Introduction

SUPPORT VECTOR MACHINES IN R



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Preliminaries

- Objective: gain understanding of how SVMs work; options available in the algorithm and situations in which they work best.
- Prerequisites: Intermediate knowledge of R; basic visualization using ggplot().
- **Approach**: Start with 1-dimensional example and gradually move on to more complex examples.

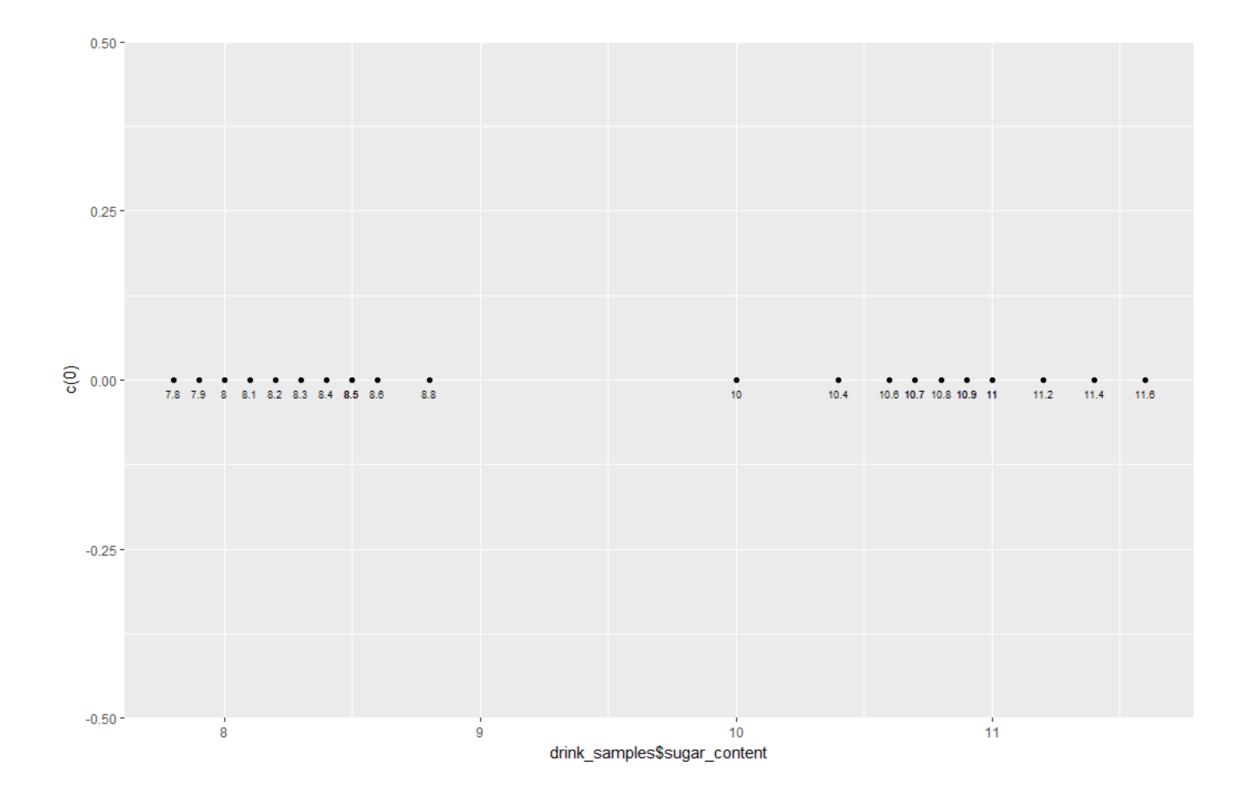
Sugar content of soft drinks

- Soft drink manufacturer has two versions of flagship brand:
 - Choke sugar content 11g/ 100 ml.
 - Choke-R sugar content 8 g/ 100 ml.
- Actual sugar content varies in practice.
- Given 25 samples chosen randomly, find a decision rule to determine brand.
- First step: visualize data!

Sugar content of soft drinks - visualization code

Data in drink_samples dataframe.

```
# Specify dataframe, set plot aesthetics in geom_point (note y = 0)
p <- ggplot(drink_samples) +</pre>
  geom_point(aes(sugar_content, 0))
# Label each point with sugar content value, adjust text size and location
p <- p +
  geom_text(aes(sugar_content, 0, label = sugar_content),
            size = 2.5,
            vjust = 2,
            hjust = 0.5)
# Display plot
p
```





Decision boundaries

- Let's pick two points in the interval as candidate boundaries:
 - 9.1 g/100 ml
 - 9.7 g/100 ml
- Classification (decision) rules:
 - if (y < 9.1) then "Choke-R" else "Choke"
 - o if (y < 9.7) then "Choke-R" else "Choke"
- · Let's visualize them on the plot shown on the previous slide.

Decision boundaries - visualization code

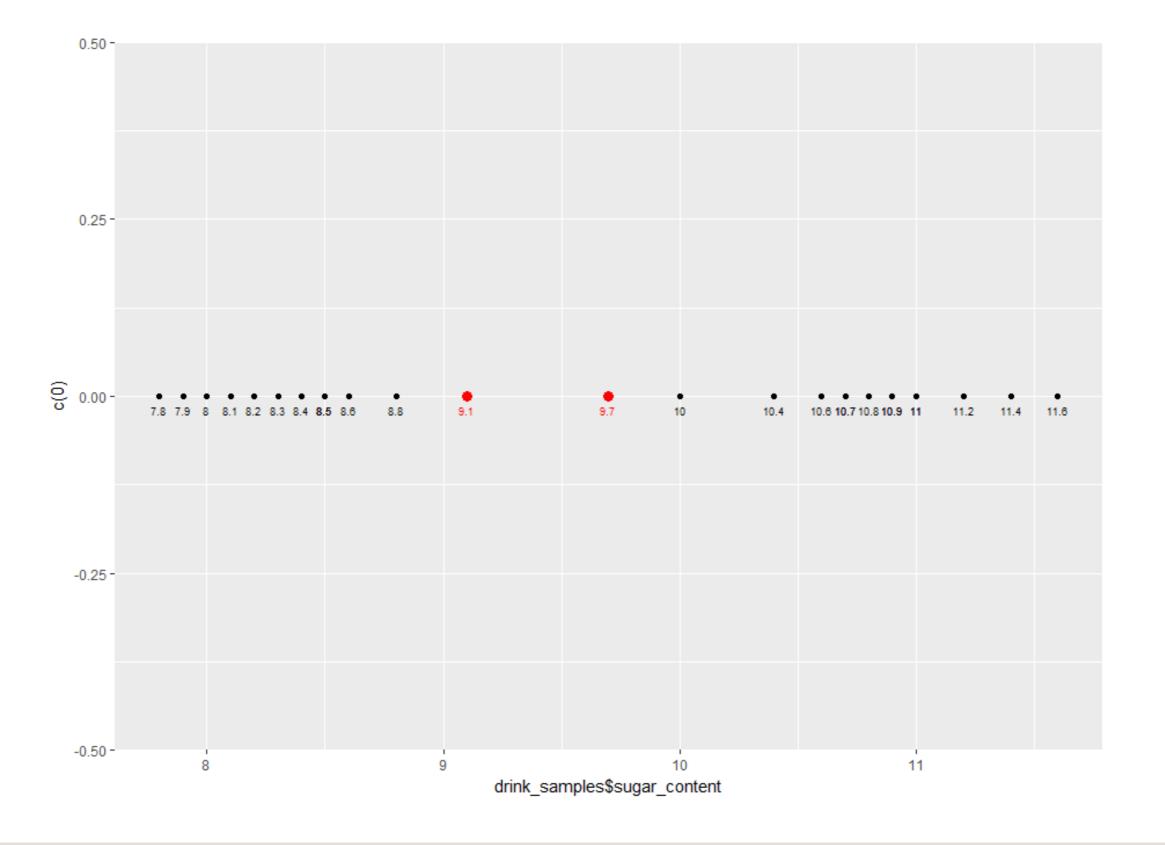
• Create a dataframe containing the two decision boundaries.

```
# Define data frame containing decision boundaries
d_bounds <- data.frame(sep = c(9.1, 9.7))</pre>
```

Decision boundaries - visualization code

Add to plot using geom_point()

