06. Support Vector Machines

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Support Vector Machines

- Here we approach the two-class classification problem in a direct way:
  - We try and find a plane that separates the classes in feature space.
- If we cannot, we get creative in two ways:
  - We soften what we mean by "separates", and
  - We enrich and enlarge the feature space so that separation is possible.
- Three methods
  - Maximal margin classifier
  - Support vector classifier (soft margin classifier)
  - Support vector machines

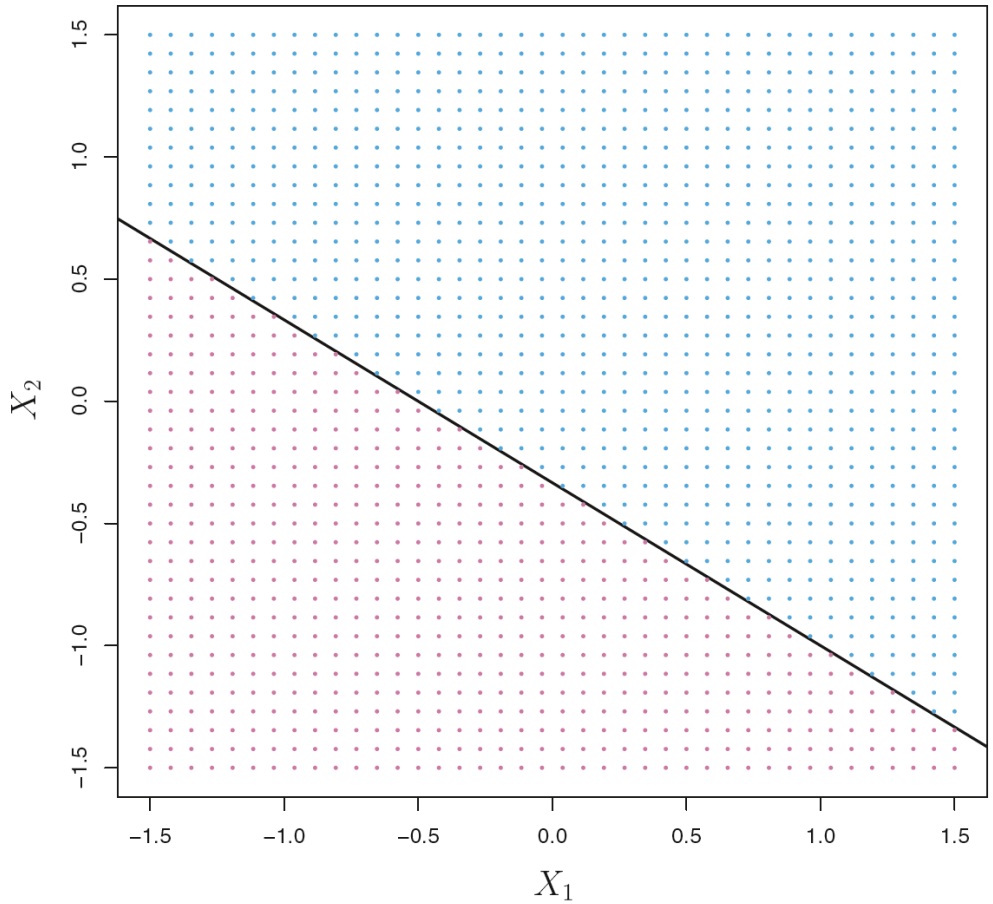
What is a Hyperplane?

- A hyperplane in p dimensions is a flat affine subspace of dimension $p - 1$.
- In general the equation for a hyperplane has the form

$$\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p = 0 \tag{1}$$

- If $X = (X_1, \ldots, X_p)^{\mathrm{T}}$ satisfies (1), then X lies on the hyperplane.
- If $X = (X_1, \ldots, X_p)^{\mathrm{T}}$ does not satisfy (1), then X lies to one side of the hyperplane.
- Which side of the hyperplane a point lies can be determined by calculating the sign of the L.H.S of (1).
- Note that a hyperplane is a line when $p = 2$.

Hyperplane in Two-dimensional Space



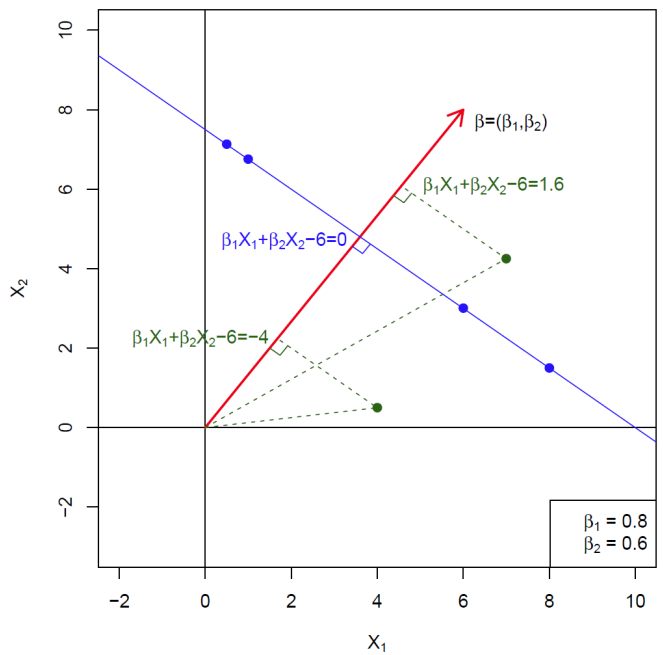
- The hyperplane $1 + 2X_1 + 3X_2 = 0$ is shown
  - Blue region : $1 + 2X_1 + 3X_2 > 0$
  - Purple region : $1 + 2X_1 + 3X_2 < 0$

Normal Vector of Hyperplane

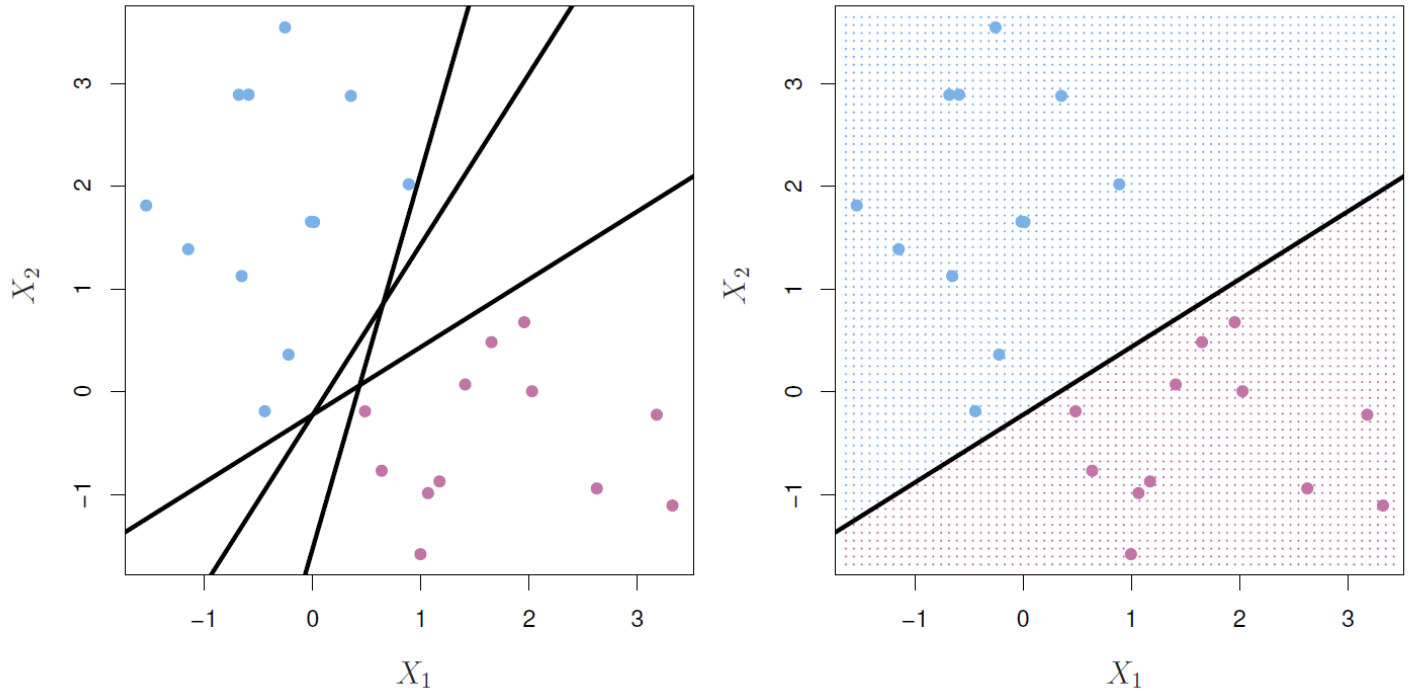
- $f(X)$ is a hyperplane in the p-dimensional feature space,

$$f(X) = \beta_0 + \boldsymbol{\beta}^{\mathrm{T}} X = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p = 0$$

- The vector $\boldsymbol{\beta} = (\beta_1, \beta_2, \ldots, \beta_p)^{\mathrm{T}}$ is called the normal vector
- It points in a direction orthogonal to the surface of a hyperplane.



Separating Hyperplanes



- If $f(X) = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p$, then $f(X) > 0$ for points on one side of the hyperplane, and $f(X) < 0$ for points on the other.
- If we code the colored points as $Y_i = 1$ for blue, and $Y_i = -1$ for pink, then if $Y_i \cdot f(X_i) > 0$ for all i, $f(X_i) = 0$ defines a separating hyperplane.

