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Generating a radially separable dataset

Generating a 2d uniformly distributed set of points

- Generate a dataset with 200 points
  - 2 predictors `x1` and `x2`, uniformly distributed between -1 and 1.

```
#set required number of datapoints
n <- 200

#set seed to ensure reproducibility
set.seed(42)

#Generate dataframe with 2 predictors x1 and x2 in (-1,1)
df <- data.frame(x1 = runif(n, min = -1, max = 1),
                 x2 = runif(n, min = -1, max = 1))
```

Create a circular boundary

- Create a circular decision boundary of radius 0.7 units
- Categorical variable y is +1 or -1 depending on the point lies outside or within boundary.

```
radius <- 0.7
radius_squared <- radius^2

#categorize data points depending on location wrt boundary
df$y <- factor(ifelse(df$x1^2 + df$x2^2 < radius_squared, -1, 1),
               levels = c(-1,1))
```

Plot the dataset

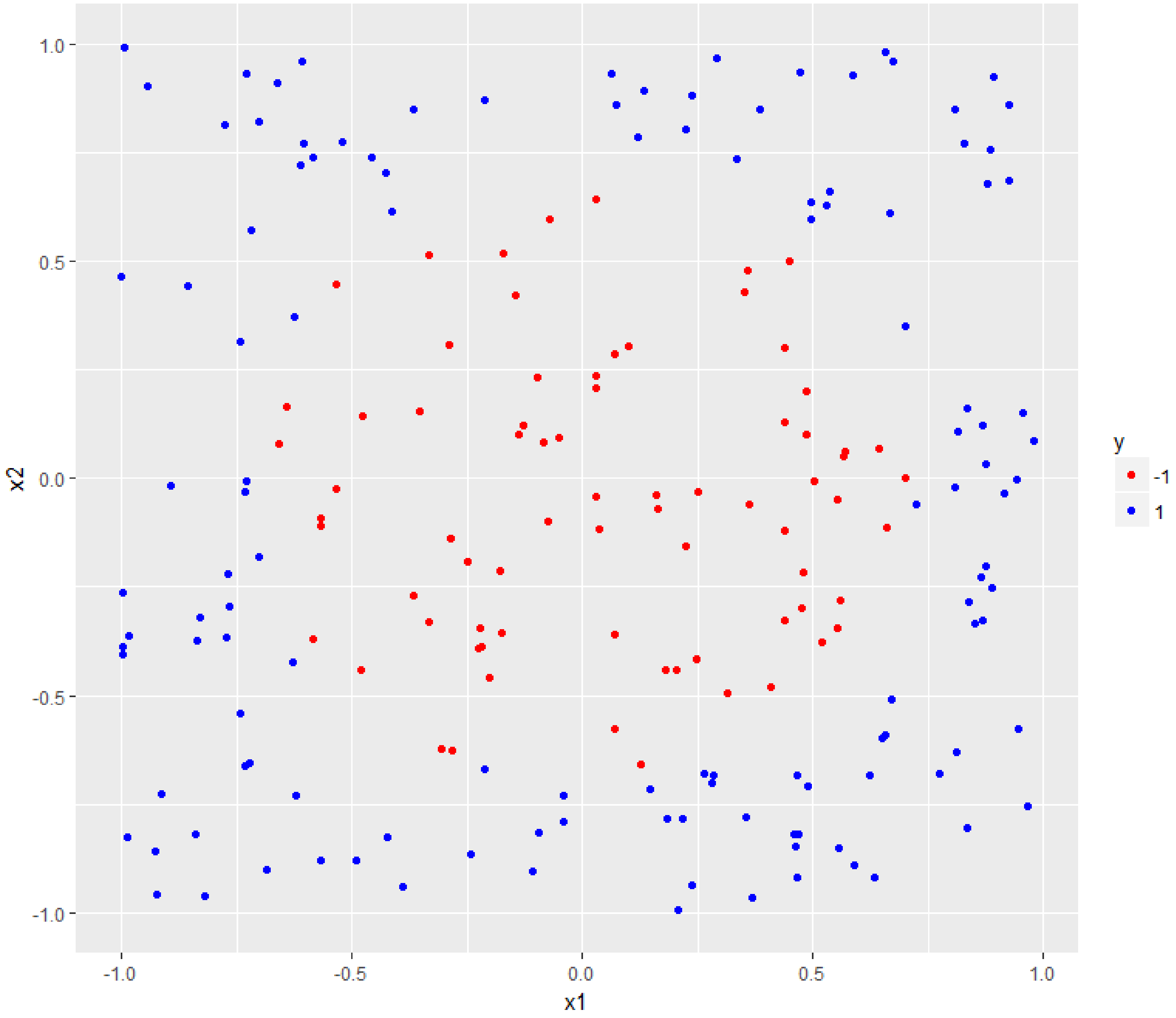
- Visualize using ggplot.

```
#load ggplot
library(ggplot2)
```