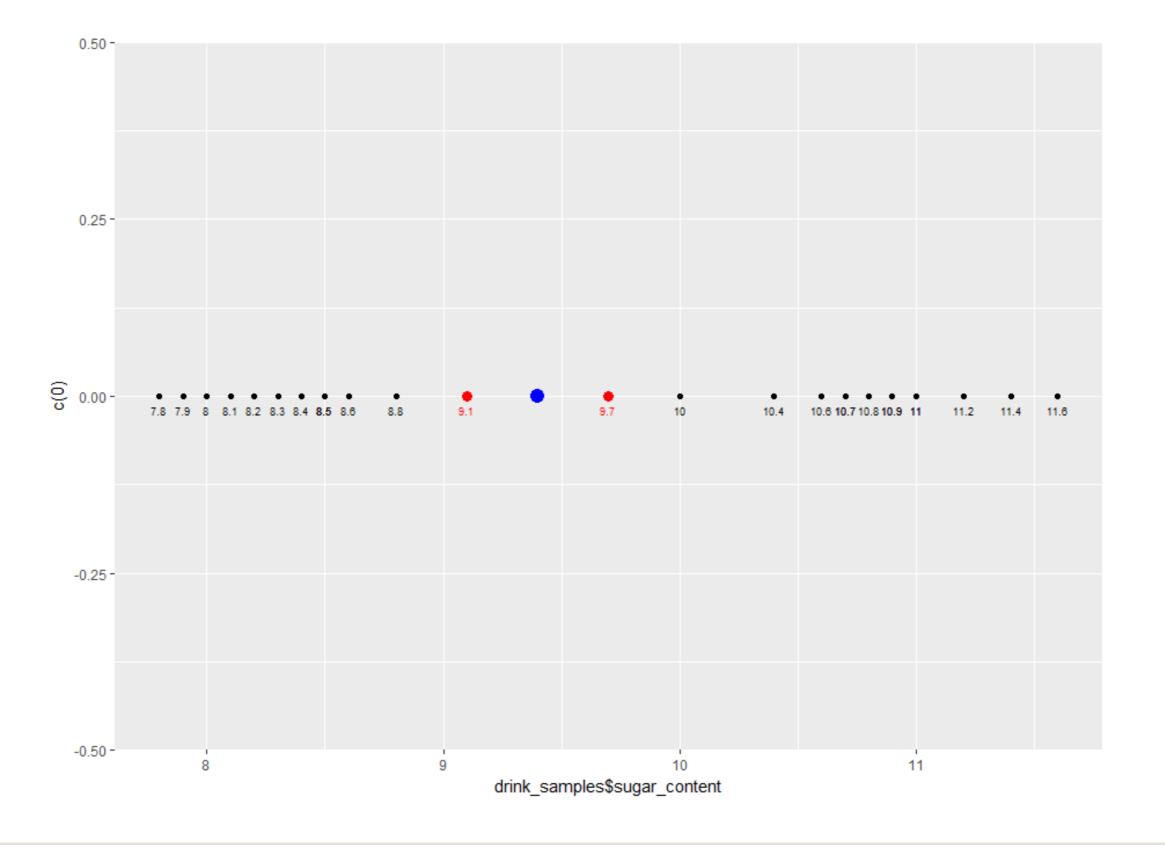
```
# Add decision boundaries to previous plot
p <- p +
  geom_point(data = d_bounds,
             aes(sep, 0),
             color = "red",
             size = 3) +
  geom_text(data = d_bounds,
            aes(sep, 0, label = sep),
            size = 2.5,
            vjust = 2,
            hjust = 0.5,
            color = "red")
# Display plot
p
```





Maximum margin separator

- The best decision boundary is one that maximizes the margin: maximal margin separator
- Maximal margin separator lies halfway between the two clusters.
- Visualize the maximal margin separator.





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Generating a linearly separable dataset

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Overview of lesson

- Create a dataset that we'll use to illustrate key principles of SVMs.
- Dataset has two variables and a linear decision boundary.

Generating a two-dimensional dataset using runif()

- Generate a two variable dataset with 200 points
- Variables x1 and x2 uniformly distributed in (0,1).

Creating two classes

- Create two classes, separated by the straight line decision boundary x1 = x2
- Line passes through (0, 0) and makes a 45 degree angle with horizontal
- Class variable y = -1 for points below line and y = 1 for points above it

```
# Classify points as -1 or +1  df\$y \leftarrow factor(ifelse(df\$x1 - df\$x2 > 0, -1, 1),   levels = c(-1, 1))
```

Visualizing dataset using ggplot

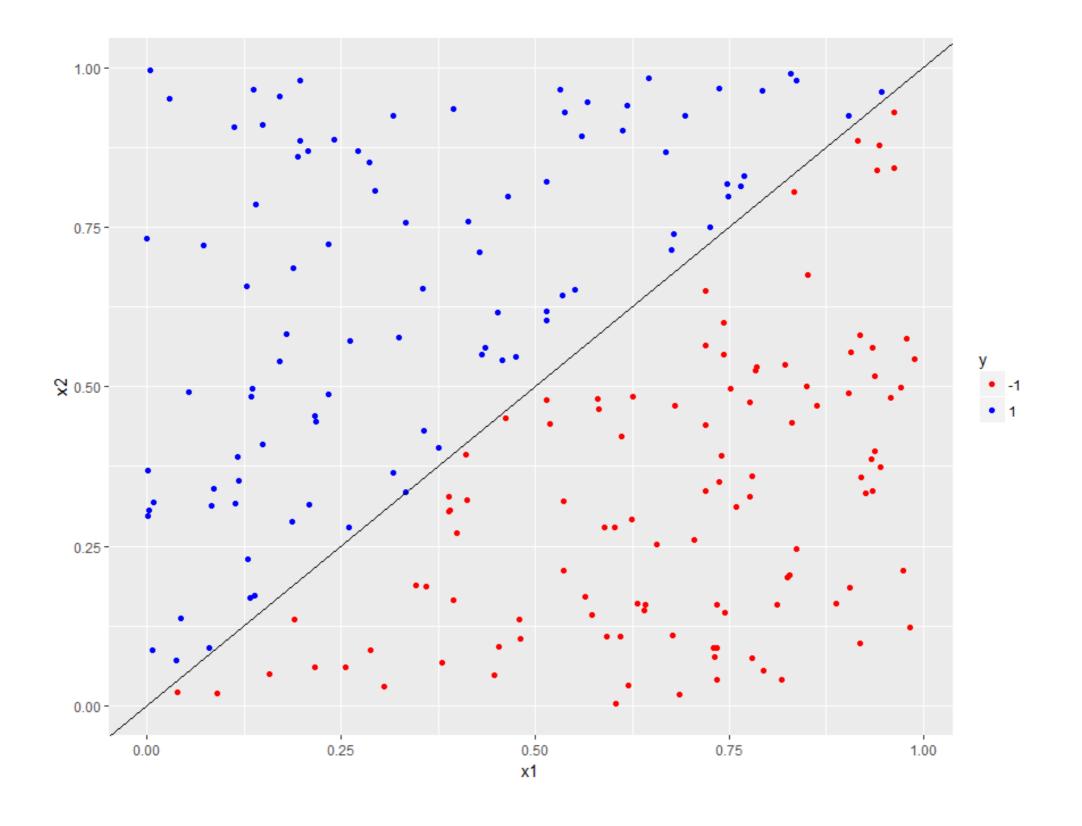
- Create 2 dimensional scatter plot with x1 on the x axis and x2 on the y-axis
- Distinguish classes by color (below line = red; above line = blue)
- Decision boundary is line x1 = x2: passes through (0, 0) and has slope = 1

```
library(ggplot2)

# Build plot

p <- ggplot(data = df, aes(x = x1, y = x2, color = y)) +
        geom_point() +
        scale_color_manual(values = c("-1" = "red", "1" = "blue")) +
        geom_abline(slope = 1, intercept = 0)

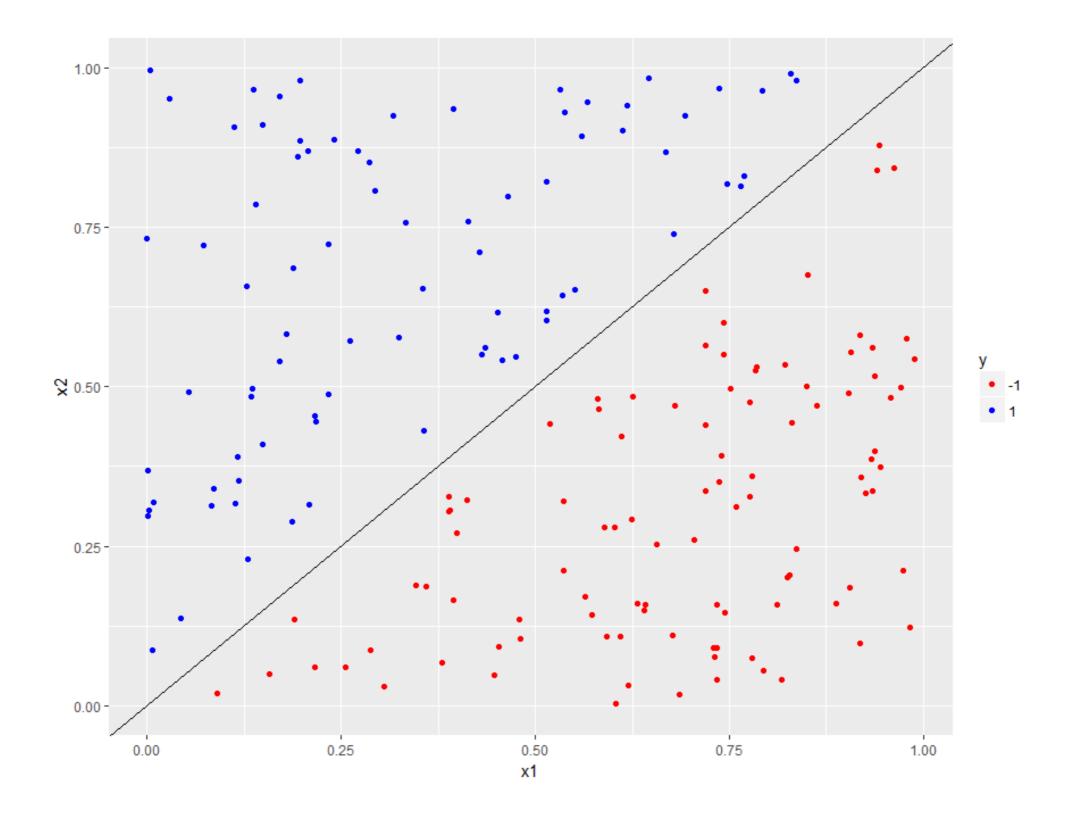
# Display it
p</pre>
```



Introducing a margin

- To create a margin we need to remove points that lie close to the boundary
- Remove points that have x1 and x2 values that differ by less than a specified value