Separating Hyperplanes

- If a separating hyperplane exists, we can use it to construct a very natural classifier.
- For a test observation x^*,

$$f(x^*) = \beta_0 + \beta_1 x_1^* + \cdots + \beta_p x_p^*$$

  - If $f(x^*) > 0$, we assign the test observation to class 1
  - If $f(x^*) < 0$, we assign the test observation to class 2
- For the magnitude of $f(x^*)$,
  - If $|f(x^*)|$ is relatively large, the class assignment is confident.
  - If $|f(x^*)|$ is relatively small, the class assignment is less confident.

Maximal Margin Classifier

- The maximal margin hyperplane is the separating hyperplane that is farthest from the training observations.
  - Among all separating hyperplanes, find the one that makes the biggest gap or margin between the two classes.
- Constrained optimization problem:

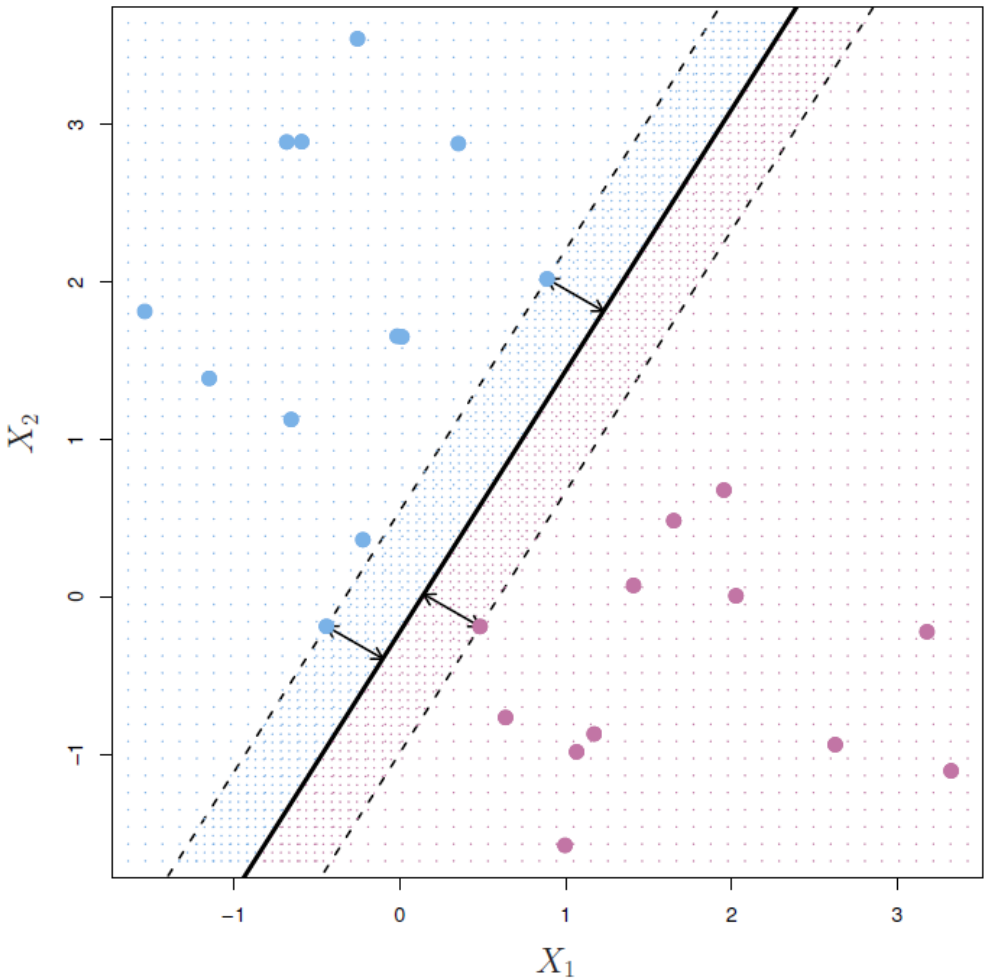
$$\underset{\beta_0,\beta_1,\ldots,\beta_p}{\text{maximize}}\, M \text{ subject to}$$

$$\sum_{j=1}^{p} \beta_j^2 = 1, \text{ and } y_i(\beta_0 + \beta_1 x_{i1} + \ldots + \beta_p x_{ip}) \geq M$$

for all $i = 1, 2, \ldots, n$.

- This can be rephrased as a convex quadratic program, and solved efficiently. The function `svm()` in an R package "`e1071`" solves this problem efficiently.

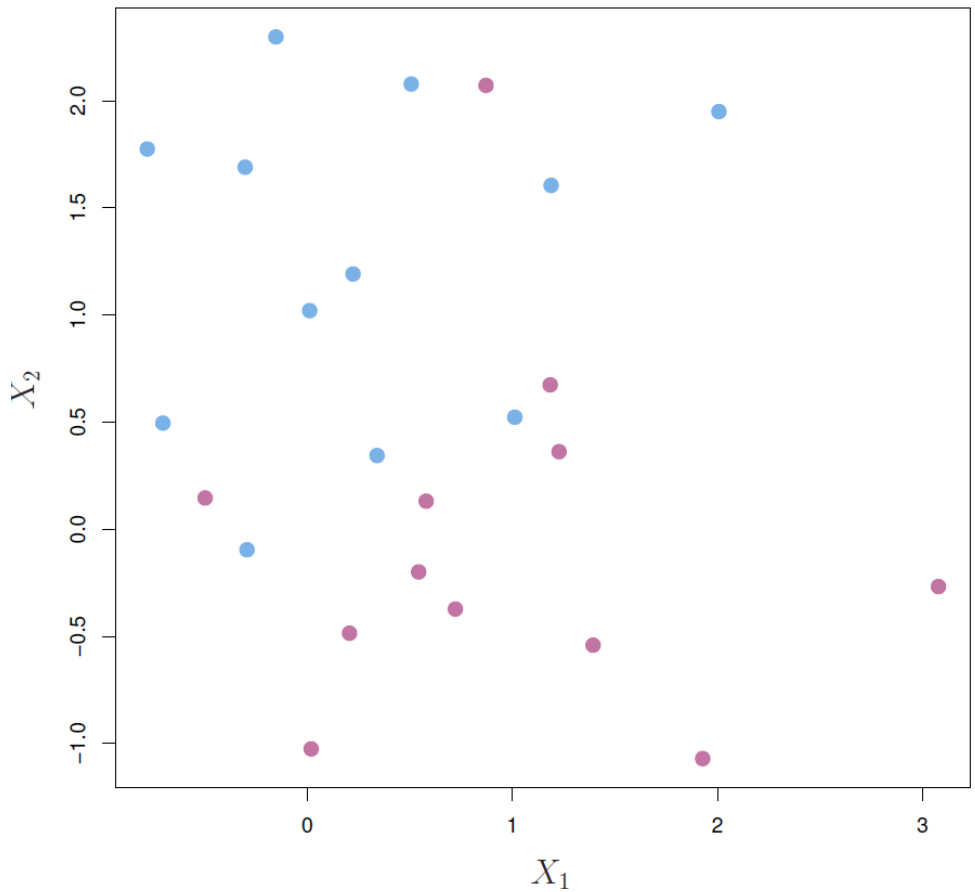
Maximal Margin Classifier



The Non-separable Case

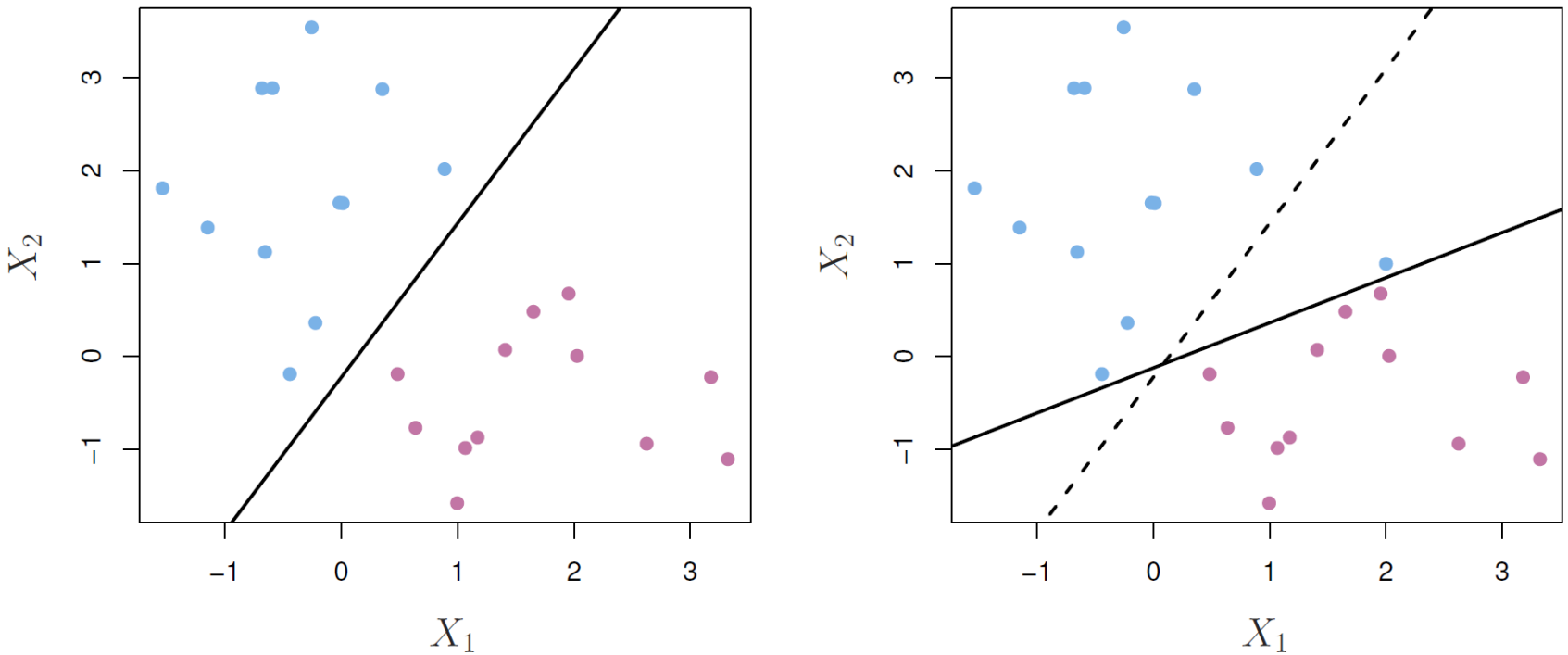
- The maximal margin classifier is a very natural way to perform classification, if a separating hyperplane exists.
- However, in many cases no separating hyperplane exists, and so there is no maximal margin classifier.
- If a separating hyperplane doesn't exist, there is no solution to M in the optimization problem.
- However, we can extend the concept of a separating hyperplane in order to develop a hyperplane that almost separates the classes, using a so-called soft margin.
- The generalization of the maximal margin classifier to the non-separable case is known as the support vector classifier.