- predictors plotted on 2 axes; classes distinguished by color.

```
#build plot
p <- ggplot(data = df, aes(x = x1, y = x2, color = y)) +
     geom_point() +
     scale_color_manual(values = c("-1" = "red","1" = "blue"))

#display plot
p
```


1.0
0.5
0.0
-0.5
-1.0
x2
-1.0
-0.5
0.0
0.5
1.0
x1
y
-1
1

Adding a circular boundary - Part 1

- We'll create a function to generate a circle

```
# function generates dataframe with points
# lying on a circle of radius r
circle <-
  function(x1_center, x2_center, r, npoint = 100){

  #angular spacing of 2*pi/npoint between points
  theta <- seq(0,2*pi,length.out = npoint)
  x1_circ <- x1_center + r * cos(theta)
  x2_circ <- x2_center + r * sin(theta)

  return(data.frame(x1c = x1_circ, x2c = x2_circ))
}
```

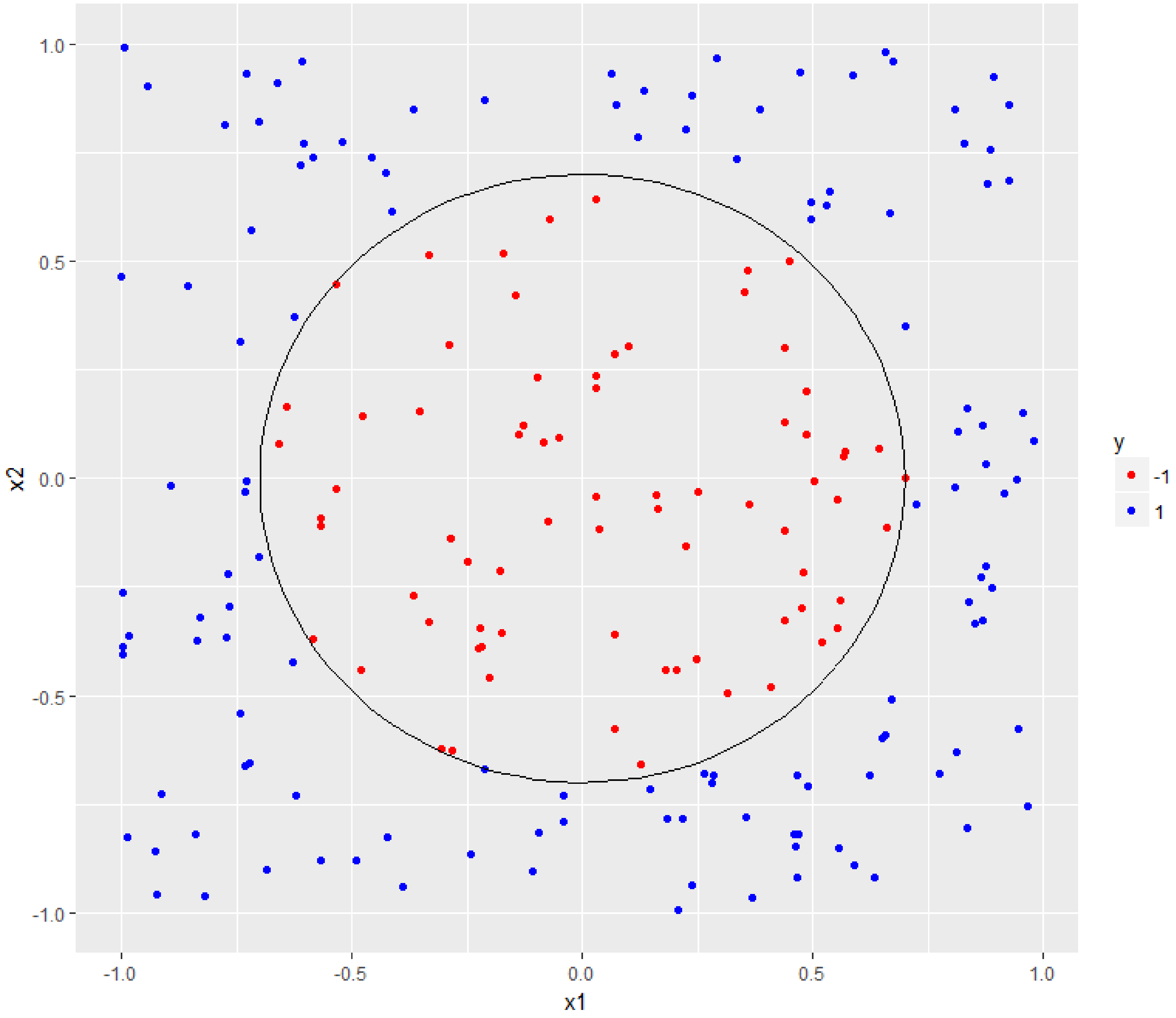
Adding a circular boundary - Part 2

- To add boundary to plot:
  - generate boundary using `circle()` function.
  - add boundary to plot using `geom_path()`

```
#generate boundary
boundary <- circle(x1_center = 0,
                   x2_center = 0,
                   r = radius)

#add boundary to previous plot
p <- p +
     geom_path(data = boundary,
               aes(x = x1c, y = x2c),
               inherit.aes = FALSE)

#display plot
p
```