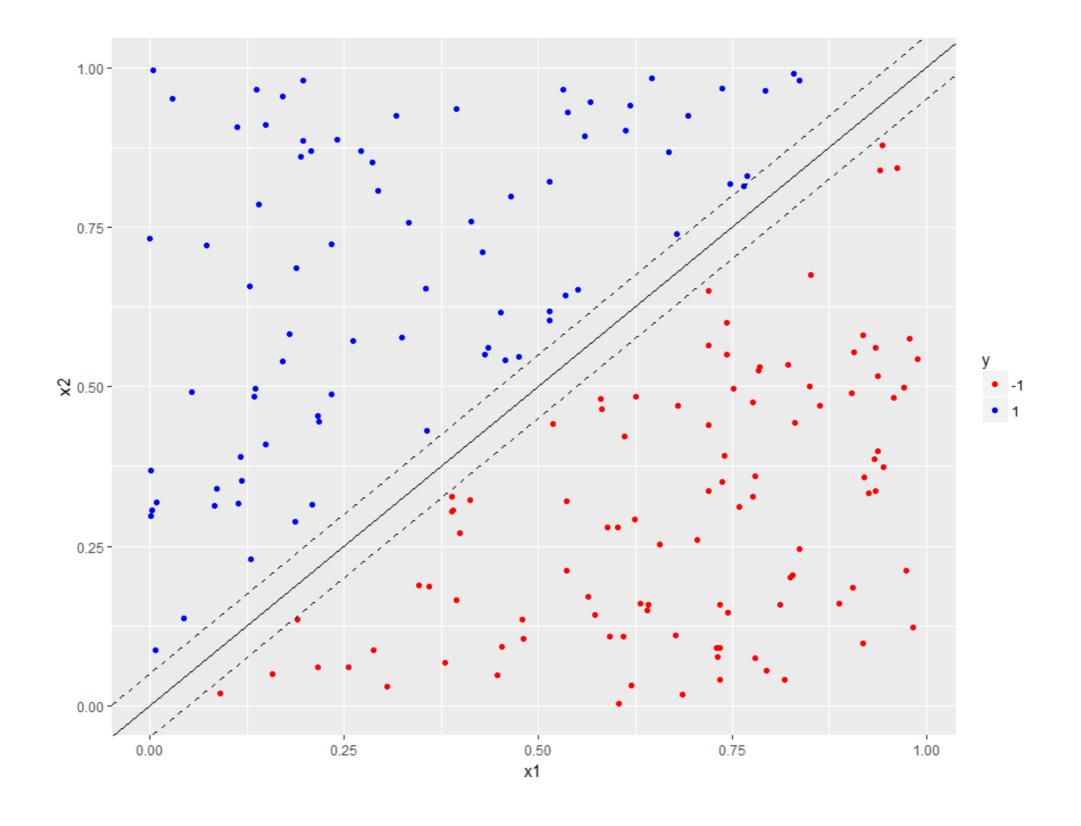
```
# Create a margin of 0.05 in dataset
delta <- 0.05
# Retain only those points that lie outside the margin
df1 \leftarrow df[abs(df$x1 - df$x2) > delta, ]
# Check number of data points remaining
nrow(df1)
# Replot dataset with margin (code is exactly same as before)
p \leftarrow qqplot(data = df1, aes(x = x1, y = x2, color = y)) +
     qeom_point() +
     scale_color_manual(values = c("red", "blue")) +
     qeom_abline(slope = 1, intercept = 0)
# Display plot
```



Plotting the margin boundaries

- The margin boundaries are:
 - parallel to the decision boundary (slope = 1).
 - located delta units on either side of it (delta = 0.05).

```
p <- p +
    geom_abline(slope = 1, intercept = delta, linetype = "dashed") +
    geom_abline(slope = 1, intercept = -delta, linetype = "dashed")
p</pre>
```



Time to practice!

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Linear Support Vector Machines

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Split into training and test sets

- The dataset generated in previous chapter is in dataframe df.
- Split dataset into training and test sets
- Random 80/20 split

```
# Set seed for reproducibility
set.seed(1)
# Set the upper bound for the number of rows to be in the training set
sample_size <- floor(0.8 * nrow(df))
# Assign rows to training/test sets randomly in 80/20 proportion
train <- sample(seq_len(nrow(df)), size = sample_size)
# Separate training and test sets
trainset <- df[train, ]
testset <- df[-train, ]</pre>
```

Decision boundaries and kernels

- Decision boundaries can have different shapes lines, polynomials or more complex functions.
- Type of decision boundary is called a **kernel**.
- Kernel must be specified upfront.
- This chapter focuses on linear kernels.

SVM with linear kernel

- We'll use the sym function from the e1071 library.
- The function has a number of parameters. We'll set the following explicitly:
 - o formula a formula specifying the dependent variable. y in our case.
 - data dataframe containing the data i.e. trainset.
 - type set to C-classification (classification problem).
 - **kernel** this is the form of the decision boundary, linear in this case.
 - o cost and gamma these are parameters that are used to tune the model.
 - o scale Boolean indicating whether to scale data.

Building a linear SVM

• Load e1071 library and invoke svm() function

```
library(e1071)
```

Overview of model

- Entering svm_model gives:
 - an overview of the model including classification and kernel type
 - tuning parameter values

```
svm_model
```

```
Call:
svm(formula = y ~ .,
    data = trainset,
    type = "C-classification",
    kernel = "linear",
    scale = FALSE)
Parameters:
  SVM-Type: C-classification
SVM-Kernel: linear
      cost: 1
             0.5
      gamma:
Number of Support Vectors: 55
```

```
# Index of support vectors in training dataset
svm_model$index
# Support vectors
svm_model$SV
# Negative intercept (unweighted)
svm_model$rho
# Weighting coefficients for support vectors
svm_model$coefs
```

```
4 8 10 11 18 37 38 39 47 59 60 74 76 77 78 80 83 ...

x1 x2

5 0.519095949 0.44232464

-0.1087075

[,1]

[1,] 1.0000000
```

- Obtain class predictions for training and test sets.
- Evaluate the training and test set accuracy of the model.

```
# Training accuracy
pred_train <- predict(svm_model, trainset)
mean(pred_train == trainset$y)</pre>
```

1

```
# Test accuracy
pred_test <- predict(svm_model, testset)
mean(pred_test == testset$y)</pre>
```

```
1
# Perfect!!
```

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Visualizing linear SVMs

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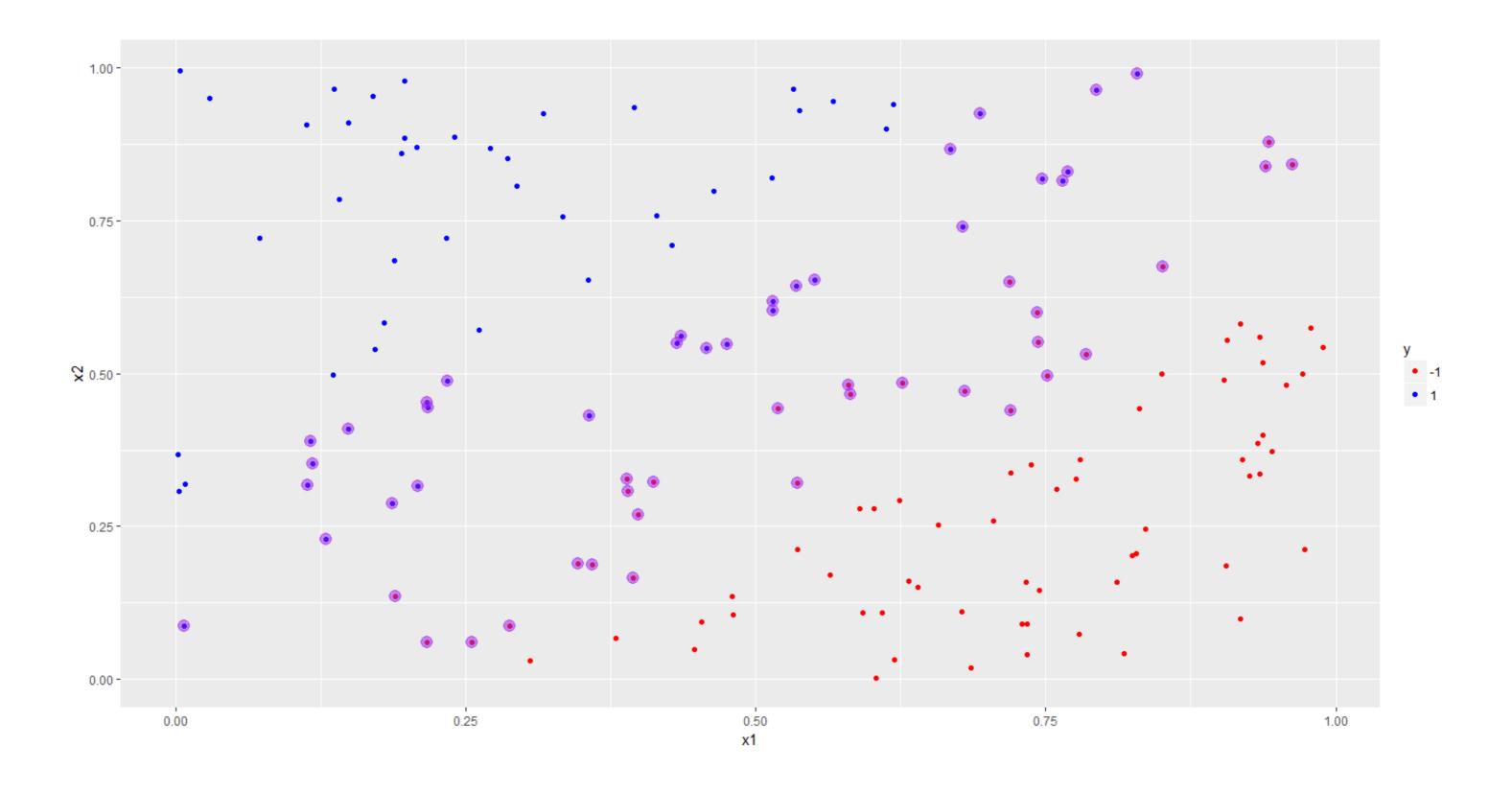
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• Plot the training data using ggplot().

```
# Visualize training data, distinguish classes using color
p <- ggplot(data = trainset, aes(x = x1, y = x2, color = y)) +
        geom_point() +
        scale_color_manual(values = c("red", "blue"))
# Render plot
p</pre>
```

Mark out the support vectors using index from svm_model.