Non-separable Data



- The data above are not separable by a linear boundary.
- This is often the case, unless $n < p$.

Separable but Noisy Data

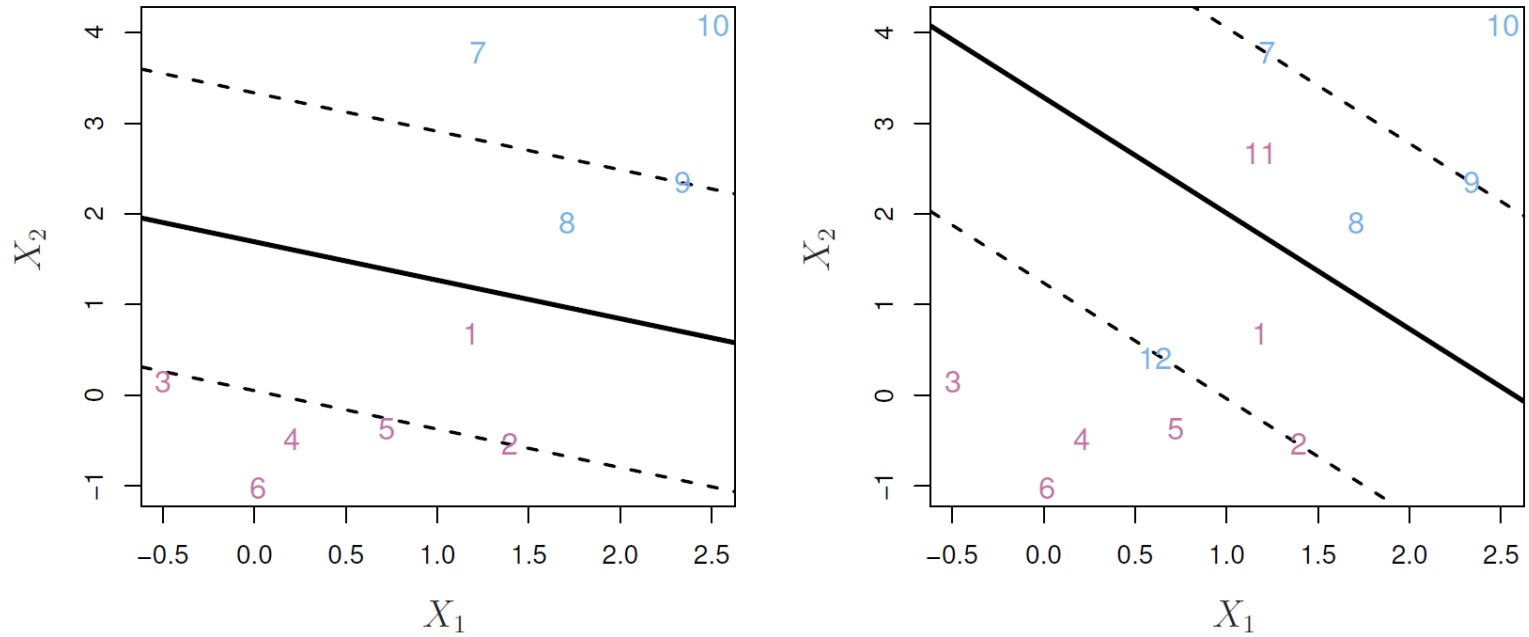


- Sometimes the data are separable, but noisy. This can lead to a poor solution for the maximal-margin classifier.
- The support vector classifier maximizes a soft margin.

Support Vector Classifier

- We need to consider a classifier based on a hyperplane that does not perfectly separate the two classes, in the interest of
  - Greater robustness to individual observations
  - Better classification of most of the training observations
- That is, it could be worthwhile to misclassify a few training observations in order to do a better job in classifying the remaining observations.
- The support vector classifier (soft margin classifier) allows some observations to be on the incorrect side of the margin, or even the incorrect side of the hyperplane.
- The margin is soft because it can be violated by some of the training observations.
- The support vector classifier classifies a test observation depending on which side of a hyperplane it lies.

Optimization of Support Vector Classifier

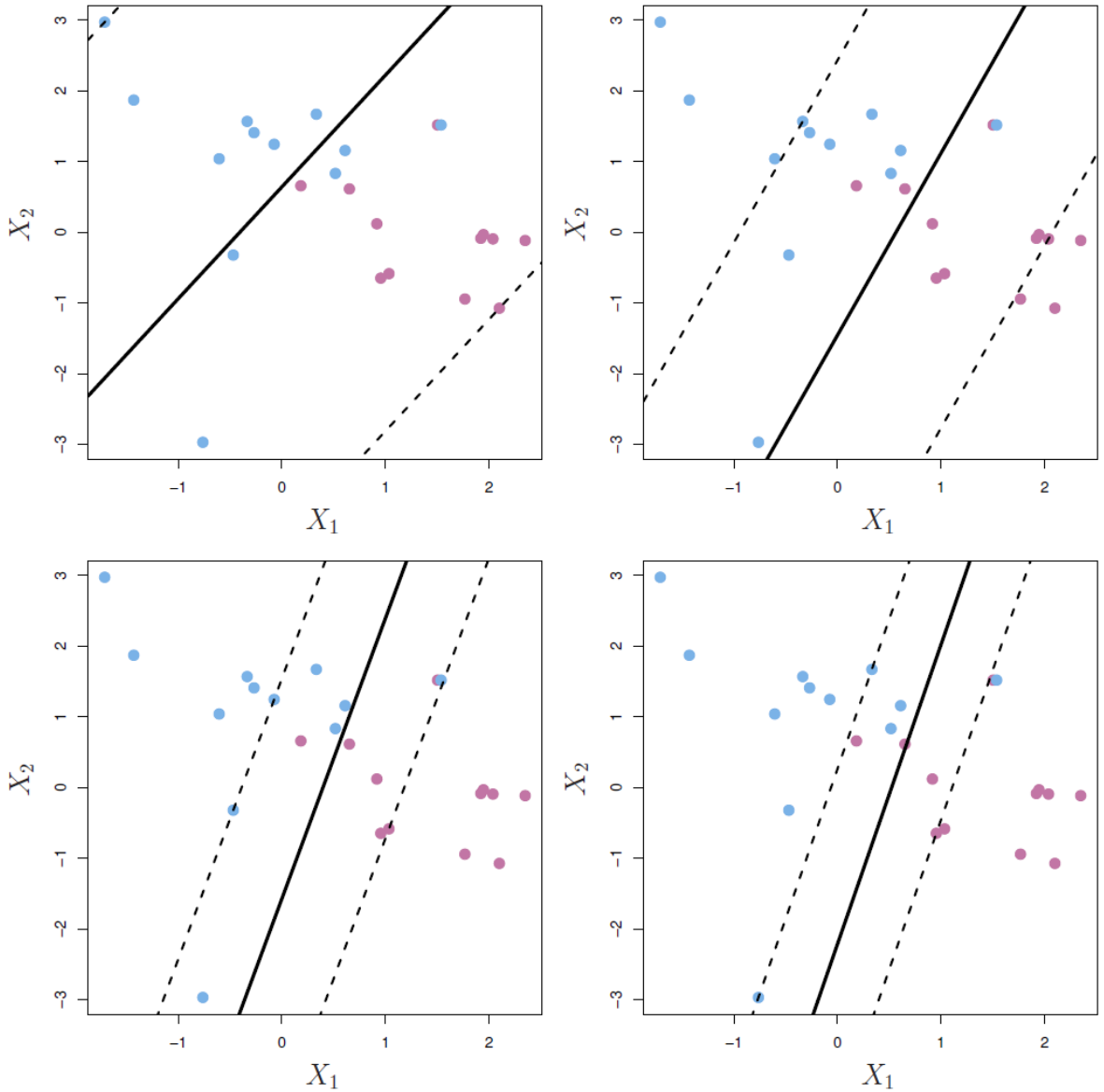


$$\underset{\beta_0,\beta_1,\ldots,\beta_p,\epsilon_1,\ldots,\epsilon_n}{\text{maximize}} \; M \text{ subject to } \sum_{j=1}^{p} \beta_j^2 = 1,$$

$$y_i(\beta_0 + \beta_1 x_{i1} + \ldots + \beta_p x_{ip}) \geq M(1 - \epsilon_i),$$

$$\epsilon_i \geq 0, \text{ and } \sum_{i=1}^{n} \epsilon_i \leq C, \text{ where } C > 0 \text{ is a tuning parameter.}$$