1.0
0.5
0.0
-0.5
-1.0
x2
-1.0
-0.5
0.0
0.5
1.0
x1
y
-1
1

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Linear SVMs on radially separable data

Linear SVM, cost = 1

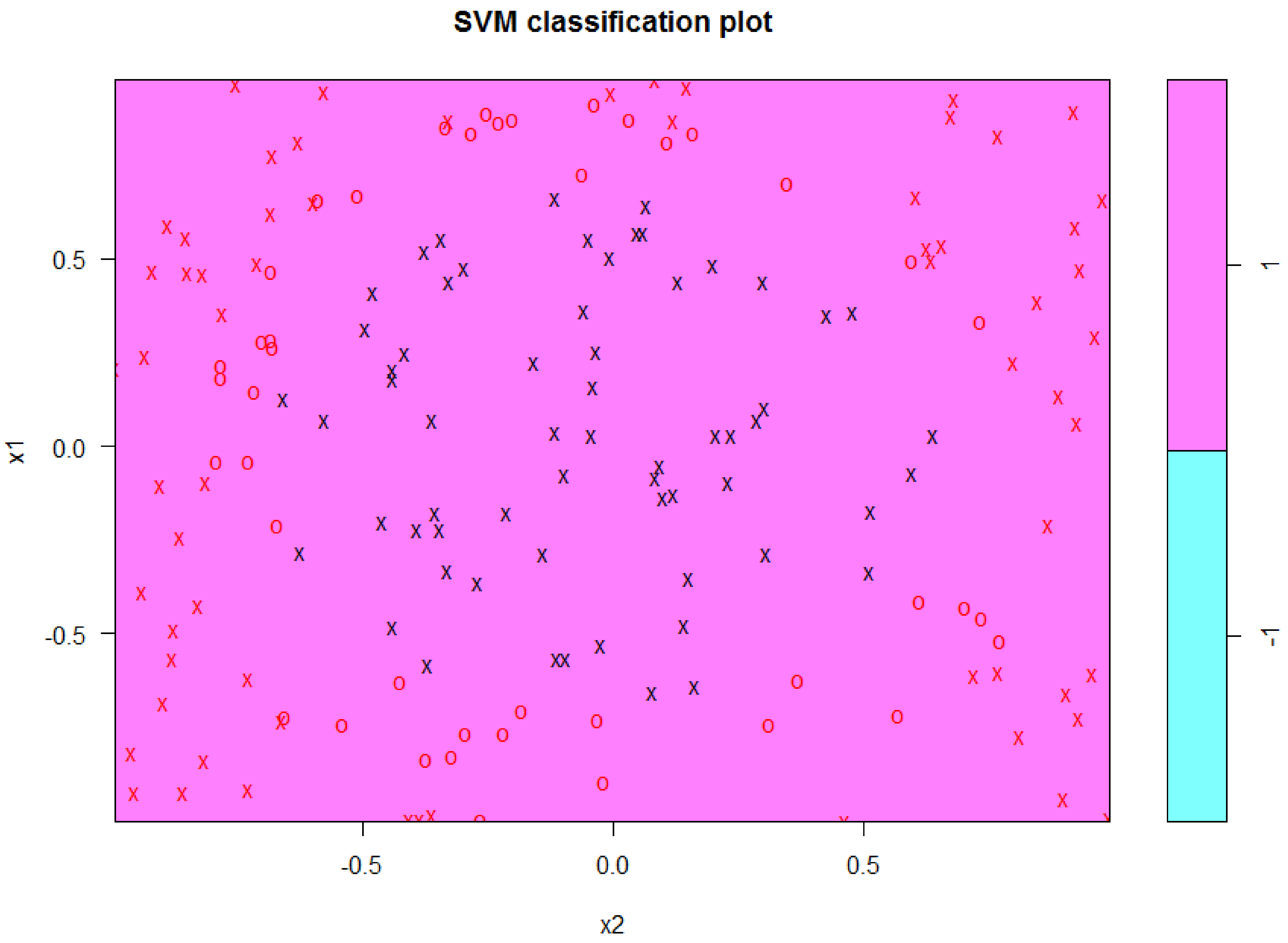
- Partition radially separable dataset into training/test (seed = 10)
- Build default cost linear SVM on training set

```
svm_model<-
  svm(y ~ ., data=trainset, type="C-classification", kernel="linear")
svm_model
....
Number of Support Vectors:  126
```

- Calculate accuracy on test set.