Find slope and intercept of the boundary:

• Build the weight vector, w, from coefs and SV elements of svm_model.

```
# Build weight vector
w <- t(svm_model$coefs) %*% svm_model$SV</pre>
```

• slope = -w[1] / w[2]

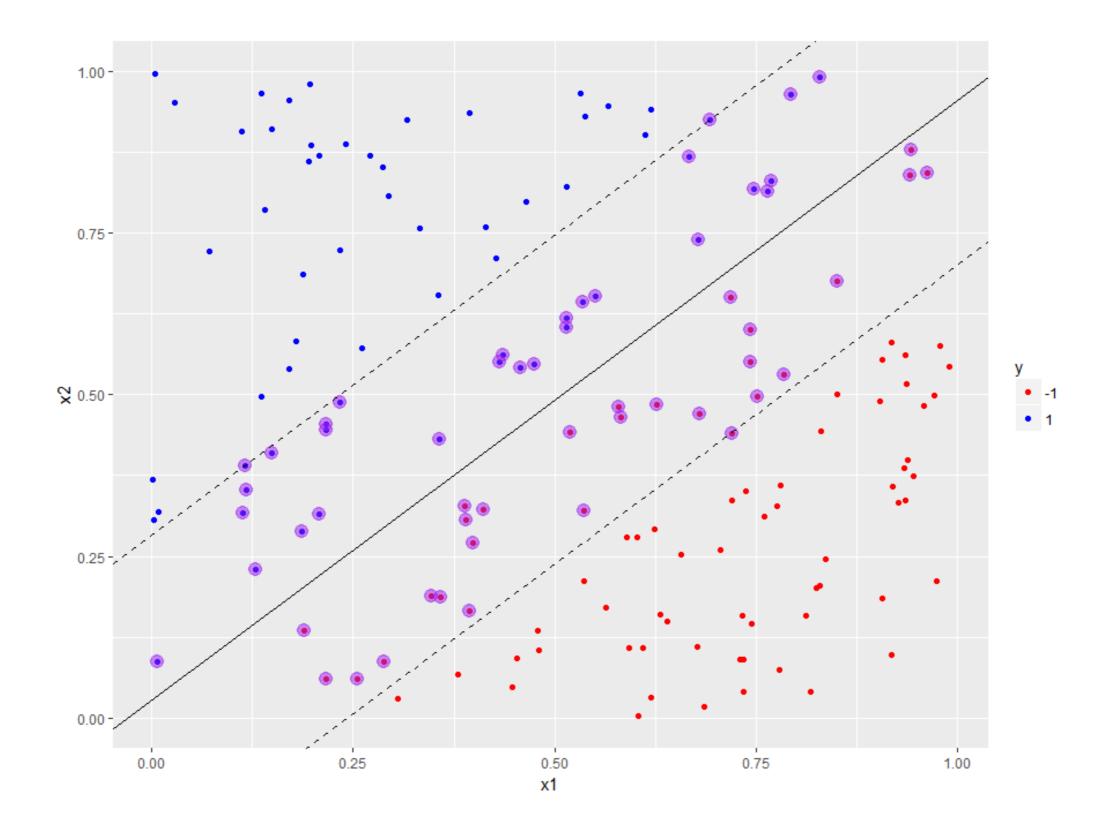
```
# Calculate slope and save it to a variable
slope_1 <- -w[1] / w[2]</pre>
```

• intercept = svm_model\$rho / w[2]

```
# Calculate intercept and save it to a variable
intercept_1 <- svm_model$rho / w[2]</pre>
```

- Add decision boundary using slope and intercept calculated in previous slide.
- We use geom_abline() to add the decision boundary to the plot.

• Margins parallel to decision boundary, offset by 1 / w[2] on either side of it.



Soft margin classifiers

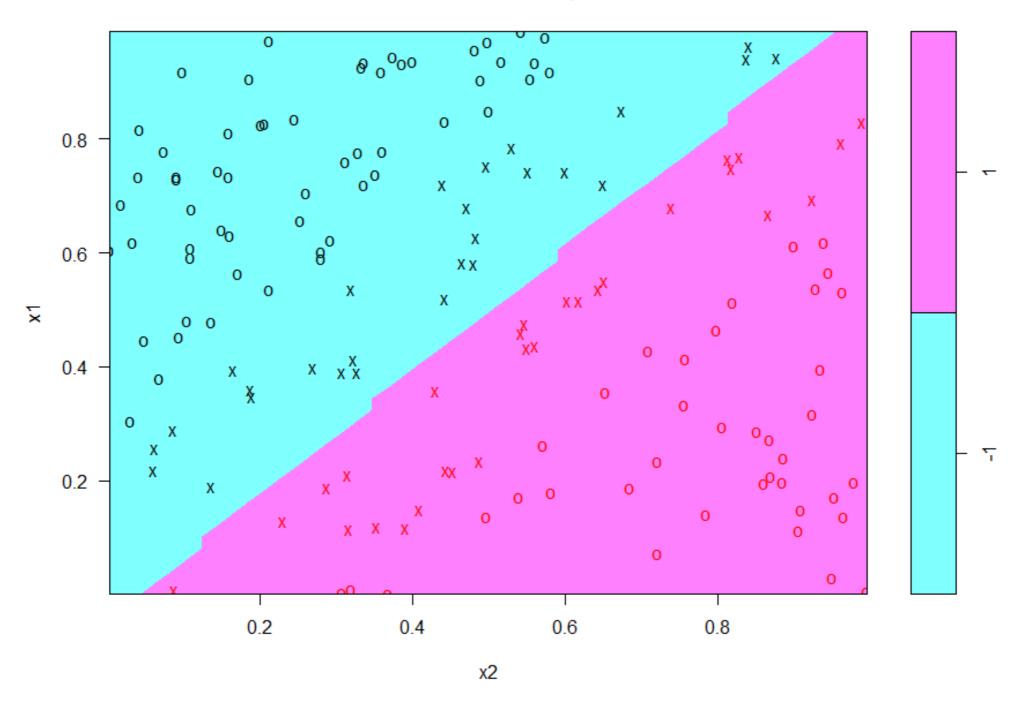
- Allow for uncertainty in location / shape of boundary
 - Never perfectly linear
 - Usually unknown
- Our decision boundary is linear, so we can reduce margin

Visualizing the decision boundary using the sym plot() function

• The svm plot() function in e1071 offers an easy way to plot the decision boundary.

```
# Visualize decision boundary using built in plot function
plot(x = svm_model,
    data = trainset)
```

SVM classification plot



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Tuning linear SVMs

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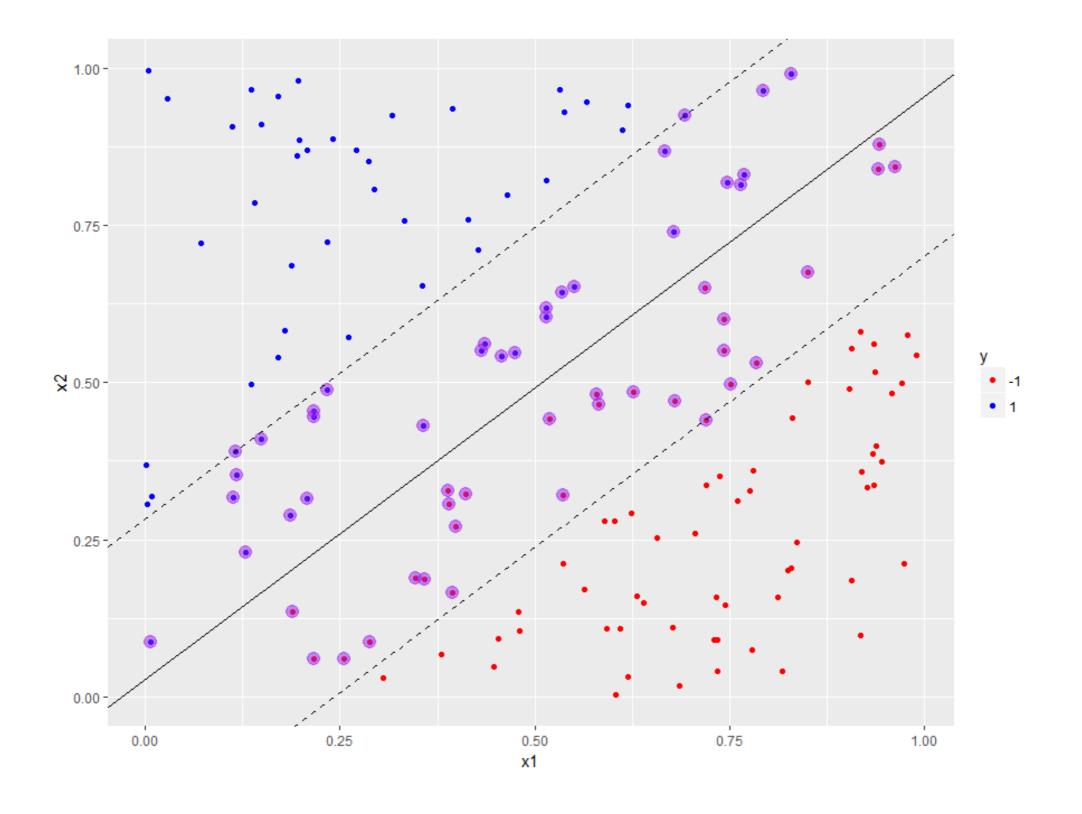