Support Vector Classifier



Margins and Slack Variables

- M is the width of the margin $-$ as large as possible.
- $\epsilon_1, \ldots, \epsilon_n$ are slack variables.
  - If $\epsilon_i = 0$, the ith obs. is on the correct side of the margin.
  - If $\epsilon_i > 0$, the ith obs. is on the wrong side of the margin.
  - If $\epsilon_i > 1$, the ith obs. is on the wrong side of the hyperplane.
- A regularization parameter C bounds the sum of the ϵ_i's
  - If C is small, we seek narrow margins that are rarely violated $-$ low bias but high variance.
  - If C is larger, the margin is wider and we allow more violations to it $-$ more bias but lower variance.
- Observations that lie directly on the margin, or on the wrong side of the margin for their class are known as support vectors.
- These observations do affect the support vector classifier.

```r
## Simple example (simulate data set)
set.seed(1)
x <- matrix(rnorm(20*2), ncol=2)
y <- c(rep(-1, 10), rep(1, 10))
x[y==1, ] <- x[y==1, ] + 1
plot(x, col=(3-y), pch=19, xlab="X1", ylab="X2")
```

```r
## Support vector classifier with cost=10
library(e1071)
dat <- data.frame(x, y=as.factor(y))
svmfit <- svm(y~., data=dat, kernel="linear", cost=10,
              scale=FALSE)
plot(svmfit, dat)
summary(svmfit)
```

```r
names(svmfit)
svmfit$index
svmfit$coefs
```

```r
## coefficient beta_0 (negative)
beta0 <- svmfit$rho
```

```
## coefficient beta_1 and beta_2
beta <- drop(t(svmfit$coefs)%*%x[svmfit$index,])
```

```
plot(x, col=(3-y), pch=19, xlab="X1", ylab="X2")
points(x[svmfit$index, ], pch=5, cex=2)
abline(beta0 / beta[2], -beta[1] / beta[2])
abline((beta0 - 1) / beta[2], -beta[1] / beta[2], lty = 2)
abline((beta0 + 1) / beta[2], -beta[1] / beta[2], lty = 2)
```

```
## Different value of tuning parameter (cost=0.1)
svmfit <- svm(y~., data=dat, kernel="linear", cost=0.1,
              scale=FALSE)
svmfit$index
beta <- drop(t(svmfit$coefs)%*%x[svmfit$index,])
beta0 <- svmfit$rho
```

```
plot(x, col=(3-y), pch=19, xlab="X1", ylab="X2")
points(x[svmfit$index, ], pch=5, cex=2)
abline(beta0 / beta[2], -beta[1] / beta[2])
abline((beta0 - 1) / beta[2], -beta[1] / beta[2], lty = 2)
abline((beta0 + 1) / beta[2], -beta[1] / beta[2], lty = 2)
```

```
## A function to create a grid of values or a lattice of values
make.grid <- function(x, n = 75) {
  ran <- apply(x, 2, range)
  x1 <- seq(from = ran[1,1], to = ran[2,1], length = n)
  x2 <- seq(from = ran[1,2], to = ran[2,2], length = n)
  expand.grid(X1 = x1, X2 = x2)
}
```

```
xgrid <- make.grid(x)
xgrid[1:76,]
```

```
## Classification of potential test set
ygrid <- predict(svmfit, xgrid)
plot(xgrid, col=c("red","blue")[as.numeric(ygrid)], pch=20,
     cex=.2)
points(x, col=y+3, pch=19)
points(x[svmfit$index, ], pch=5, cex=2)
```

```
## Cross validation to find the optimal tuning parameter (cost)
set.seed(1)
tune.out <- tune(svm, y~., data=dat, kernel="linear",
            ranges=list(cost=c(0.001, 0.01, 0.1, 1, 5, 10, 100)))
summary(tune.out)
bestmod <- tune.out$best.model
summary(bestmod)
```

```
## Generate test set
set.seed(4321)
xtest <- matrix(rnorm(20*2), ncol=2)
ytest <- sample(c(-1,1), 20, rep=TRUE)
xtest[ytest==1, ] <- xtest[ytest==1, ] + 1
testdat <- data.frame(xtest, y=as.factor(ytest))
```

```
## Compute misclassification rate for the optimal model
ypred <- predict(bestmod, testdat)
table(predict=ypred, truth=testdat$y)
mean(ypred!=testdat$y)
```

```
## Misclassification rate for other value of cost (cost=0.01)
svmfit <- svm(y~., data=dat, kernel="linear", cost=.01,
              scale=FALSE)
ypred <- predict(svmfit, testdat)
table(predict=ypred, truth=testdat$y)
mean(ypred!=testdat$y)
```

```
## Misclassification rate for other value of cost (cost=1)
svmfit <- svm(y~., data=dat, kernel="linear", cost=1,
              scale=FALSE)
ypred <- predict(svmfit, testdat)
table(predict=ypred, truth=testdat$y)
mean(ypred!=testdat$y)
```

```
## Misclassification rate for other value of cost (cost=100)
svmfit <- svm(y~., data=dat, kernel="linear", cost=100,
              scale=FALSE)
ypred <- predict(svmfit, testdat)
table(predict=ypred, truth=testdat$y)
mean(ypred!=testdat$y)
```

```
library(mnormt)
library(e1071)
```

```
## Misclassification Rate of SVC
SVC.MCR <- function(x.tran, x.test, y.tran, y.test,
                    cost=c(0.01,0.1,1,10,100)) {
    dat <- data.frame(x.tran, y=as.factor(y.tran))
    testdat <- data.frame(x.test, y=as.factor(y.test))
    MCR <- rep(0, length(cost)+1)
    for (i in 1:length(cost)) {
        svmfit <- svm(y~., data=dat, kernel="linear",
                      cost=cost[i])
        MCR[i] <- mean(predict(svmfit, testdat)!=testdat$y)
    }
    tune.out <- tune(svm, y~., data=dat, kernel="linear",
                ranges=list(cost=cost))
    pred <- predict(tune.out$best.model, testdat)
    MCR[length(cost)+1] <- mean(pred!=testdat$y)
MCR
}
```

```
set.seed(123)
K <- 100
RES <- matrix(NA, K, 6)
colnames(RES) <- c("0.01", "0.1" ,"1" , "10" ,"100", "CV")
```

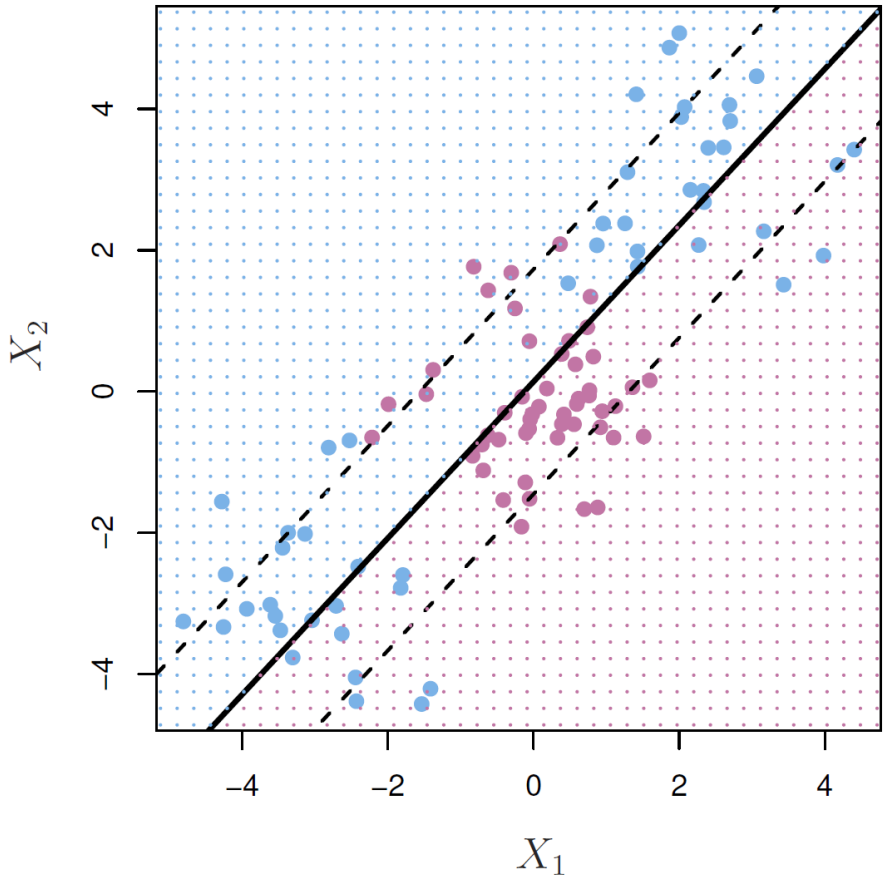
```
for (i in 1:K) {
    x.A <- rmnorm(100, rep(0, 2), matrix(c(1,-0.5,-0.5,1),2))
    x.B <- rmnorm(100, rep(1, 2), matrix(c(1,-0.5,-0.5,1),2))
    x.tran <- rbind(x.A[1:50, ], x.B[1:50, ])
    x.test <- rbind(x.A[-c(1:50), ], x.B[-c(1:50), ])
    y.tran <- factor(rep(0:1, each=50))
    y.test <- factor(rep(0:1, each=50))
    RES[i,] <- SVC.MCR(x.tran, x.test, y.tran, y.test)
}
```

```
apply(RES, 2, summary)
boxplot(RES, boxwex=0.5, col=2:7,
        names=c("0.01", "0.1", "1", "10", "100", "CV"),
        main="", ylab="Classification Error Rates")
```

Non-linear Decision Boundaries

- The support vector classifier is a natural approach for classification in the two-class setting, if the boundary between the two classes is linear.
- In practice, we can be faced with non-linear class boundaries.
- The performance of linear regression can suffer when there is a nonlinear relationship between the predictors and the outcome.
- We need to consider enlarging the feature space using functions of the predictors such as quadratic and cubic terms, in order to address this non-linearity.
- In the case of the support vector classifier, we can also enlarge the feature space using quadratic, cubic, and even higher-order polynomial functions of the predictors.