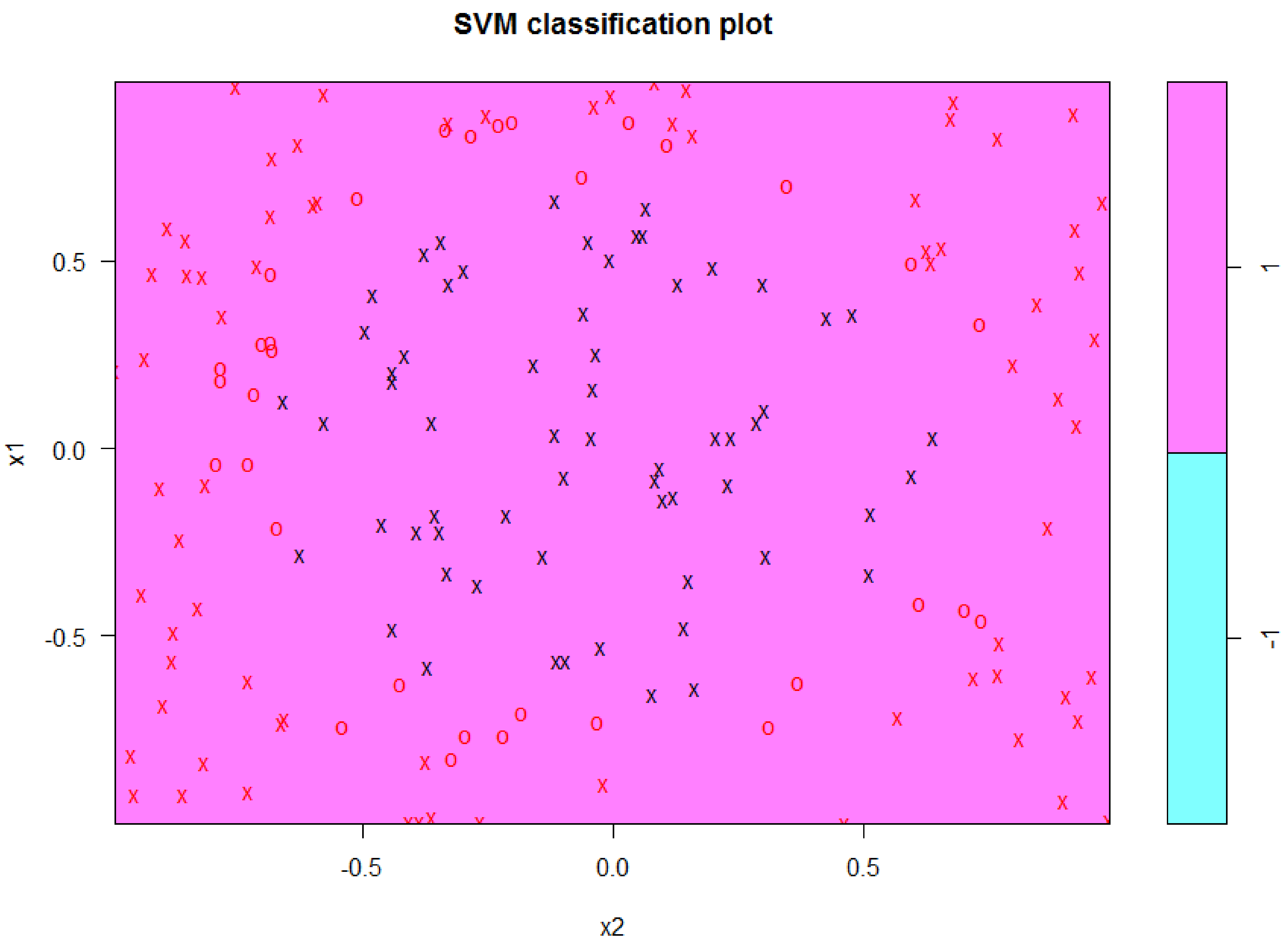
```
#accuracy
pred_test <- predict(svm_model,testset)
mean(pred_test==testset$y)
[1] 0.6129032

#plot
plot(svm_model,trainset)
```


SVM classification plot
x1
0.5
0.0
-0.5
x2
-0.5
0.0
0.5
1
-1

Linear SVM, cost = 100

```
svm_model<-
  svm(y ~ ., data=trainset, type="C-classification", kernel="linear")
svm_model
....
Number of Support Vectors:  136
#accuracy
pred_test <- predict(svm_model,testset)
mean(pred_test==testset$y)
[1] 0.6129032
plot(svm_model,trainset)
```


SVM classification plot
x1
0.5
0.0
-0.5
x2
-0.5
0.0
0.5
1
-1

A better estimate of accuracy

- Calculate average accuracy over a number of independent train/test splits.
- Check standard deviation of result to get an idea of variability.

Average accuracy for default cost SVM

```
accuracy <- rep(NA, 100)
set.seed(10)

for (i in 1:100){
  df[,"train"] <- ifelse(runif(nrow(df))<0.8,1,0)
  trainset <- df[df$train==1,]
  testset <- df[df$train==0,]
  trainColNum <- grep("train",names(trainset))
  trainset <- trainset[,-trainColNum]
  testset <- testset[,-trainColNum]
  svm_model<-
    svm(y ~ ., data = trainset,
        type = "C-classification",
        cost = 1,
        kernel = "linear")
  pred_test <- predict(svm_model, testset)
  accuracy[i] <- mean(pred_test==testset$y)
}

mean(accuracy)
[1] 0.642843
sd(accuracy)
[1] 0.07606017
```

How well does a linear SVM perform?