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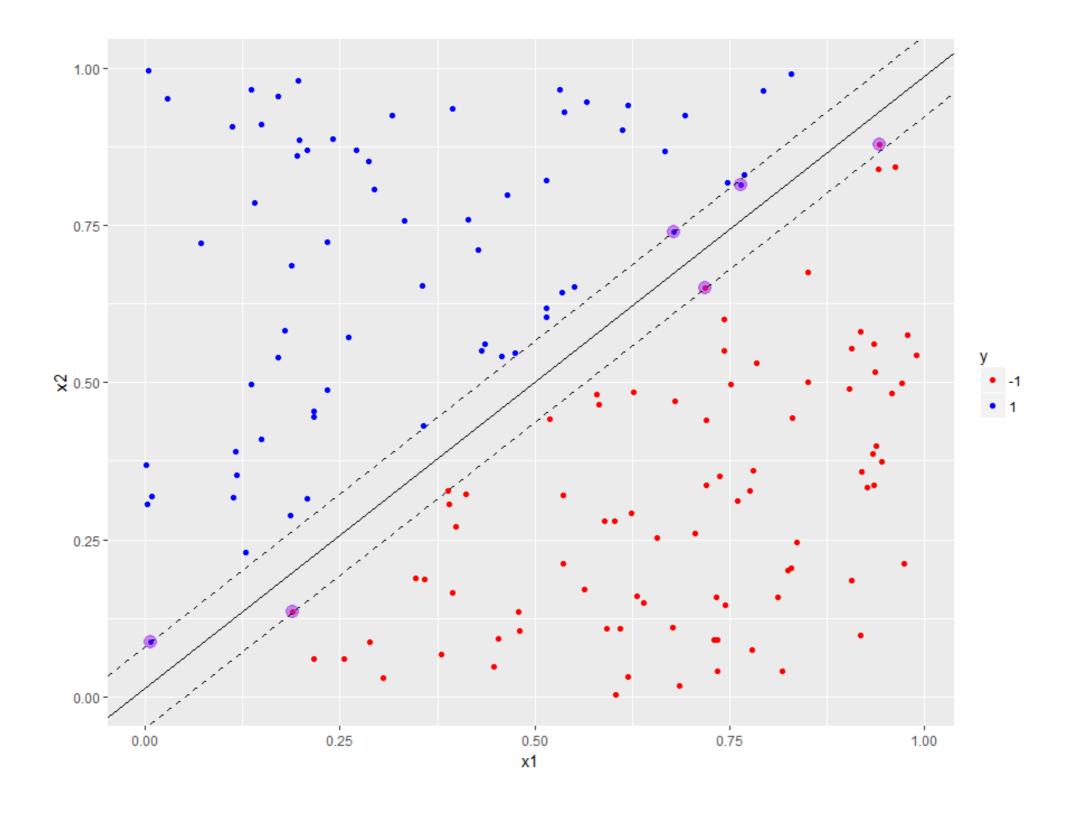
Linear SVM, default cost

```
Call:
svm(formula = y ~ .,
   data = trainset,
   type = "C-classification",
   kernel = "linear",
   scale = FALSE)
Parameters:
SVM-Type: C-classification
SVM-Kernel: linear
      cost: 1
      gamma: 0.5
Number of Support Vectors: 55
```



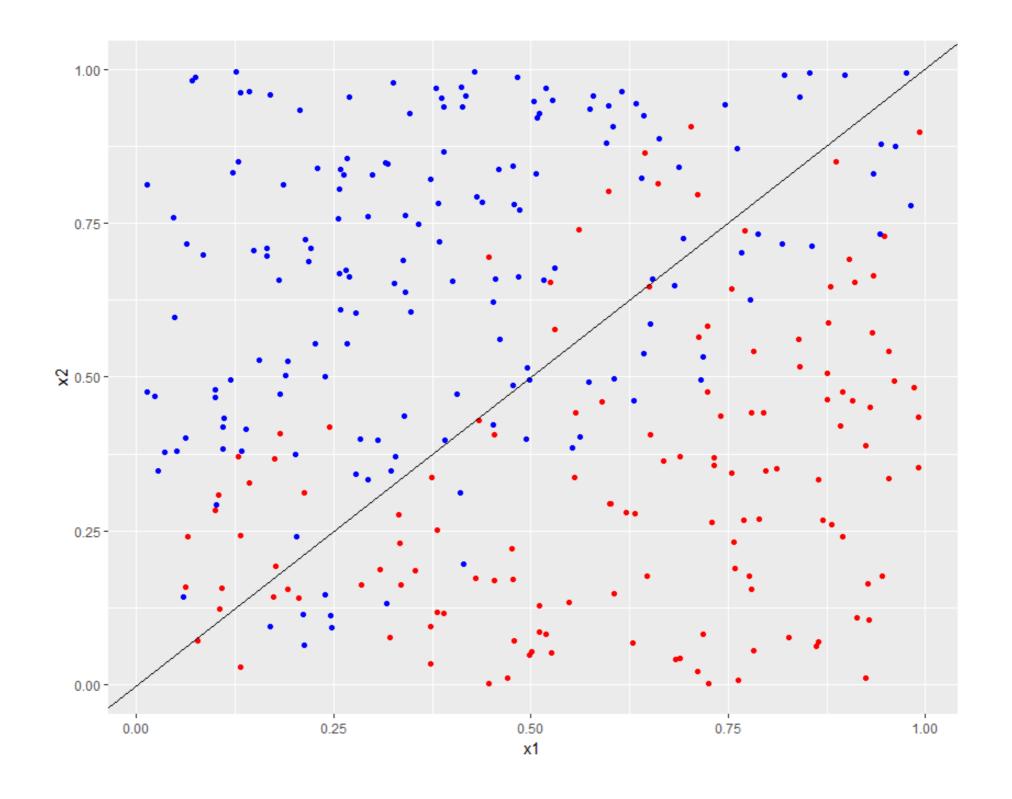
Linear SVM with cost = 100

```
Call:
svm(formula = y ~ .,
   data = trainset,
   type = "C-classification",
   kernel = "linear",
   cost = 100,
   scale = FALSE)
Parameters:
SVM-Type: C-classification
SVM-Kernel: linear
      cost: 100
     gamma: 0.5
Number of Support Vectors: 6
```



Implication

- Can be useful to reduce margin if decision boundary is known to be linear
- ...but this is rarely the case in real life



Nonlinear dataset, linear SVM (cost = 100)

 Build cost=100 model using training set composed of 80% of data

Calculate accuracy

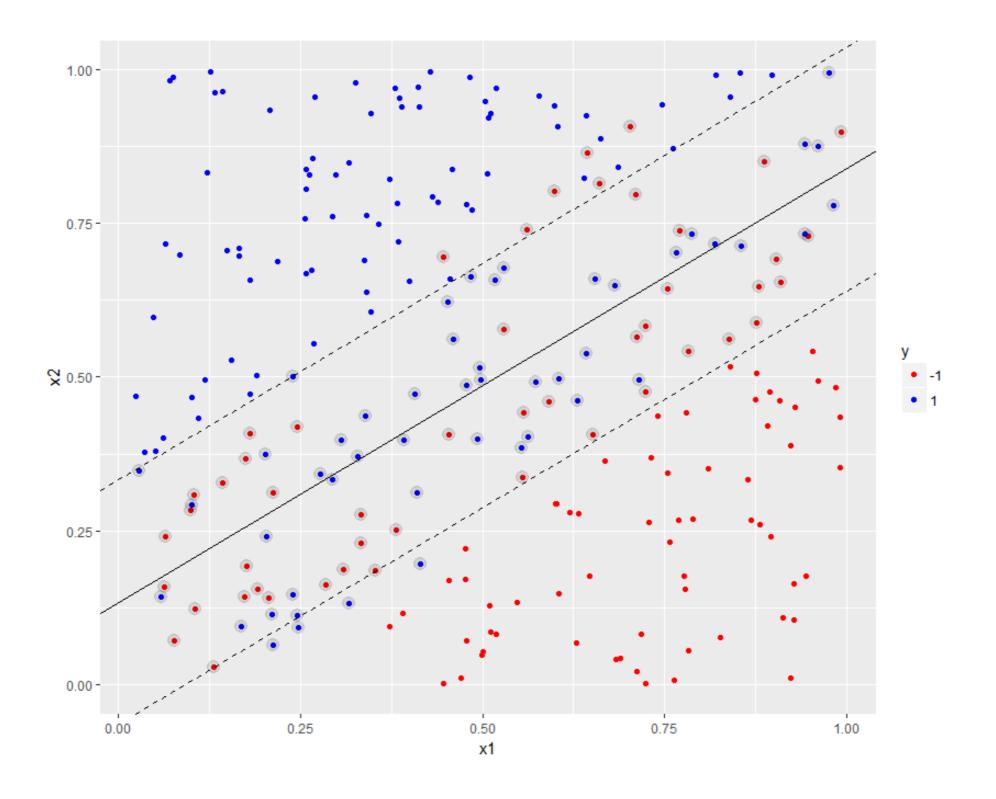
```
# Train and test accuracy
pred_train <- predict(svm_model, trainset)
mean(pred_train == trainset$y)</pre>
```

0.8208333

```
pred_test <- predict(svm_model, testset)
mean(pred_test == testset$y)</pre>
```

0.85

 Average test accuracy over 50 random train/test splits: 82.9%



Nonlinear dataset, linear SVM (cost = 1)

