 package.

Linearly Non-separable SVM with Slack Variables

When we cannot have a perfect separation of the two classes, the original SVM cannot find a solution. Hence, a slack was introduce to incorporate such observations:

$$y_i(\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\beta} + \beta_0) \ge (1 - \xi_i)$$

for a positive ξ . Note that when $\xi=0$, the observation is lying at the correct side, with enough margin. When $1>\xi>0$, the observation is lying at the correct side, but the margin is not sufficiently large. When $\xi>1$, the observation is lying on the wrong side of the separation hyperplane.



This new optimization problem can be formulated as

$$\min \quad \frac{1}{2} \|\boldsymbol{\beta}\|^2 + C \sum_{i=1}^n \xi_i$$

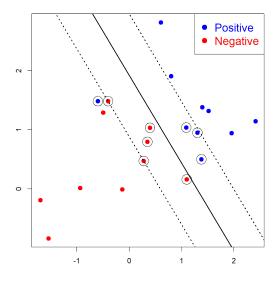
subject to $y_i(\mathbf{x}_i^{\mathsf{T}} \boldsymbol{\beta} + \beta_0) \ge (1 - \xi_i), \ i = 1, \dots, n,$
and $\xi_i \ge 0, \ i = 1, \dots, n,$

where C is a tuning parameter that controls the emphasis on the slack variable. Large C will be less tolerable on having positive slacks. We can again write the Lagrangian and convert that to the dual form. Details can be found at our SMLR textbook (https://teazrq.github.io/SMLR/support-vector-machines.html#linearly-non-separable-svm-with-slack-variables). The dual form is given by

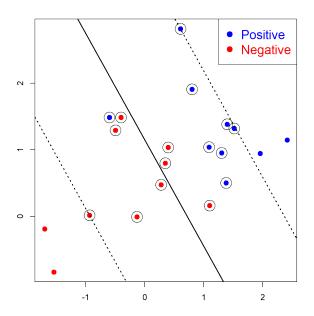
$$\max_{\alpha} \sum_{i=1}^{n} \alpha_{i} - \frac{1}{2} \sum_{i,j=1}^{n} y_{i} y_{j} \alpha_{i} \alpha_{j} \langle \mathbf{x}_{i}, \mathbf{x}_{j} \rangle$$
subject to $0 \le \alpha_{i} \le C, i = 1, ..., n,$
and $\sum_{i=1}^{n} \alpha_{i} y_{i} = 0.$

Here, the inner product $\langle \mathbf{x}_i, \mathbf{x}_j \rangle$ is nothing but $\mathbf{x}_i^T \mathbf{x}_j$. The observations with $0 < \alpha_i < C$ are the that lie on the margin. Hence, we can obtain these observations and perform the same calculations as before to obtain $\hat{\boldsymbol{\beta}}_0$. The following code generates some data for this situation and fit SVM. We use the default C=1.

```
set.seed(70)
n <- 10 # number of data points for each class
p <- 2 # dimension
# Generate the positive and negative examples
xneg <- matrix(rnorm(n*p,mean=0,sd=1),n,p)</pre>
xpos <- matrix(rnorm(n*p,mean=1.5,sd=1),n,p)</pre>
x <- rbind(xpos,xneg)</pre>
y <- matrix(as.factor(c(rep(1,n),rep(-1,n))))</pre>
# Visualize the data
plot(x,col=ifelse(y>0,"blue","red"), pch = 19, cex = 1.2, lwd = 2,
     xlab = "X1", ylab = "X2", cex.lab = 1.5)
legend("topright", c("Positive","Negative"),col=c("blue","red"),
       pch=c(19, 19),text.col=c("blue","red"), cex = 1.5)
svm.fit <- svm(y \sim ., data = data.frame(x, y), type='C-classification',
               kernel='linear',scale=FALSE, cost = 1)
b <- t(svm.fit$coefs) %*% svm.fit$SV
b0 <- -svm.fit$rho
points(x[svm.fit$index, ], col="black", cex=3)
abline(a= -b0/b[1,2], b=-b[1,1]/b[1,2], col="black", lty=1, lwd = 2)
abline(a= (-b0-1)/b[1,2], b=-b[1,1]/b[1,2], col="black", lty=3, lwd = 2)
abline(a= (-b0+1)/b[1,2], b=-b[1,1]/b[1,2], col="black", lty=3, lwd = 2)
```