- **Marginally better than a coin toss!**
- We can use our knowledge of the boundary to do much better.

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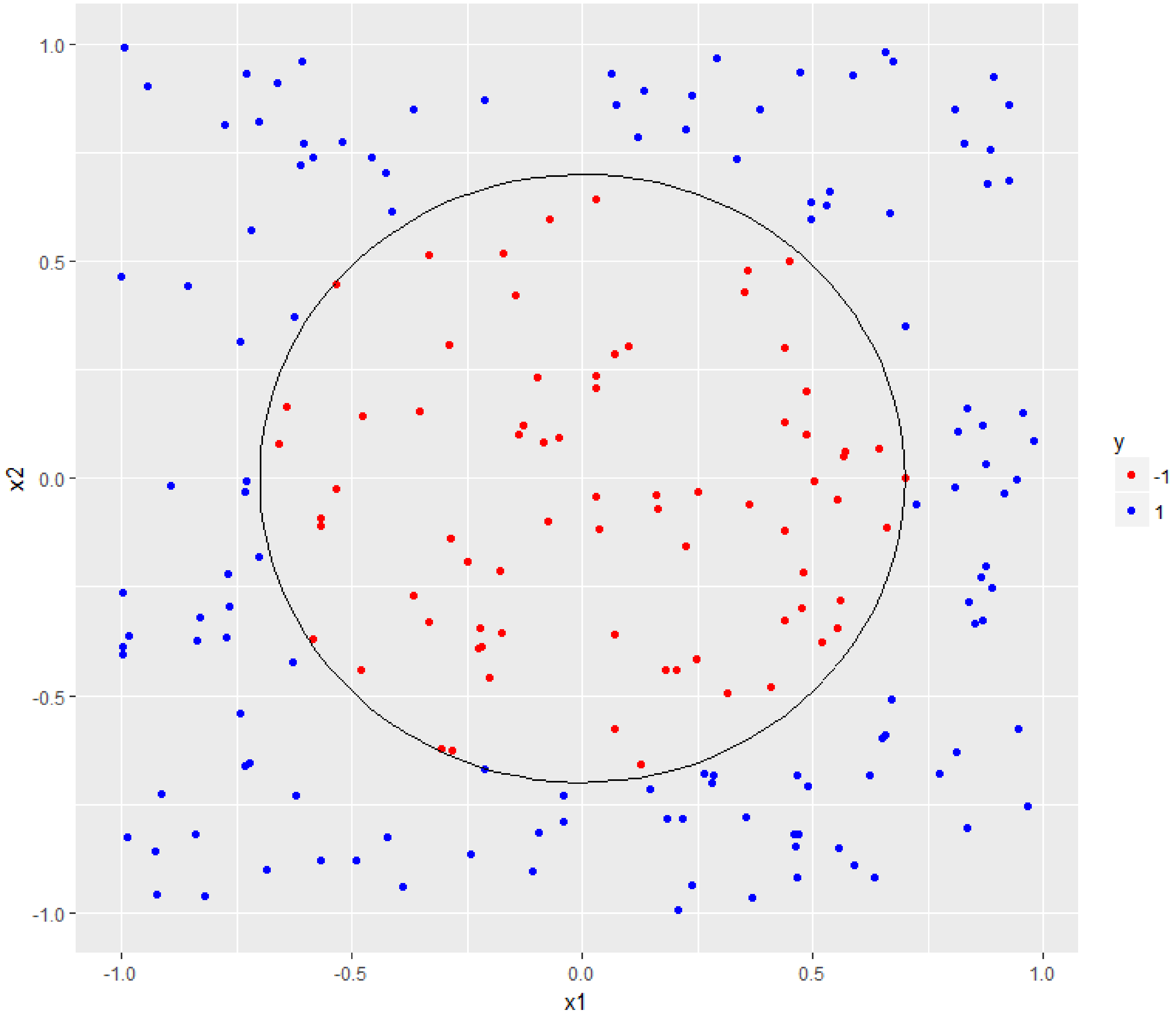
The Kernel Trick

The basic idea

- Devise a transformation that makes the problem linearly separable.
- We'll see how to do this for a radially separable dataset.