Failure of Linear Boundary



- Sometime a linear boundary simply won't work, no matter what value of C.
- The example above is such a case. What to do?

Feature Expansion

- Enlarge the space of features by including transformations;

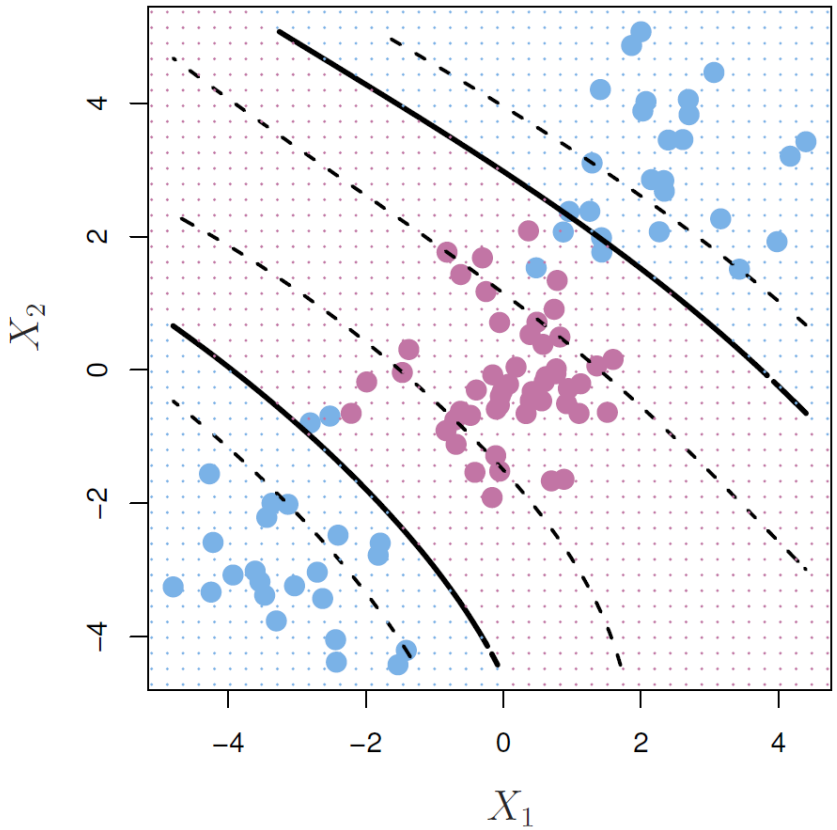
$$X_1^2, X_1^3, X_1X_2, X_1X_2^2, \ldots$$

  Hence, go from a p-dimensional space to a M-dimensional space ($M > p$).
- Fit a support-vector classifier in the enlarged space.
- This results in non-linear decision boundaries in the space.
- For example,

$$\beta_0 + \beta_1X_1 + \beta_2X_2 + \beta_3X_1^2 + \beta_4X_2^2 + \beta_5X_1X_2 = 0$$

  This leads to nonlinear decision boundaries in the original space (quadratic conic sections).

Cubic Polynomials



- Here we use a basis expansion of cubic polynomials.
- The support vector classifier in the enlarged space solves the problem in the lower-dimensional space.

Computational Issues for High-dimensional Polynomials

- Cubic polynomial is

$$\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1^2 + \beta_4 X_2^2 + \beta_5 X_1 X_2 + \\ \beta_6 X_1^3 + \beta_7 X_2^3 + \beta_8 X_1 X_2^2 + \beta_9 X_1^2 X_2 = 0$$

- However, high-dimensional polynomials get wild rather fast.
- There are many possible ways to enlarge the feature space, but computations would become unmanageable for a huge number of features .
- There is a more elegant and controlled way to introduce nonlinearities in support vector classifiers, using kernels.
- Before we discuss these, we must understand the role of inner products in support vector classifiers.

Inner Products

- Inner product between vectors

$$\langle x_i, x_{i'} \rangle = \sum_{j=1}^{p} x_{ij} x_{i'j}$$

- The linear support vector classifier can be represented as

$$f(x) = \beta_0 + \sum_{i=1}^{n} \alpha_i \langle x, x_i \rangle$$

- To estimate the parameters $\alpha_1, \ldots, \alpha_n$ and β_0, all we need are the $\binom{n}{2}$ inner products $\langle x_i, x_{i'} \rangle$ between all pairs of training observations.
- To evaluate $f(x)$, we need to compute the inner product between the new point x and each of the training points x_i.

Kernels and Support Vector Machines

- It turns out that most of the $\hat{\alpha}_i$ can be zero:

$$f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \hat{\alpha}_i \langle x, x_i \rangle$$

  $\mathcal{S}$ is the support set of indices i such that $\hat{\alpha}_i > 0$.
- A generalization of the inner product of the form $K(x_i, x_{i'})$ is called a kernel.
- A kernel is a function that quantifies the similarity of two observations.
- When the support vector classifier is combined with a non-linear kernel, the resulting classifier is known as a support vector machine.

$$f(x) = \beta_0 + \sum_{i \in \mathcal{S}} \hat{\alpha}_i K(x, x_i)$$

Examples of Kernels

- Standard linear kernel

$$K(x_i, x_{i'}) = \sum_{j=1}^{p} x_{ij} x_{i'j}$$

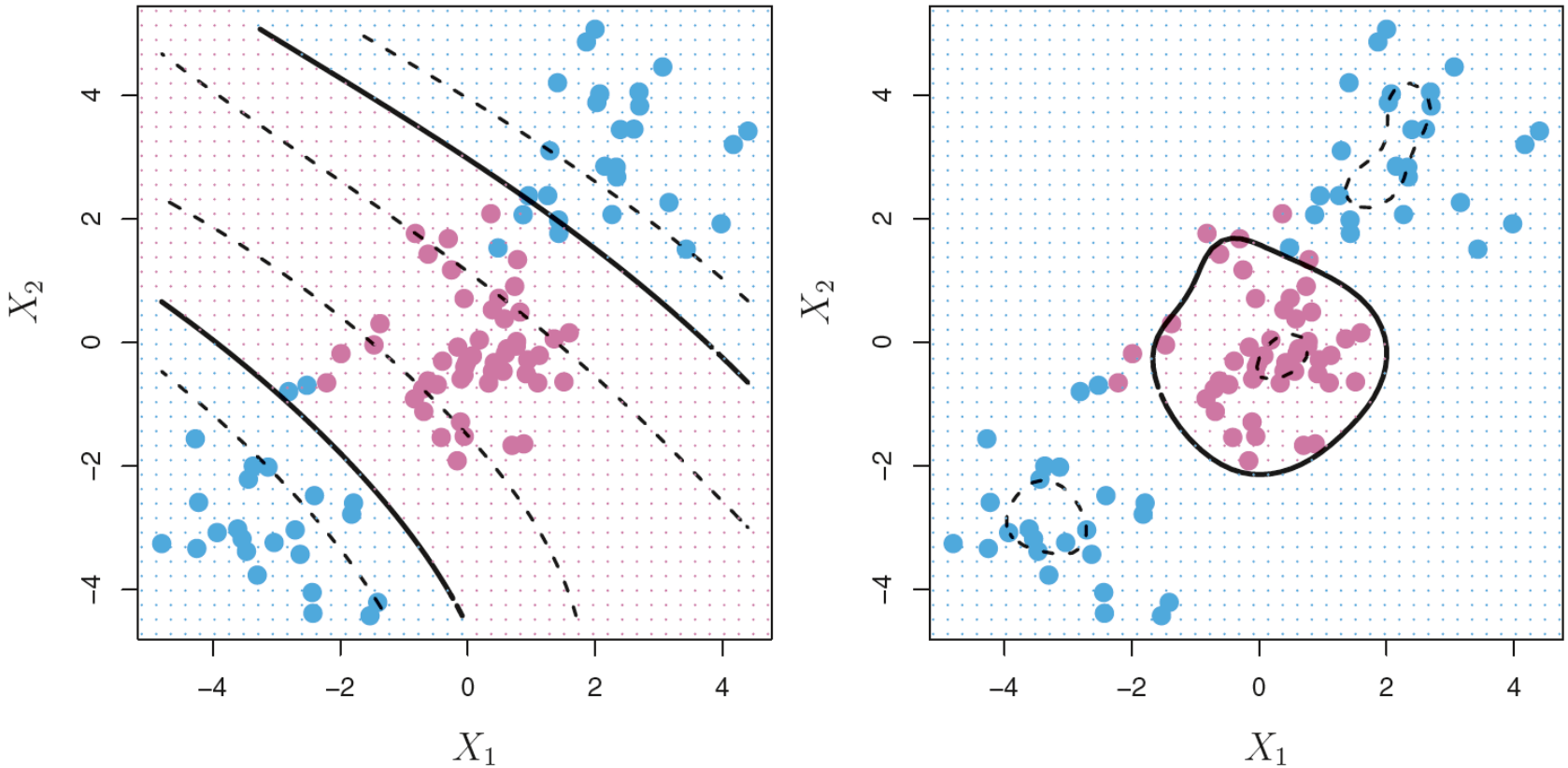
- Polynomial kernel of degree $d > 1$

$$K(x_i, x_{i'}) = \left(1 + \sum_{j=1}^{p} x_{ij} x_{i'j}\right)^d$$

- Radial kernel

$$K(x_i, x_{i'}) = \exp\left(-\gamma \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2\right)$$