If we instead use a smaller *C*:



Example: SAheart Data

If you want to use the 1071e package and perform cross-validation, you could consider using the caret package. Make sure that you specify method = "svmLinear2" so that 1071e is used. The following code is using the SAheart as an example.

```
library(ElemStatLearn)
  data(SAheart)
  library(caret)
## Loading required package: ggplot2
## Loading required package: lattice
  cost.grid = expand.grid(cost = seq(0.01, 2, length = 20))
  train_control = trainControl(method="repeatedcv", number=10, repeats=3)
  svm2 <- train(as.factor(chd) ~., data = SAheart, method = "svmLinear2",</pre>
               trControl = train_control,
               tuneGrid = cost.grid)
  # see the fitted model
  svm2
## Support Vector Machines with Linear Kernel
##
## 462 samples
    9 predictor
##
    2 classes: '0', '1'
##
##
## No pre-processing
## Resampling: Cross-Validated (10 fold, repeated 3 times)
## Summary of sample sizes: 416, 416, 416, 416, 416, ...
## Resampling results across tuning parameters:
##
##
    cost Accuracy Kappa
    0.0100000 0.7142923 0.2844994
##
   0.1147368 0.7200123 0.3520308
##
##
   0.2194737 0.7164354 0.3454492
    0.3242105 0.7171600 0.3467866
##
##
   0.4289474 0.7164354 0.3453015
##
    0.5336842 0.7164354 0.3450704
    0.6384211 0.7157108 0.3438517
##
##
    0.7431579 0.7171600 0.3472755
    0.8478947 0.7157108 0.3437850
##
##
    0.9526316 0.7157108 0.3437850
    1.0573684 0.7171600 0.3479914
##
##
    1.1621053 0.7164354 0.3459484
##
    1.2668421 0.7164354 0.3459484
##
    1.3715789 0.7178847 0.3500130
    1.4763158 0.7171600 0.3479914
##
    1.5810526 0.7178847 0.3500130
##
    1.6857895 0.7171600 0.3479914
##
    1.7905263 0.7171600 0.3479914
##
    1.8952632 0.7171600 0.3479914
##
##
    2.0000000 0.7164354 0.3459484
## Accuracy was used to select the optimal model using the largest value.
## The final value used for the model was cost = 0.1147368.
```

Note that when you fit the model, there are a few things you could consider:

- You can consider centering and scaling the covariates. This can be done during pre-processing. Or you may specify preProcess = c("center", "scale") in the train() function.
- You may want to start with a wider range of cost values, then narrow down to a smaller range, since SVM can be quite sensitive to tuning in some cases.
- There are many other SVM libraries, such as kernlab. This can be specified by using method = "svmLinear". However, kernlab uses C as the parameter name for cost. We will show an example later.

Nonlinear SVM via Kernel Trick

The essential idea of kernel trick can be summarized as using the kernel function of two observations \mathbf{x} and \mathbf{z} to replace the inner product between some feature mapping of the two covariate vectors. In other words, if we want to create some nonlinear features of \mathbf{x} , such as x_1^2 , $\exp(x_2)$, $\sqrt{x_3}$, etc., we may in general write them as

$$\Phi: \square \rightarrow \square, \ \Phi(\mathbf{x}) = (\phi_1(\mathbf{x}), \phi_2(\mathbf{x}), \ldots),$$

where \Box has either finite or infinite dimensions. Then, we can still treat this as a linear SVM by constructing the decision rule as

$$f(\mathbf{x}) = \langle \Phi(\mathbf{x}), \boldsymbol{\beta} \rangle = \Phi(\mathbf{x})^{\mathrm{T}} \boldsymbol{\beta}.$$