1.0
0.5
0.0
-0.5
-1.0
x2
-1.0
-0.5
0.0
0.5
1.0
x1
y
-1
1

Transforming the problem

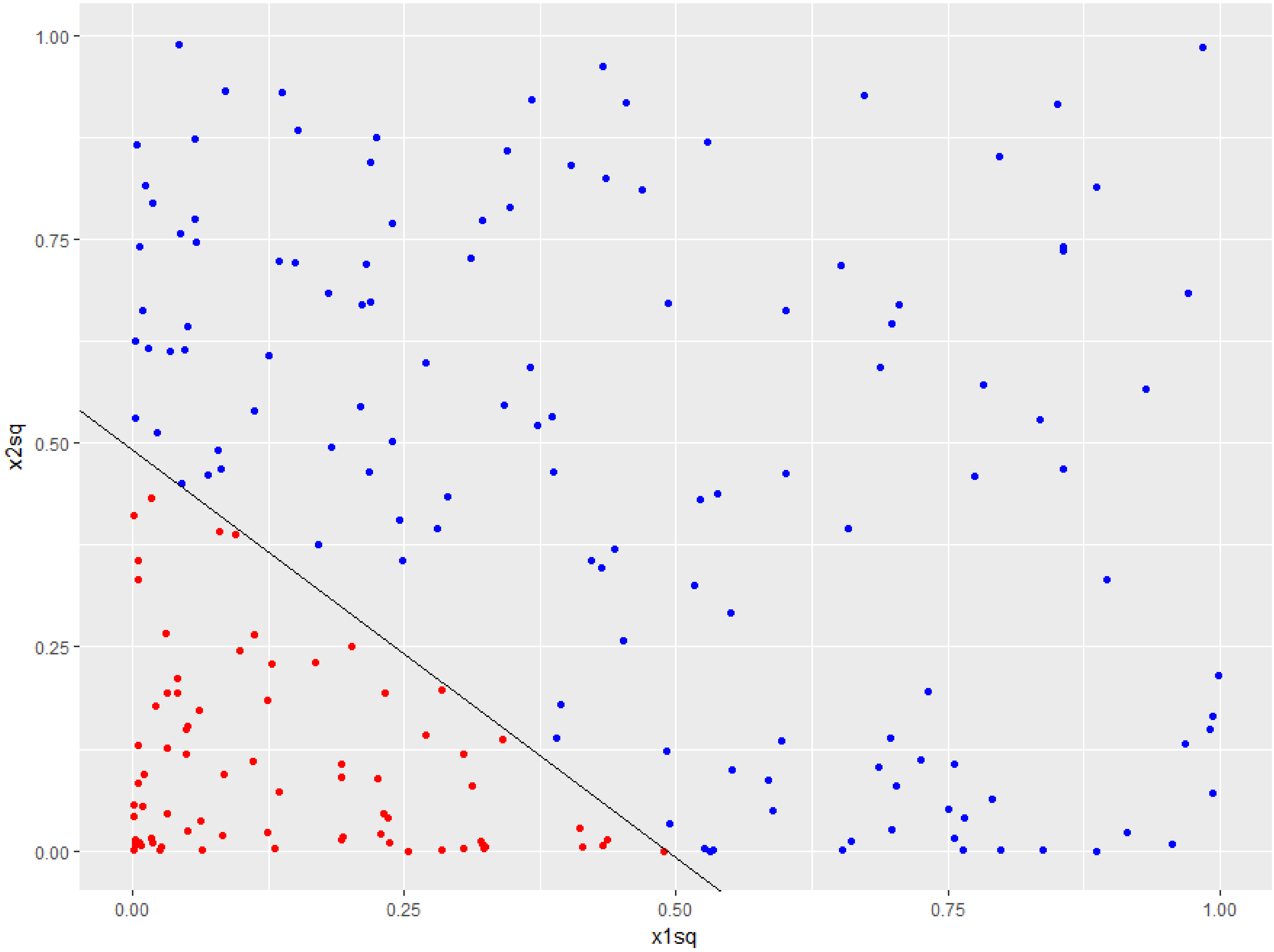
- Equation of boundary is x1^2 + x2^2 = 0.49
- Map x1^2 to a new variable X1 and x2^2 to X2
- The equation of boundary in the X1-X2 space becomes...
- X1 + X2 = 0.49 (a line!!)

Plot in X1-X2 space - code

- Use `ggplot()` to plot the dataset in X1-X2 space
- Equation of boundary X2 = -X1 + 0.49:
  - slope=-1
  - y-intercept=0.49

```
p <- ggplot(data = df4, aes(x = x1sq, y = x2sq, color = y)) +
  geom_point()+
  scale_color_manual(values = c("red","blue"))+
  geom_abline(slope = -1, intercept = 0.49)

p
```


1.00
0.75
0.50
0.25
0.00
x2sq
0.00
0.25
0.50
0.75
1.00
x1sq

The Polynomial Kernel - Part 1

- Polynomial kernel: (gamma*(u.v)+coef0)^degree
  - degree = degree of polynomial
  - gamma and coef0- tuning parameters
  - u, v - vectors (datapoints) belonging to the dataset
- We can guess we need a 2nd degree polynomial (transformation)

Kernel functions

- The math formulation of SVMs requires transformations with specific properties.
- Functions satisfying these properties are called **kernel functions**
- Kernel functions are generalizations of vector dot products
- *Basic idea** - use a kernel that separates the data well!