Polynomial Kernel and Radial Kernel



- Left: SVM with a polynomial kernel of degree 3
- Right: SVM with a radial kernel

Computational Advantages

- One advantage of using kernels over enlarging the feature space using functions of the original features is computational efficiency.
  - Just compute $K(x_i, x_i')$ for all $\binom{n}{2}$ distinct pairs i and i'.
  - This can be done without explicitly working in the enlarged feature space.
- This is important because in many applications of SVMs, the enlarged feature space is so large that computations are intractable.
- For radial kernel, the feature space is implicit and infinite-dimensional, so we could never do the computations there anyway.

```
## Simulate non-linear data set
set.seed(1)
x <- matrix(rnorm(200*2), ncol=2)
x[1:100, ] <- x[1:100, ] + 2
x[101:150, ] <- x[101:150, ] - 2
y <- c(rep(-1, 150), rep(1, 50))
dat <- data.frame(x, y=as.factor(y))
plot(x, col=y+3, pch=19)
```

```
fit <- svm(y~.,data=dat, kernel="radial", gamma=0.5, cost=0.1)
plot(fit, dat)
summary(fit)
```

```
fit <- svm(y~.,data=dat, kernel="radial", gamma=0.5, cost=5)
plot(fit, dat)
summary(fit)
```

```
fit <- svm(y~.,data=dat, kernel="radial", gamma=0.5, cost=1)
```

```
px1 <- seq(round(min(x[,1]),1), round(max(x[,1]),1), 0.1)
px2 <- seq(round(min(x[,2]),1), round(max(x[,2]),1), 0.1)
xgrid <- expand.grid(X1=px1, X2=px2)
ygrid <- as.numeric(predict(fit, xgrid))
ygrid[ygrid==1] <- -1
ygrid[ygrid==2] <- 1
```

```
plot(xgrid, col=ygrid+3, pch = 20, cex = .2)
points(x, col = y+3, pch = 19)
```

```
pred <- predict(fit, xgrid, decision.values=TRUE)
func <- attributes(pred)$decision
contour(px1, px2, matrix(func, length(px1), length(px2)),
        level=0, col="purple", lwd=2, lty=2, add=TRUE)
```

```
## Separate training and test sets
set.seed(1234)
tran <- sample(200, 100)
test <- setdiff(1:200, tran)
```

```
gamma <- c(0.5, 1, 5, 10)
cost <- c(0.01, 1, 10, 100)
R <- NULL
```

```
for (i in 1:length(gamma)) {
    for (j in 1:length(cost)) {
        svmfit <- svm(y~., data=dat[tran, ], kernel="radial",
                      gamma=gamma[i] , cost=cost[j])
        pred <- predict(svmfit, dat[test, ])
        R0 <- c(gamma[i], cost[j], mean(pred!=dat[test, "y"]))
        R <- rbind(R, R0)
    }
}
```

```
colnames(R) <- c("gamma", "cost", "error")
rownames(R) <- seq(dim(R)[1])
R
```

```
## Find the optimal tuning parameters
set.seed(1)
tune.out <- tune(svm, y~., data=dat[tran, ], kernel="radial",
          ranges=list(gamma=gamma, cost=cost))
summary(tune.out)
tune.out$best.parameters
```

```
pred <- predict(tune.out$best.model, dat[test,])
table(pred=pred, true=dat[test, "y"])
mean(pred!=dat[test, "y"])
```

```
degree <- c(1, 2, 3, 4)
R <- NULL
```

```
for (i in 1:length(degree)) {
    for (j in 1:length(cost)) {
        svmfit <- svm(y~., data=dat[tran, ], kernel="polynomial",
                      degree=degree[i] , cost=cost[j])
        pred <- predict(svmfit, dat[test, ])
        R0 <- c(degree[i], cost[j], mean(pred!=dat[test, "y"]))
        R <- rbind(R, R0)
    }
}
```

```
colnames(R) <- c("degree", "cost", "error")
rownames(R) <- seq(dim(R)[1])
R
```

```
tune.out <- tune(svm, y~., data=dat[tran, ], kernel="polynomial",
           ranges=list(degree=degree, cost=cost))
summary(tune.out)
tune.out$best.parameters
```

```
pred <- predict(tune.out$best.model, dat[test,])
table(pred=pred, true=dat[test, "y"])
mean(pred!=dat[test, "y"])
```

```
R <- NULL
for (i in 1:length(gamma)) {
    for (j in 1:length(cost)) {
        svmfit <- svm(y~., data=dat[tran, ], kernel="sigmoid",
                      gamma=gamma[i] , cost=cost[j])
        pred <- predict(svmfit, dat[test, ])
        R0 <- c(gamma[i], cost[j], mean(pred!=dat[test, "y"]))
        R <- rbind(R, R0)
    }
}
```

```
colnames(R) <- c("gamma", "cost", "error")
rownames(R) <- seq(dim(R)[1])
R
```

```
tune.out <- tune(svm, y~., data=dat[tran, ], kernel="sigmoid",
                 ranges=list(gamma=gamma, cost=cost))
summary(tune.out)
tune.out$best.parameters
```

```
pred <- predict(tune.out$best.model, dat[test,])
table(pred=pred, true=dat[test, "y"])
mean(pred!=dat[test, "y"])
```

```
set.seed(123)
N <- 20
RES <- matrix(0, N, 3)
colnames(RES) <- c("radial", "poly", "sigmoid")
```

```
for (i in 1:N) {
    tran <- sample(200, 100)
    test <- setdiff(1:200, tran)

    tune1 <- tune(svm, y~., data=dat[tran, ], kernel="radial",
                  ranges=list(gamma=gamma, cost=cost))
    pred1 <- predict(tune1$best.model, dat[test,])
    RES[i, 1] <- mean(pred1!=dat[test, "y"])

    tune2 <- tune(svm, y~., data=dat[tran, ], kernel="polynomial",
                  ranges=list(degree=degree, cost=cost))
    pred2 <- predict(tune2$best.model, dat[test,])
    RES[i, 2] <- mean(pred2!=dat[test, "y"])

    tune3 <- tune(svm, y~., data=dat[tran, ], kernel="sigmoid",
                  ranges=list(gamma=gamma, cost=cost))
    pred3 <- predict(tune3$best.model, dat[test,])
    RES[i, 3] <- mean(pred3!=dat[test, "y"])
}
```

```
apply(RES, 2, summary)
```

```
## A function to plot an ROC curve given pred and truth
library(ROCR)
rocplot <- function(pred, truth, ...){
    predob <- prediction(pred, truth)
    perf <- performance(predob, "tpr", "fpr")
plot(perf, ...)}
```

```
## Radial kernel with cost = 0.1 (gamma=1)
svmfit.opt <- svm(y ~., data=dat[tran, ], kernel="radial",
                  gamma=1, cost=0.1, decision.values=T)
fitted <- attributes(predict(svmfit.opt, dat[tran, ],
                    decision.values=TRUE))$decision.values
```

```
ry <- y
ry[y==-1] <- 1
ry[y==1] <- -1
```

```
## ROC plot
par(mfrow=c(1,2))
rocplot(fitted, ry[tran], main="Training Data", col=4, lwd=2)
```

```
## Radial kernel with cost = 1000 (gamma=1)
svmfit.flex <- svm(y~., data=dat[tran, ], kernel ="radial",
                   gamma=1, cost=1000, decision.values=T)
fitted2 <- attributes(predict(svmfit.flex, dat[tran, ],
                     decision.values=TRUE))$decision.values
rocplot(fitted2, ry[tran], add=T, col="red", lwd=2)
```

```
## ROC curves for test set
fitted3 <- attributes(predict(svmfit.opt, dat[test, ],
                      decision.values=T))$decision.values
rocplot(fitted3, ry[test], main="Test Data", col=4, lwd=2)
fitted4 <- attributes(predict(svmfit.flex, dat[test, ],
                      decision.values=T))$decision.values
rocplot(fitted4, ry[test], add=T, col="red", lwd=2)
```