This is why we used the $\langle \cdot, \cdot \rangle$ operator in the previous example. Now, the kernel trick is essentially skipping the explicit calculation of $\Phi(\mathbf{x})$ by utilizing the property that

$$K(\mathbf{x}, \mathbf{z}) = \langle \Phi(\mathbf{x}), \Phi(\mathbf{z}) \rangle$$

for some kernel function $K(\mathbf{x}, \mathbf{z})$. Since $\langle \Phi(\mathbf{x}), \Phi(\mathbf{z}) \rangle$ is all we need in the dual form, we can simply replace it by $K(\mathbf{x}, \mathbf{z})$, which gives the kernel form:

$$\max_{\alpha} \sum_{i=1}^{n} \alpha_{i} - \frac{1}{2} \sum_{i,j=1}^{n} y_{i} y_{j} \alpha_{i} \alpha_{j} K(\mathbf{x}_{i}, \mathbf{x}_{j})$$
subject to $0 \le \alpha_{i} \le C, i = 1, ..., n,$
and
$$\sum_{i=1}^{n} \alpha_{i} y_{i} = 0.$$

One most apparent advantage of doing this is to save computational cost. This maybe understood using the following example:

- Consider kernel function $K(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^T \mathbf{z})^2$
- Consider $\Phi(\mathbf{x})$ being the basis expansion that contains all second order interactions: $x_k x_l$ for $1 \le k, l \le p$

We can show that the two gives equivalent results, however, the kernel version is much faster. $K(\mathbf{x}, \mathbf{z})$ takes p+1 operations, while $\langle \Phi(\mathbf{x}_i), \Phi(\mathbf{x}_i) \rangle$ requires $3p^2$.

$$K(\mathbf{x}, \mathbf{z}) = \left(\sum_{k=1}^{p} x_k z_k\right) \left(\sum_{l=1}^{p} x_l z_l\right)$$

$$= \sum_{k=1}^{p} \sum_{l=1}^{p} x_k z_k x_l z_l$$

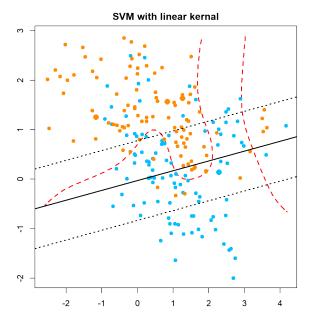
$$= \sum_{k,l=1}^{p} (x_k x_l) (z_k z_l)$$

$$= \langle \Phi(\mathbf{x}), \Phi(\mathbf{z}) \rangle$$

Example: mixture.example Data

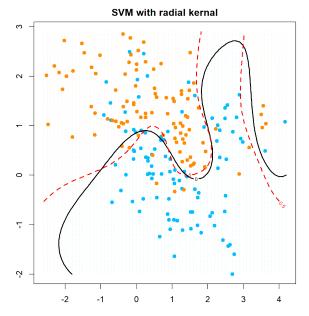
We use the mixture.example data in the ElemStatLearn package. In addition, we use a different package kernlab. The red dotted line indicates the true decision boundary.

```
library(ElemStatLearn)
    data(mixture.example)
    # redefine data
    px1 = mixture.example$px1
    px2 = mixture.example$px2
    x = mixture.example$x
    y = mixture.example$y
    # plot the data and true decision boundary
    prob <- mixture.example$prob</pre>
    prob.bayes <- matrix(prob,</pre>
                          length(px1),
                          length(px2))
    contour(px1, px2, prob.bayes, levels=0.5, lty=2,
            labels="", xlab="x1",ylab="x2",
            main="SVM with linear kernal", col = "red", lwd = 2)
    points(x, col=ifelse(y==1, "darkorange", "deepskyblue"), pch = 19)
    # train linear SVM using the kernlab package
    library(kernlab)
    cost = 10
    svm.fit <- ksvm(x, y, type="C-svc", kernel='vanilladot', C=cost)</pre>
## Setting default kernel parameters
    # plot the SVM decision boundary
    # Extract the indices of the support vectors on the margin:
    sv.alpha<-alpha(svm.fit)[[1]][which(alpha(svm.fit)[[1]]<cost)]</pre>
    sv.index<-alphaindex(svm.fit)[[1]][which(alpha(svm.fit)[[1]]<cost)]</pre>
    sv.matrix<-x[sv.index,]</pre>
    points(sv.matrix, pch=16, col=ifelse(y[sv.index] == 1, "darkorange", "deepskybl
ue"), cex=1.5)
    # Plot the hyperplane and the margins:
    w <- t(cbind(coef(svm.fit)[[1]])) %*% xmatrix(svm.fit)[[1]]</pre>
    b <- - b(svm.fit)
    abline(a= -b/w[1,2], b=-w[1,1]/w[1,2], col="black", lty=1, lwd = 2)
    abline(a= (-b-1)/w[1,2], b=-w[1,1]/w[1,2], col="black", lty=3, lwd = 2)
    abline(a= (-b+1)/w[1,2], b=-w[1,1]/w[1,2], col="black", lty=3, lwd = 2)
```