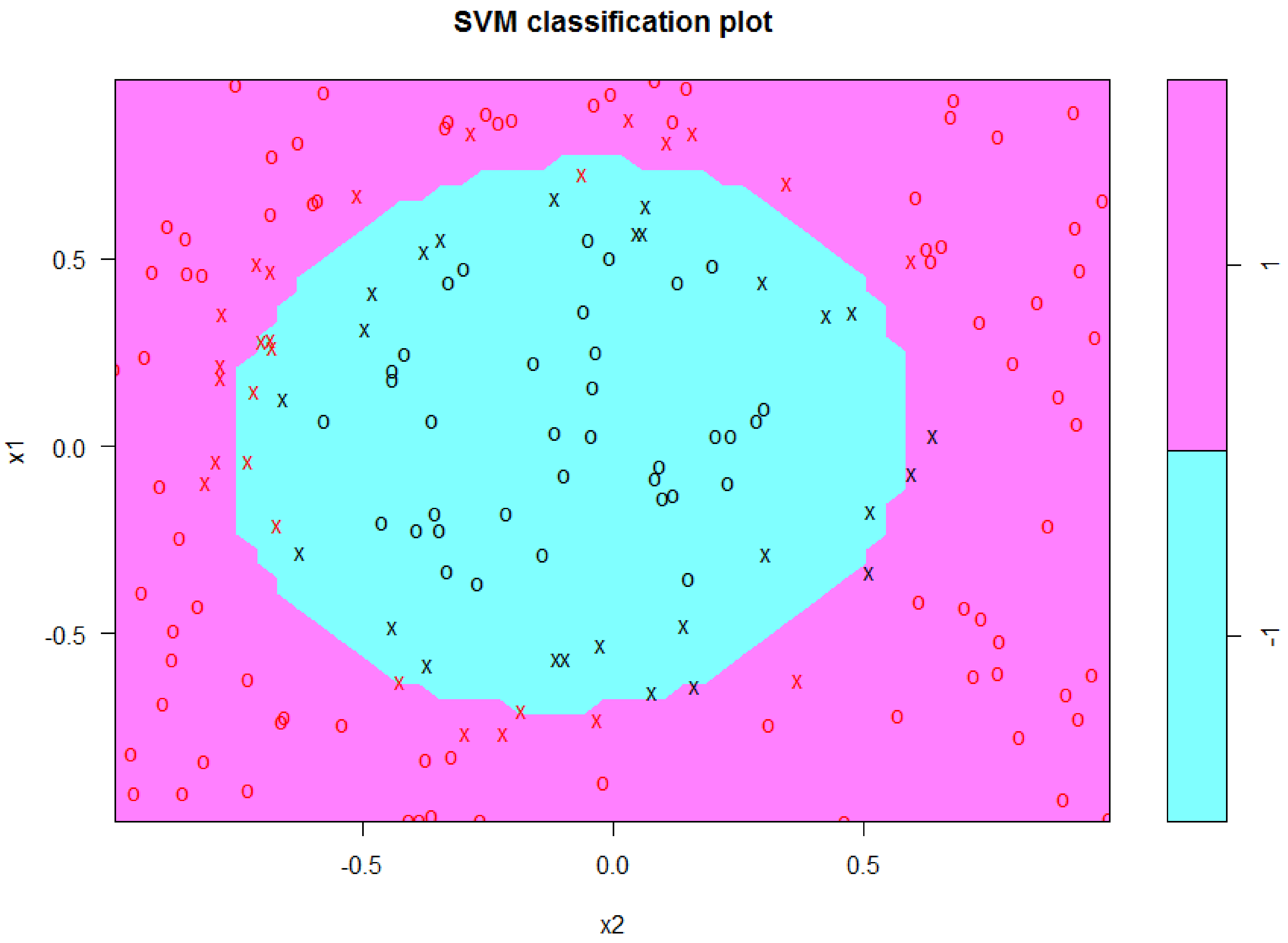
Radially separable dataset - quadratic kernel

- 80/20 train/test split
- Build a quadratic SVM for the radially separable dataset:
  - degree =2
  - default values of cost, gamma and coef0 (1, 1/2 and 0)

```
svm_model<-
  svm(y ~ ., data = trainset, type = "C-classification",
      kernel = "polynomial", degree = 2)

#predictions
pred_test <- predict(svm_model, testset)
mean(pred_test==testset$y)
[1] 0.9354839

#visualize model
plot(svm_model, trainset)
```


SVM classification plot
x1
0.5
0.0
-0.5
x2
-0.5
0.0
0.5
1
-1

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Tuning SVMs

Objective of tuning

- Hard to find optimal values of parameters manually for complex kernels.
- **Objective**: to find optimal set of parameters using `tune.svm()` function.

Tuning in a nutshell

- How it works:
  - set a range of search values for each parameter. Examples: cost = 10^(-1:3), gamma = c(0.1,1,10), coef0 = c(0.1,1,10)
  - Build an SVM model for each possible combination of parameter values and evaluate accuracy.
  - Return the parameter combination that yields the best accuracy.
- Computationally intensive procedure!