Example: Heart Data

- These data contain a binary outcome `AHD` for 303 patients who presented with chest pain.
- An outcome value of `Yes` indicates the presence of heart disease based on an angiographic test, while `No` means no heart disease.
- There are 13 predictors including `Age`, `Sex`, `Chol` (a cholesterol measurement), and other heart and lung function measurements.
- We can find some missing values from data, so we need to remove the samples with missing values. Then, the sample size is reduced down to 297.

```
url.ht <- "https://www.statlearning.com/s/Heart.csv"
Heart <- read.csv(url.ht, h=T)
summary(Heart)
```

```
Heart <- Heart[, colnames(Heart)!="X"]
Heart[,"Sex"] <- factor(Heart[,"Sex"], 0:1, c("female", "male"))
Heart[,"Fbs"] <- factor(Heart[,"Fbs"], 0:1, c("false", "true"))
Heart[,"ExAng"] <- factor(Heart[,"ExAng"], 0:1, c("no", "yes"))
Heart[,"ChestPain"] <- as.factor(Heart[,"ChestPain"])
Heart[,"Thal"] <- as.factor(Heart[,"Thal"])
Heart[,"AHD"] <- as.factor(Heart[,"AHD"])
```

```
summary(Heart)
dim(Heart)
sum(is.na(Heart))
```

```
Heart <- na.omit(Heart)
dim(Heart)
summary(Heart)
```

```
## Separate training and test sets
set.seed(123)
train <- sample(1:nrow(Heart), nrow(Heart)/2)
test <- setdiff(1:nrow(Heart), train)
```

```
## Classification tree
library(tree)
tree.tran <- tree(AHD ~., Heart, subset = train)
tree.pred <- predict(tree.tran, Heart[test,], type="class")
mean(tree.pred!=Heart$AHD[test])
```

```
## Cross-validated tree
set.seed(1234)
cv.heart <- cv.tree(tree.tran, FUN=prune.misclass, K=5)
w <- cv.heart$size[which.min(cv.heart$dev)]
prune.heart <- prune.misclass(tree.tran, best=w)
heart.pred <- predict(prune.heart, Heart[test,], type="class")
mean(heart.pred!=Heart$AHD[test])
```

```
set.seed(1111)
```

```
## Bagging and random forest (m=2, 4, and 6)
library(randomForest)
bag.heart <- randomForest(x=Heart[train,-14], y=Heart[train,14],
            xtest=Heart[test,-14], ytest=Heart[test,14], mtry=13)
bag.heart$test$err.rate[500,1]
```

```
rf.heart <- randomForest(x=Heart[train,-14], y=Heart[train,14],
            xtest=Heart[test,-14], ytest=Heart[test,14], mtry=6)
rf.heart$test$err.rate[500,1]
```

```
rf.heart <- randomForest(x=Heart[train,-14], y=Heart[train,14],
            xtest=Heart[test,-14], ytest=Heart[test,14], mtry=4)
rf.heart$test$err.rate[500,1]
```

```
rf.heart <- randomForest(x=Heart[train,-14], y=Heart[train,14],
            xtest=Heart[test,-14], ytest=Heart[test,14], mtry=2)
rf.heart$test$err.rate[500,1]
```

```
library(e1071)
```

```
## SVM with a linear kernel
tune.out <- tune(svm, AHD~., data=Heart[train, ],
                 kernel="linear", ranges=list(
                 cost=c(0.001, 0.01, 0.1, 1, 5, 10, 100)))
heart.pred <- predict(tune.out$best.model, Heart[test,])
table(heart.pred, Heart$AHD[test])
mean(heart.pred!=Heart$AHD[test])
```

```
## SVM with a radial kernel
tune.out <- tune(svm, AHD~., data=Heart[train, ],
                 kernel="radial", ranges=list(
                 cost=c(0.1,1,10,100), gamma=c(0.5,1,2,3)))
heart.pred <- predict(tune.out$best.model, Heart[test,])
table(heart.pred, Heart$AHD[test])
mean(heart.pred!=Heart$AHD[test])
```

```
## SVM with a polynomial kernel
tune.out <- tune(svm, AHD~.,data=Heart[train, ],
                 kernel="polynomial", ranges=list(
                 cost=c(0.1,1,10,100), degree=c(1,2,3)))
heart.pred <- predict(tune.out$best.model, Heart[test,])
table(heart.pred, Heart$AHD[test])
mean(heart.pred!=Heart$AHD[test])
```

```
## SVM with a sigmoid kernel
tune.out <- tune(svm, AHD~.,data=Heart[train, ],
                 kernel="sigmoid", ranges=list(
                 cost=c(0.1,1,10,100), gamma=c(0.5,1,2,3)))
heart.pred <- predict(tune.out$best.model, Heart[test,])
table(heart.pred, Heart$AHD[test])
mean(heart.pred!=Heart$AHD[test])
```

```
set.seed(123)
N <- 20
Err <- matrix(0, N, 5)
```

```
for (i in 1:N) {
    train <- sample(1:nrow(Heart), floor(nrow(Heart)*2/3))
    test <- setdiff(1:nrow(Heart), train)

    g1 <- randomForest(x=Heart[train,-14], y=Heart[train,14],
            xtest=Heart[test,-14], ytest=Heart[test,14], mtry=4)
    Err[i,1] <- g1$test$err.rate[500,1]

    g2 <- tune(svm, AHD~., data=Heart[train, ], kernel="linear",
          ranges=list(cost=c(0.001, 0.01, 0.1, 1, 5, 10, 100)))
    p2 <- predict(g2$best.model, Heart[test,])
    Err[i,2] <- mean(p2!=Heart$AHD[test])

    g3 <- tune(svm, AHD~., data=Heart[train, ], kernel="radial",
          ranges=list(cost=c(0.1,1,10,100), gamma=c(0.5,1,2,3)))
    p3 <- predict(g3$best.model, Heart[test,])
    Err[i,3] <- mean(p3!=Heart$AHD[test])
```

```
    g4 <- tune(svm, AHD~.,data=Heart[train, ],kernel="polynomial",
               ranges=list(cost=c(0.1,1,10,100), degree=c(1,2,3)))
    p4 <- predict(g4$best.model, Heart[test,])
    Err[i,4] <- mean(p4!=Heart$AHD[test])

    g5 <- tune(svm, AHD~.,data=Heart[train, ],kernel="sigmoid",
            ranges=list(cost=c(0.1,1,10,100), gamma=c(0.5,1,2,3)))
    p5 <- predict(g5$best.model, Heart[test,])
    Err[i,5] <- mean(p5!=Heart$AHD[test])
}
```

```
dev.off()
labels <- c("RF","SVM.linear","SVM.radial","SVM.poly","SVM.sig")
boxplot(Err, boxwex=0.5, main="Random Forest and SVM", col=2:6,
        names=labels, ylab="Classification Error Rates",
        ylim=c(0,0.4))
```

```
colnames(Err) <- labels
apply(Err, 2, summary)
```

SVM: More Than 2 Classes

- The SVM as defined works for $K = 2$ classes. What do we do if we have $K > 2$ classes?
- One-Versus-All Classification (OVA)
  - Fit K different 2-class SVM classifiers $\hat{f}_k(x)$ for $k = 1, 2, \ldots, K$; each class versus the rest. Classify x^* to the class for which $\hat{f}_k(x^*)$ is largest.
- One-Versus-One Classification (OVO)
  - Fit all $\binom{K}{2}$ pairwise classifiers $\hat{f}_{kl}(x)$. Classify x^* to the class that wins the most pairwise competitions.
- If K is not too large, OVO is preferred.

```
## Generate 2-classes data
set.seed(1)
x <- matrix(rnorm(200*2), ncol=2)
x[1:100, ] <- x[1:100, ] + 2
x[101:150, ] <- x[101:150, ] - 2
y <- c(rep(1, 150), rep(2, 50))
```

```
## Add one more class
set.seed(1)
x <- rbind(x, matrix (rnorm(50*2), ncol=2))
y <- c(y, rep (0,50))
x[y==0, 2] <- x[y==0, 2] + 2
dat <- data.frame(x=x, y=as.factor (y))
plot(x, col=(y+1), pch=19)
```

```
## Fit SVM based on one-versus-one classification
svmfit <- svm(y~., data=dat, kernel="radial",
              cost=10, gamma=1)
plot(svmfit, dat)
```

```
library(e1071)
library(randomForest)
data(iris)
str(iris)
```

```
set.seed(123)
K <- 50
Err2 <- matrix(0, K, 7)
```

```
for (i in 1:K) {
    tran <- sample(nrow(iris), size=floor(nrow(iris)*2/3))
    for (k in 1:4) {
        g <- randomForest(x=iris[tran, -5], y=iris[tran, 5],
             xtest=iris[-tran, -5], ytest=iris[-tran, 5], mtry=k)
        Err2[i, k] <- g$test$err.rate[500, 1]
    }
    g2 <- tune(svm, Species~., data=iris[tran, ], kernel="linear",
          ranges=list(cost=c(0.001, 0.01, 0.1, 1, 5, 10, 100)))
    p2 <- predict(g2$best.model, iris[-tran,])
    Err2[i, 5] <- mean(p2!=iris$Species[-tran])
```

```
    g3 <- tune(svm, Species~., data=iris[tran, ], kernel="radial",
          ranges=list(cost=c(0.1,1,10,100), gamma=c(0.5,1,2,3)))
    p3 <- predict(g3$best.model, iris[-tran,])
    Err2[i, 6] <- mean(p3!=iris$Species[-tran])
    g4 <- tune(svm, Species~., data=iris[tran, ],
          kernel="polynomial", ranges=list(cost=c(0.1,1,10,100),
          degree=c(1,2,3)))
    p4 <- predict(g4$best.model, iris[-tran,])
    Err2[i, 7] <- mean(p4!=iris$Species[-tran])
}
```

```
labels <- c("RF1", "RF2", "RF3", "RF4", "SVM.linear",
            "SVM.radial", "SVM.poly")
boxplot(Err2, boxwex=0.5, main="Random Forest and SVM", col=2:8,
        names=labels, ylab="Classification Error Rates",
        ylim=c(0, 0.15))
```

```
colnames(Err2) <- labels
apply(Err2, 2, summary)
```

```
library(rattle.data)
data(wine)
str(wine)
```

```
set.seed(1234)
K <- 50
Err3 <- matrix(0, K, 7)
m <- c(1, 3, 5, 13)
```

```
for (i in 1:K) {
    tran <- sample(nrow(wine), size=floor(nrow(wine)*2/3))
    for (k in 1:4) {
        g <- randomForest(x=wine[tran, -1], y=wine[tran, 1],
            xtest=wine[-tran,-1], ytest=wine[-tran,1], mtry=m[k])
        Err3[i, k] <- g$test$err.rate[500, 1]
    }
    g2 <- tune(svm, Type~., data=wine[tran, ], kernel="linear",
          ranges=list(cost=c(0.001, 0.01, 0.1, 1, 5, 10, 100)))
    p2 <- predict(g2$best.model, wine[-tran,])
    Err3[i, 5] <- mean(p2!=wine$Type[-tran])
```

```
    g3 <- tune(svm, Type~., data=wine[tran, ], kernel="radial",
          ranges=list(cost=c(0.1,1,10,100), gamma=c(0.5,1,2,3)))
    p3 <- predict(g3$best.model, wine[-tran,])
    Err3[i, 6] <- mean(p3!=wine$Type[-tran])
    g4 <- tune(svm, Type~., data=wine[tran, ],
          kernel="polynomial", ranges=list(cost=c(0.1,1,10,100),
          degree=c(1,2,3)))
    p4 <- predict(g4$best.model, wine[-tran,])
    Err3[i, 7] <- mean(p4!=wine$Type[-tran])
}
```

```
labels <- c("RF1", "RF3", "RF5", "RF13", "SVM.linear",
            "SVM.radial", "SVM.poly")
boxplot(Err3, boxwex=0.5, main="Random Forest and SVM", col=2:8,
        names=labels, ylab="Classification Error Rates",
        ylim=c(0, 0.3))
```

```
colnames(Err3) <- labels
apply(Err3, 2, summary)
```