Let's also try a nonlinear SVM, using the radial kernel.

```
# fit SVM with radial kernel, with cost = 5
dat = data.frame(y = factor(y), x)
fit = svm(y \sim ., data = dat, scale = FALSE, kernel = "radial", cost = 5)
# extract the prediction
xgrid = expand.grid(X1 = px1, X2 = px2)
func = predict(fit, xgrid, decision.values = TRUE)
func = attributes(func)$decision
# visualize the decision rule
ygrid = predict(fit, xgrid)
plot(xgrid, col = ifelse(ygrid == 1, "bisque", "cadetblue1"),
     pch = 20, cex = 0.2, main="SVM with radial kernal")
points(x, col=ifelse(y==1, "darkorange", "deepskyblue"), pch = 19)
# our estimated function value, cut at 0
contour(px1, px2, matrix(func, 69, 99), level = 0, add = TRUE, lwd = 2)
# the true probability, cut at 0.5
contour(px1, px2, matrix(prob, 69, 99), level = 0.5, add = TRUE,
        col = "red", lty=2, lwd = 2)
```



You may also consider some other popular kernels. The following ones are implemented in the e1071 package, with additional tuning parameters $coef_0$ and γ .

• Linear: $K(\mathbf{x}, \mathbf{z}) = \mathbf{x}^{\mathrm{T}} \mathbf{z}$

• dth degree polynomial: $K(\mathbf{x}, \mathbf{z}) = (\cos f_0 + \gamma \mathbf{x}^T \mathbf{z})^d$ • Radial basis: $K(\mathbf{x}, \mathbf{z}) = \exp(-\gamma \|\mathbf{x} - \mathbf{z}\|^2)$

• Sigmoid: $tanh(\gamma \mathbf{x}^T \mathbf{z} + coef_0)$

Cross-validation can also be doing using the caret package. To specify the kernel, one must correctly specify the method parameter in the train() function. For this example, we use the method = "svmRadial" that uses the kernlab package to fit the model. For this choice, you need to tune just sigma and C (cost). More details are refereed to the caret documentation (https://topepo.github.io/caret/train-models-by-tag.html#support-vector-machines).

```
svm.radial <- train(y ~ ., data = dat, method = "svmRadial",</pre>
                preProcess = c("center", "scale"),
                  tuneGrid = expand.grid(C = c(0.01, 0.1, 0.5, 1), sigma = c(1, 2, 1)
3)),
                trControl = trainControl(method = "cv", number = 5))
  svm.radial
## Support Vector Machines with Radial Basis Function Kernel
##
## 200 samples
##
     2 predictor
     2 classes: '0', '1'
##
##
## Pre-processing: centered (2), scaled (2)
## Resampling: Cross-Validated (5 fold)
## Summary of sample sizes: 160, 160, 160, 160, 160
## Resampling results across tuning parameters:
##
     С
           sigma Accuracy Kappa
##
     0.01 1
                  0.715
                            0.43
##
##
    0.01 2
                  0.760
                            0.52
##
     0.01 3
                  0.770
                            0.54
                            0.44
##
     0.10 1
                  0.720
##
     0.10 2
                  0.790
                            0.58
##
    0.10 3
                  0.800
                            0.60
    0.50 1
                  0.795
                            0.59
##
##
     0.50 2
                  0.815
                            0.63
##
    0.50 3
                  0.830
                            0.66
                  0.795
                            0.59
##
     1.00 1
     1.00 2
                  0.825
                            0.65
##
##
     1.00 3
                  0.835
                            0.67
##
## Accuracy was used to select the optimal model using the largest value.
## The final values used for the model were sigma = 3 and C = 1.
```