Introducing tune.svm()

- Tune SVM model for the radially separable dataset created earlier
  - Built polynomial kernel SVM in previous lesson
  - Accuracy of SVM was ~94%.
- Can we do better by tuning gamma, cost and coef0?

```
tune_out <-
  tune.svm(x = trainset[,-3], y = trainset[,3],
        type = "C-classification", kernel = "polynomial", degree = 2,
        cost = 10^(-1:2), gamma = c(0.1,1,10), coef0 = c(0.1,1,10))

#print out tuned parameters
tune_out$best.parameters$cost
[1] 0.1
tune_out$best.parameters$gamma
[1] 10
tune_out$best.parameters$coef0
[1] 1
```

Build and examine optimal model

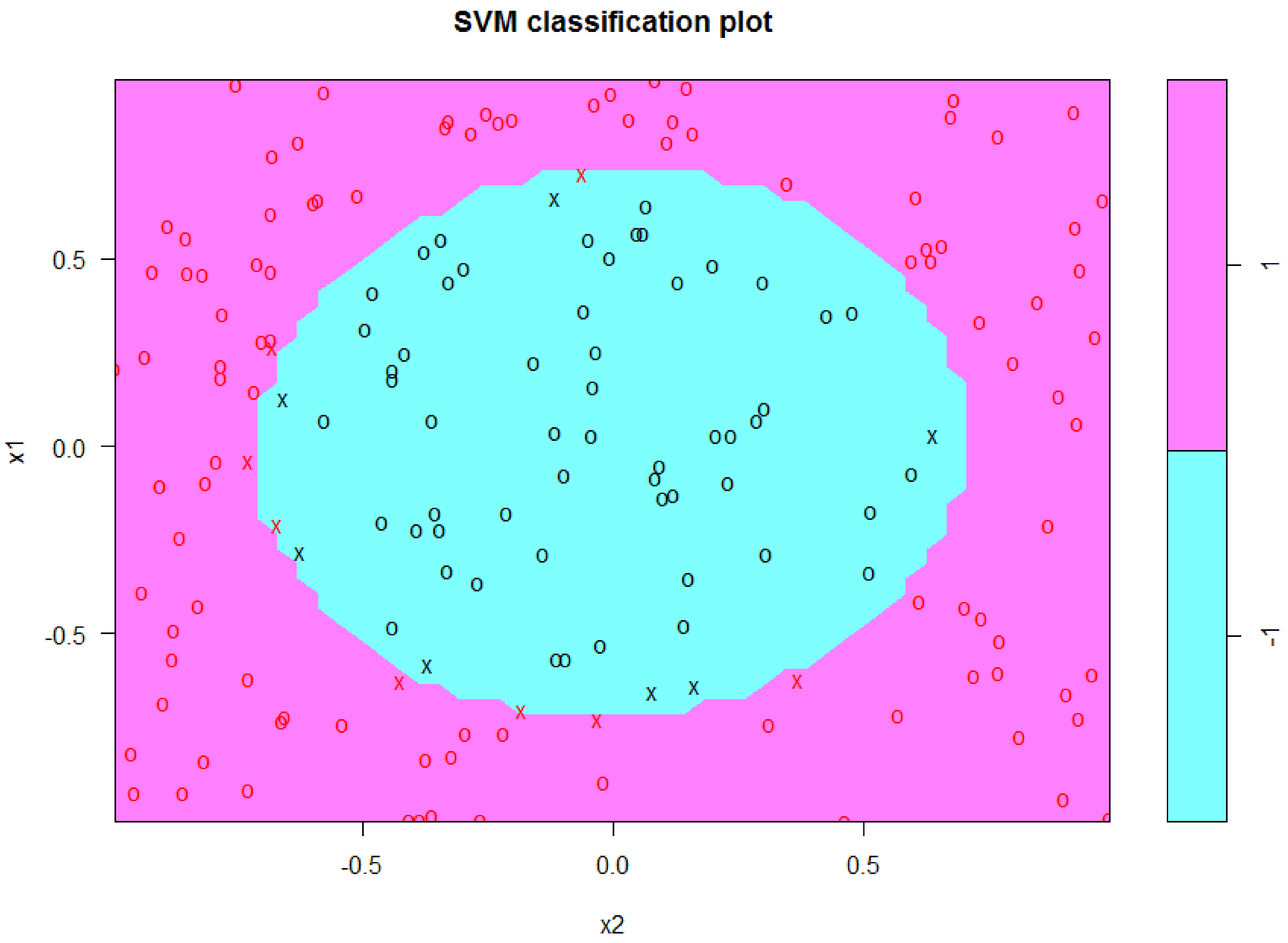
- Build SVM model using best values of parameters from `tune.svm()`.

```
svm_model <- svm(y~ ., data = trainset, type = "C-classification",
        kernel = "polynomial", degree = 2,
        cost = tune_out$best.parameters$cost,
        gamma = tune_out$best.parameters$gamma,
        coef0 = tune_out$best.parameters$coef0)
```

- evaluate training and test accuracy

```
pred_train <-predict(svm_model, trainset)
mean(pred_train==trainset$y)
[1] 1
pred_test <-predict(svm_model, testset)
mean(pred_test==testset$y)
[1] 0.9677419

#plot using svm plot
plot(svm_model, trainset)
```


SVM classification plot
x1
0.5
0.0
-0.5
x2
-0.5
0.0
0.5
1
-1

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