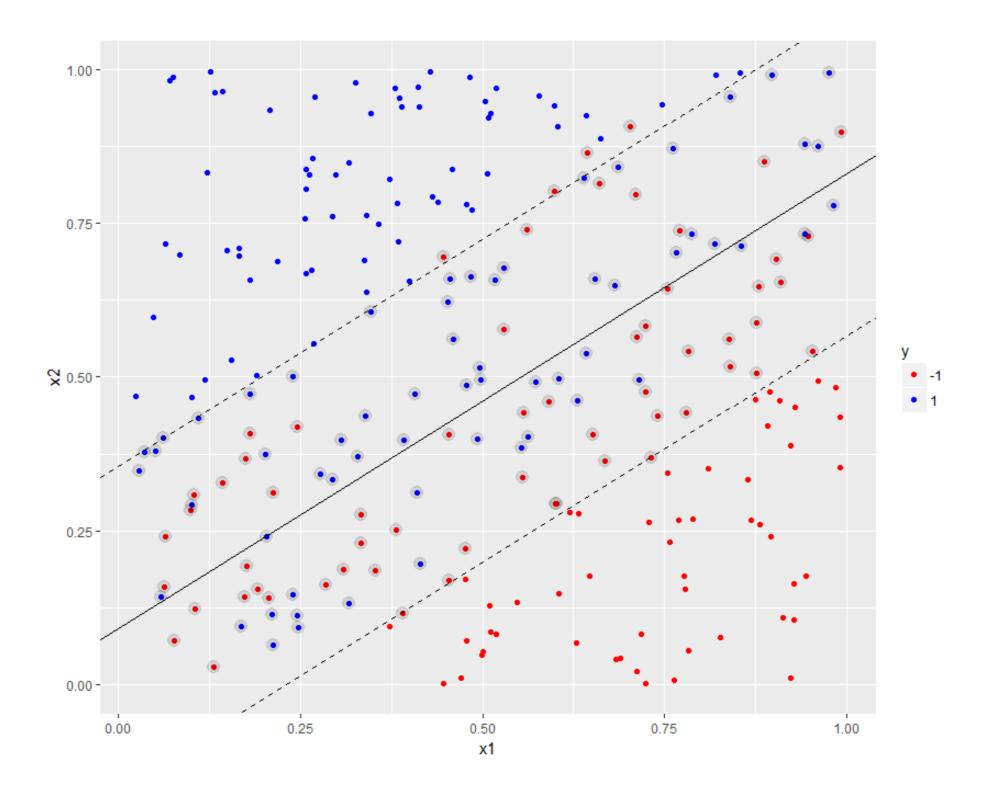
Rebuild model setting cost =1

Calculate test accuracy

```
# Test accuracy
pred_test <- predict(svm_model, testset)
mean(pred_test == testset$y)</pre>
```

0.8666667

 Average test accuracy over 50 random train/test splits: 83.7%



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Multiclass problems

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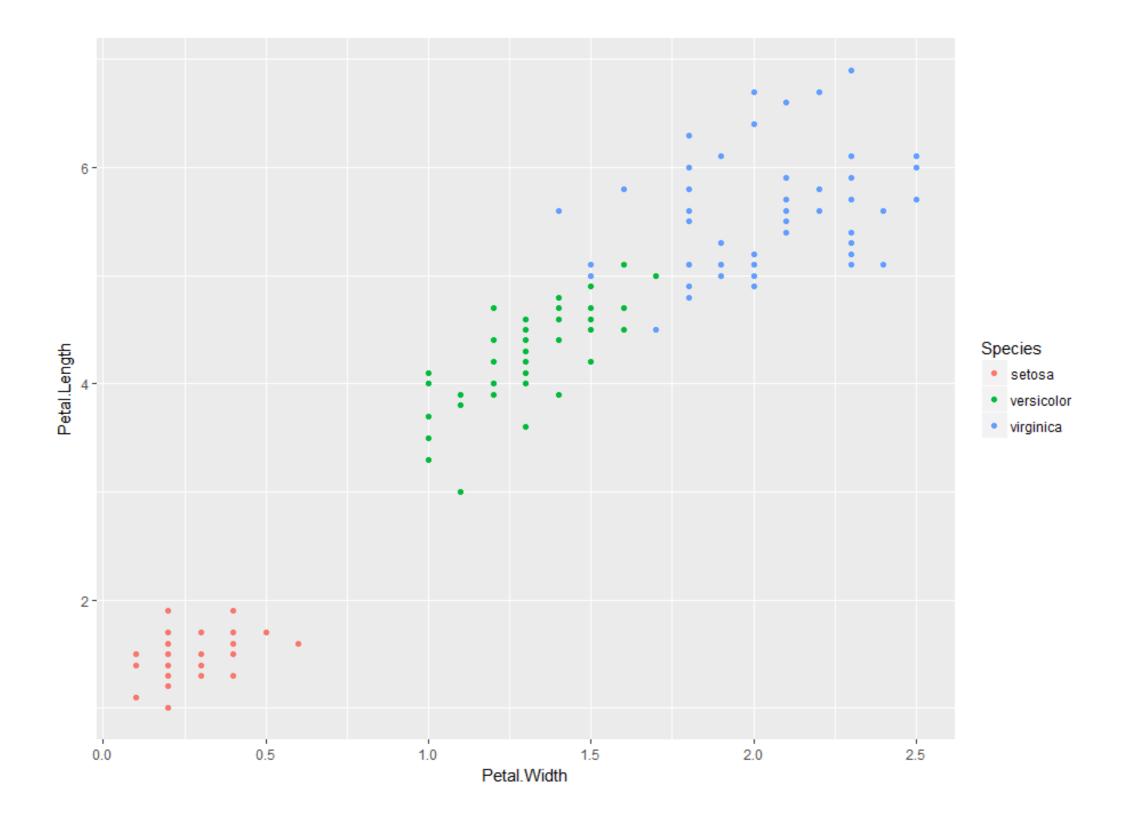
The iris dataset - an introduction

- 150 measurements of 5 attributes
 - Petal width and length number (predictor variables)
 - Sepal width and length number (predictor variables)
 - Species category: setosa, virginica or versicolor (predicted variable)
- Dataset available from UCI ML repository

Visualizing the iris dataset

Plot petal length vs petal width.

```
library(ggplot2)
# Plot petal length vs width for dataset, distinguish species by color
p <- ggplot(data = iris,</pre>
            aes(x = Petal.Width,
                 y = Petal.Length,
                color = Species)) +
     geom_point()
# Display plot
p
```



How does the SVM algorithm deal with multiclass problems?

- SVMs are essentially binary classifiers.
- Can be applied to multiclass problems using the following voting strategy:
 - Partition the data into subsets containing two classes each.
 - Solve the binary classification problem for each subset.
 - Use majority vote to assign a class to each data point.
- Called one-against-one classification strategy.

Building a multiclass linear SVM

- Build a linear SVM for the iris dataset
 - 80/20 training / test split (seed 10), default cost

Calculate accuracy

```
pred_train <- predict(svm_model, trainset)
mean(pred_train == trainset$Species)</pre>
```

0.9756098

```
pred_test <- predict(svm_model, testset)
mean(pred_test == testset$Species)</pre>
```

0.962963

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Generating a radially separable dataset

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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.

Create a circular boundary

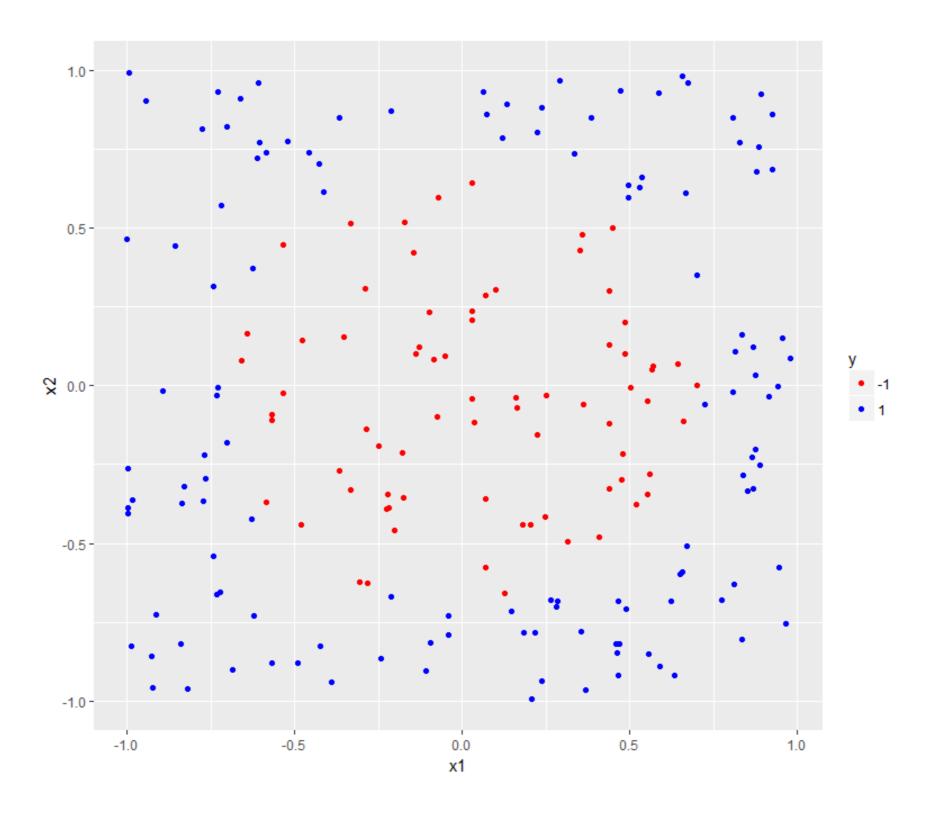
- Create a circular decision boundary of radius 0.7 units.
- Categorical variable y is +1 or -1 depending on the point lies outside or within boundary.