Another Optimization Form of SVM

- When SVMs were first introduced in the mid-1990s, they made quite a splash in the statistical and machine learning communities.
- However, it turns out that the solution to the support vector classifier

$$f(x) = \beta_0 + \beta_1 x_1 + \ldots + \beta_p x_p$$

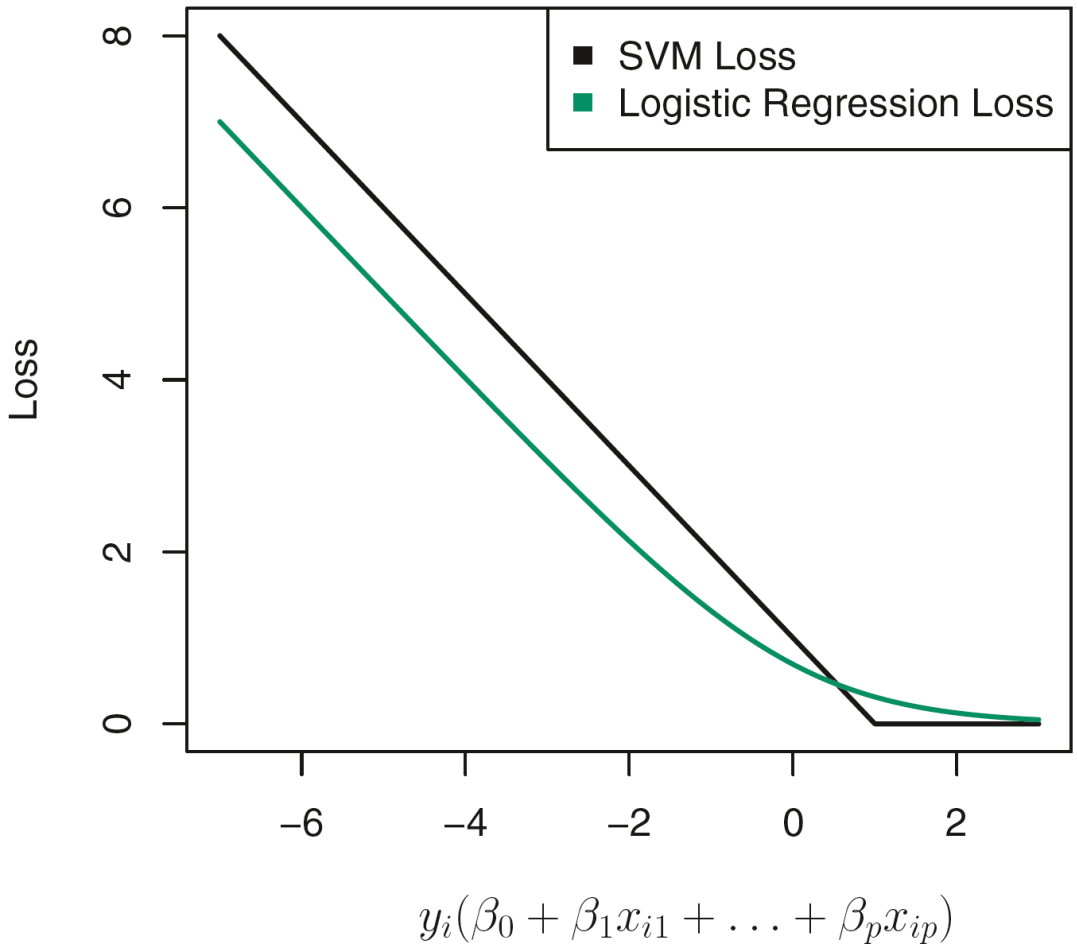
is equivalent to

$$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} \left\{ \sum_{i=1}^{n} \max[0, 1 - y_i f(x_i)] + \lambda \sum_{j=1}^{p} \beta_j^2 \right\},$$

where $\lambda > 0$ is a tuning parameter.

- This has the form 'hinge loss + penalty'
- The hinge loss function is closely related to the loss function used in logistic regression.

Loss Functions of SVM and Logistic Regression



- SVM: hinge loss
- Logistic regression: negative likelihood

SVM vs. Logistic Regression

- An interesting characteristic of the support vector classifier is that only support vectors play a role in the classifier obtained.
- This is due to the fact that the loss is exactly zero for observations for which

$$y_i(\beta_0 + \beta_1 x_{i1} + \ldots + \beta_p x_{ip}) \geq 1$$

- In contrast, the loss function for logistic regression is not exactly zero, anywhere although it is very small for observations that are far from the decision boundary.
- Due to similarities of loss functions, logistic regression and support vector classifier give very similar results.
  - If the classes are well separated, SVM is better
  - If not, logistic regression (with ridge penalty) is better.

More on SVMs

- If you wish to estimate prediction probabilities, logistic regression (with ridge penalty) is the choice.
- For nonlinear boundaries, SVMs are popular. Although using kernels with logistic regression (with ridge penalty) is feasible, computational cost are more expensive.
- The use of non-linear kernels is much more widespread in SVMs than in logistic regression or other methods.
- Support vector regression is an extension of the SVM for regression (with a quantitative response). It seeks coefficients that minimize a different type of loss.
- SVM can be applied to high-dimensional data, where the number of variables is much greater than the sample size.

```
library(ISLR)
data(Khan)
?Khan
names(Khan)
dim(Khan$xtrain)
dim(Khan$xtest)
```

```
x <- c(Khan$xtrain, Khan$xtest)
summary(x)
hist(x, nclass=50, col="purple")
```

```
length(Khan$ytrain)
table(Khan$ytrain)
length(Khan$ytest)
table(Khan$ytest)
```

```
Tran <- data.frame(x=Khan$xtrain, y=as.factor(Khan$ytrain))
Test <- data.frame(x=Khan$xtest, y=as.factor(Khan$ytest))
```

```
library(e1071)
```

```
## SVM with a linear kernel
g1 <- tune(svm, y~., data=Tran, kernel="linear",
           ranges=list(cost=c(0.001, 0.01, 0.1, 1, 5, 10)))
p1 <- predict(g1$best.model, Test)
table(p1, Test$y)
mean(p1!=Test$y)
```

```
## SVM with a radial kernel
g2 <- tune(svm, y~., data=Tran, kernel="radial",
           ranges=list(cost=c(0.1,1,10,100),
                       gamma=c(0.5,1,2,3)))
p2 <- predict(g2$best.model, Test)
table(p2, Test$y)
mean(p2!=Test$y)
```

```
## SVM with a polynomial kernel
g3 <- tune(svm, y~., data=Tran, kernel="polynomial",
           ranges=list(cost=c(0.1,1,10,100),
                       degree=c(1,2,3)))
p3 <- predict(g3$best.model, Test)
table(p3, Test$y)
mean(p3!=Test$y)
```

```
## SVM with a sigmoid kernel
g4 <- tune(svm, y~., data=Tran, kernel="sigmoid",
           ranges=list(cost=c(0.1,1,10,100),
                       gamma=c(0.5,1,2,3)))
p4 <- predict(g4$best.model, Test)
table(p4, Test$y)
mean(p4!=Test$y)
```