Plot the dataset

Visualize using ggplot.

```
library(ggplot2)
```

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



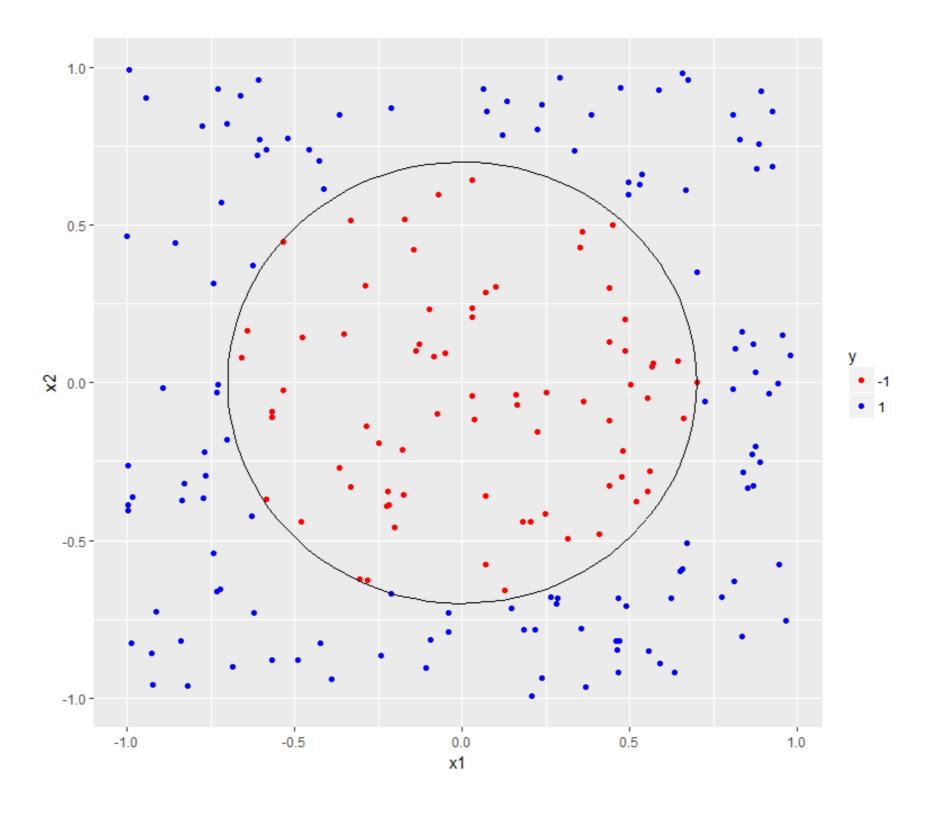
Adding a circular boundary - Part 1

• 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 \leftarrow seq(0, 2 * pi, length.out = npoint)
  x1_circ <- x1_center + r * cos(theta)</pre>
  x2_circ <- x2_center + r * sin(theta)
  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()



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Linear SVMs on radially separable data

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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", cost = 1)
svm_model</pre>
```

Number of Support Vectors: 126

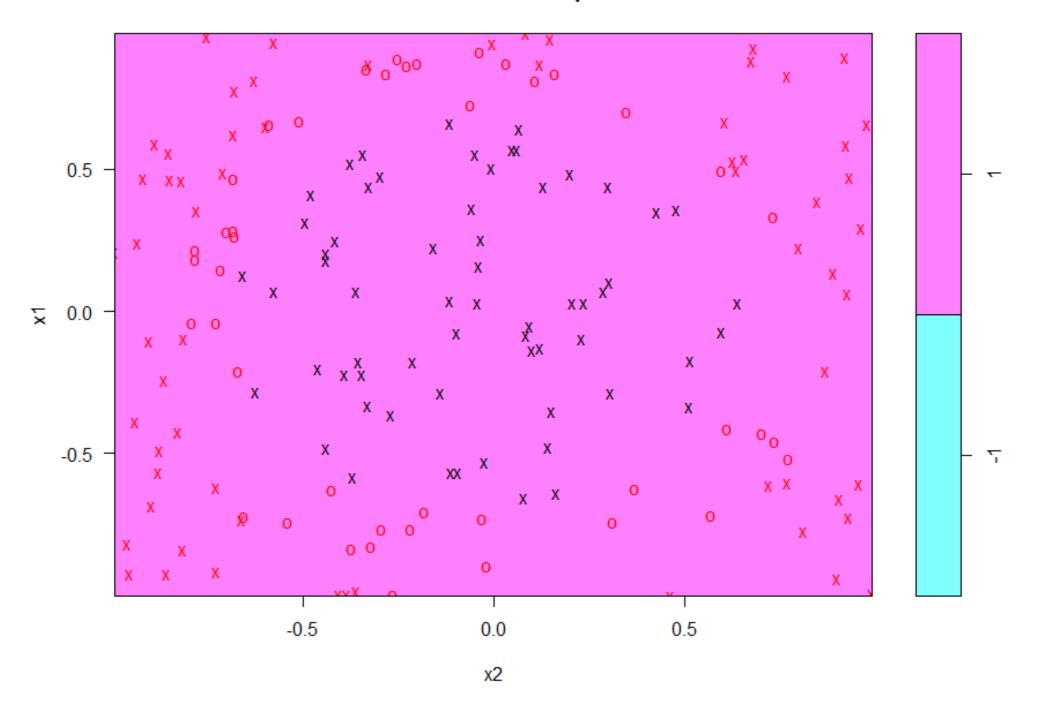
```
# Calculate accuracy on test set
pred_test <- predict(svm_model, testset)
mean(pred_test == testset$y)</pre>
```

0.6129032

```
plot(svm_model, trainset)
```



SVM classification plot



Linear SVM, cost = 100

```
svm_model <- svm(y ~ ., data = trainset, type = "C-classification", kernel = "linear", cost = 100)
svm_model</pre>
```

Number of Support Vectors: 136

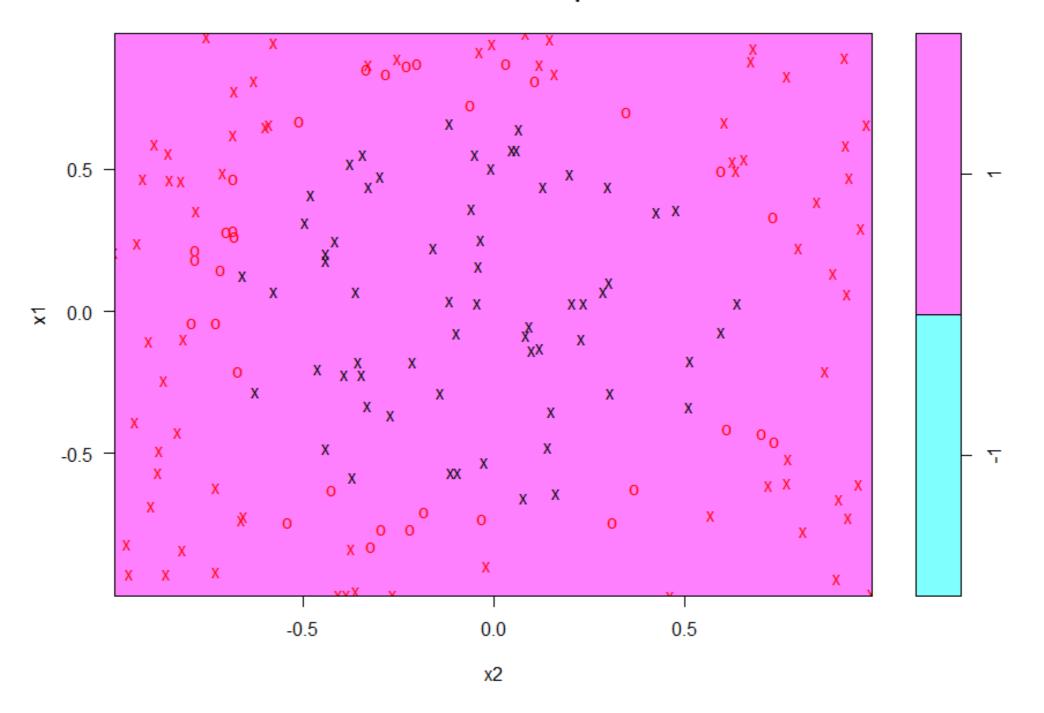
```
# Accuracy
pred_test <- predict(svm_model, testset)
mean(pred_test == testset$y)</pre>
```

0.6129032

```
plot(svm_model, trainset)
```



SVM classification plot



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) {
    sample_size <- floor(0.8 * nrow(df))
    train <- sample(seq_len(nrow(df)), size = sample_size)
    trainset <- df[train, ]
    testset <- df[-train, ]
    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)
sd(accuracy)</pre>
```

```
0.5440.04273184
```



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.

Time to practice!

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The kernel trick

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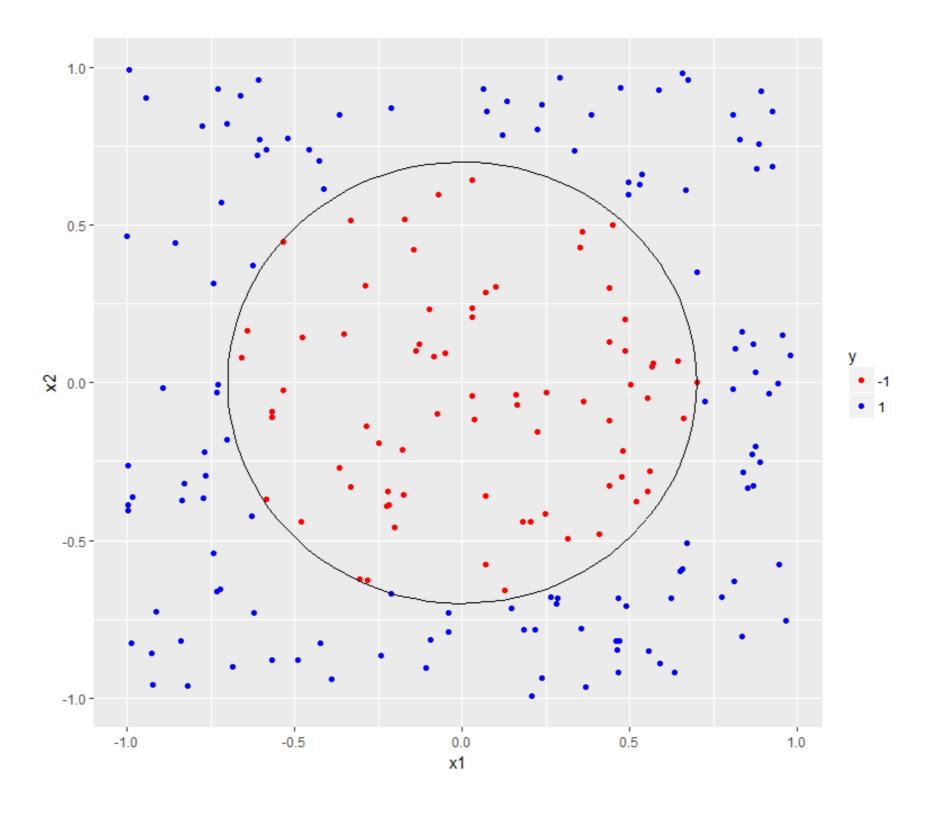


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The basic idea

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



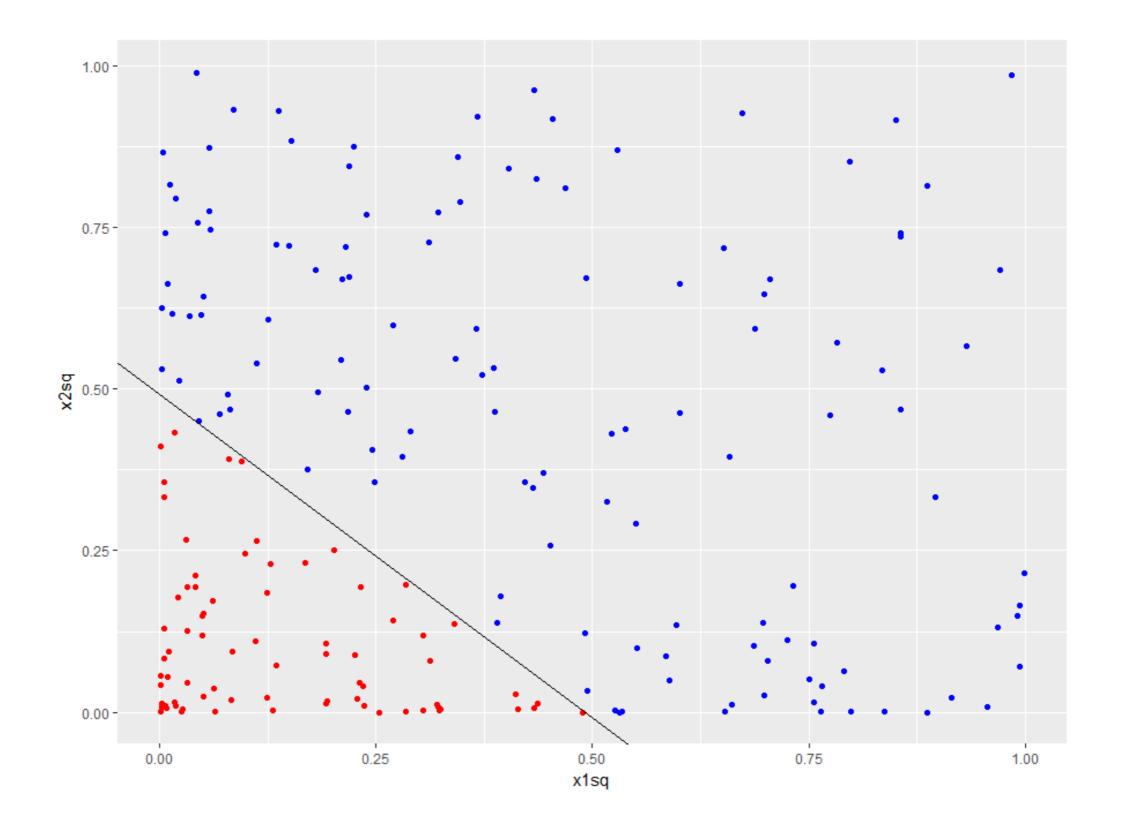
Transforming the problem

- ullet Equation of boundary is $x_1^2+x_2^2=0.49$
- ullet Map x_1^2 to a new variable X_1 and x_2^2 to X_2
- ullet The equation of boundary in the X_1-X_2 space becomes...
- $X_1 + X_2 = 0.49$ (a line!!)

Plot in X1-X2 space - code

- ullet Use ggplot() to plot the dataset in X_1-X_2 space
- Equation of boundary $X_2 = -X_1 + 0.49$:
 - \circ slope = -1
 - $\circ yintercept = 0.49$

```
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)</pre>
```





The Polynomial Kernel - Part 1

- Polynomial kernel: (gamma * (u.v) + coef0) ^ degree
 - degree is the degree of the polynomial
 - o gamma and coef0 are tuning parameters
 - o u, v are 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:
 - Set degree = 2
 - Set default values of cost, gamma and coef0 (1, 1/2 and 0)

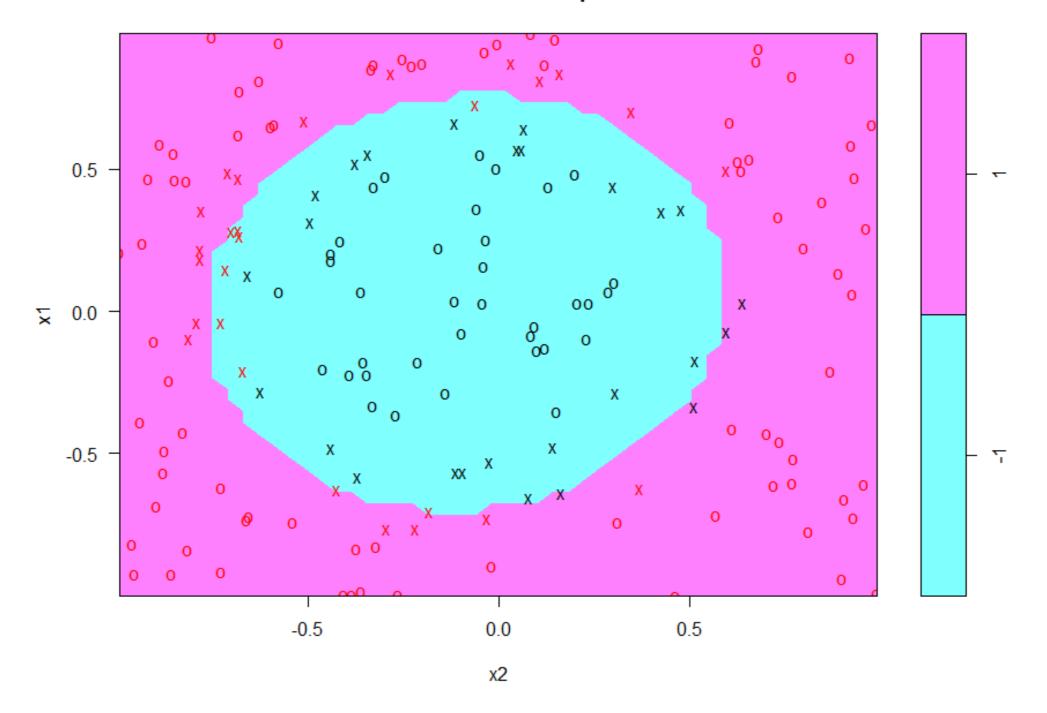
```
svm_model <- svm(y ~ ., data = trainset, type = "C-classification", kernel = "polynomial", degree = 2)
# Predictions
pred_test <- predict(svm_model, testset)
mean(pred_test == testset$y)</pre>
```

0.9354839

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



SVM classification plot



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Tuning SVMs

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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!

- 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?

```
0.1
10
1
```

• 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)</pre>
```

evaluate training and test accuracy

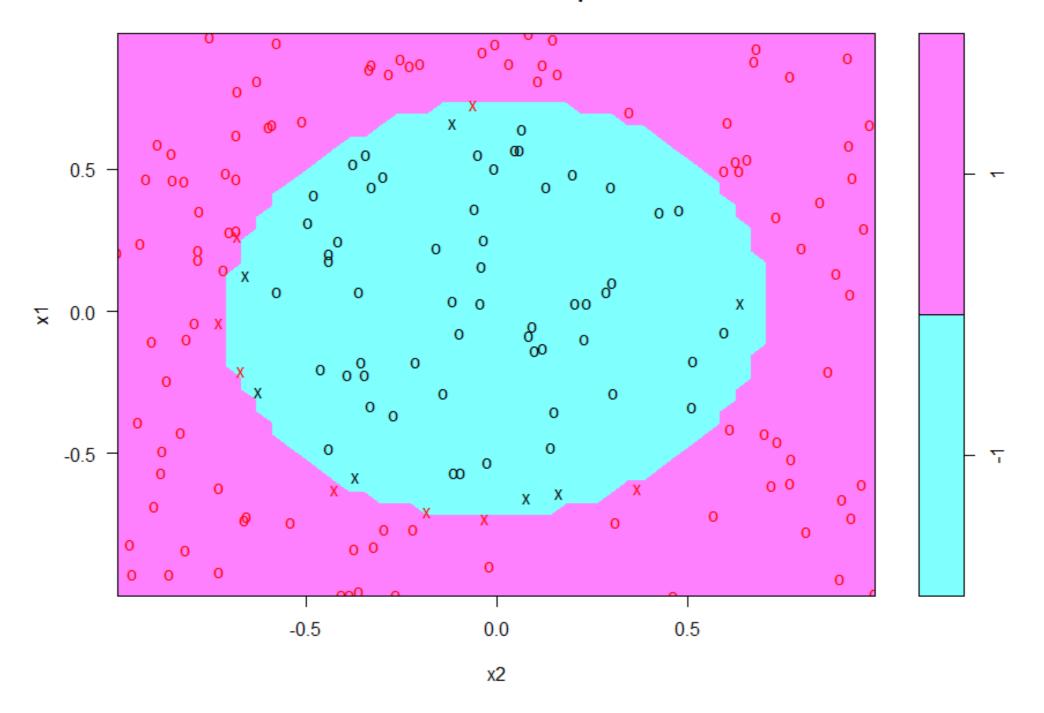
```
pred_train <- predict(svm_model, trainset)
mean(pred_train == trainset$y)
pred_test <- predict(svm_model, testset)
mean(pred_test == testset$y)</pre>
```

```
1
0.9677419
```

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



SVM classification plot



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RBF Kernels: Generating a complex dataset

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A bit about RBF Kernels

- Highly flexible kernel.
 - Can fit complex decision boundaries.
- Commonly used in practice.

Generate a complex dataset

- 600 points (x1, x2)
- x1 and x2 distributed differently

Generate boundary

Boundary consists of two equi-radial circles with a single point in common.

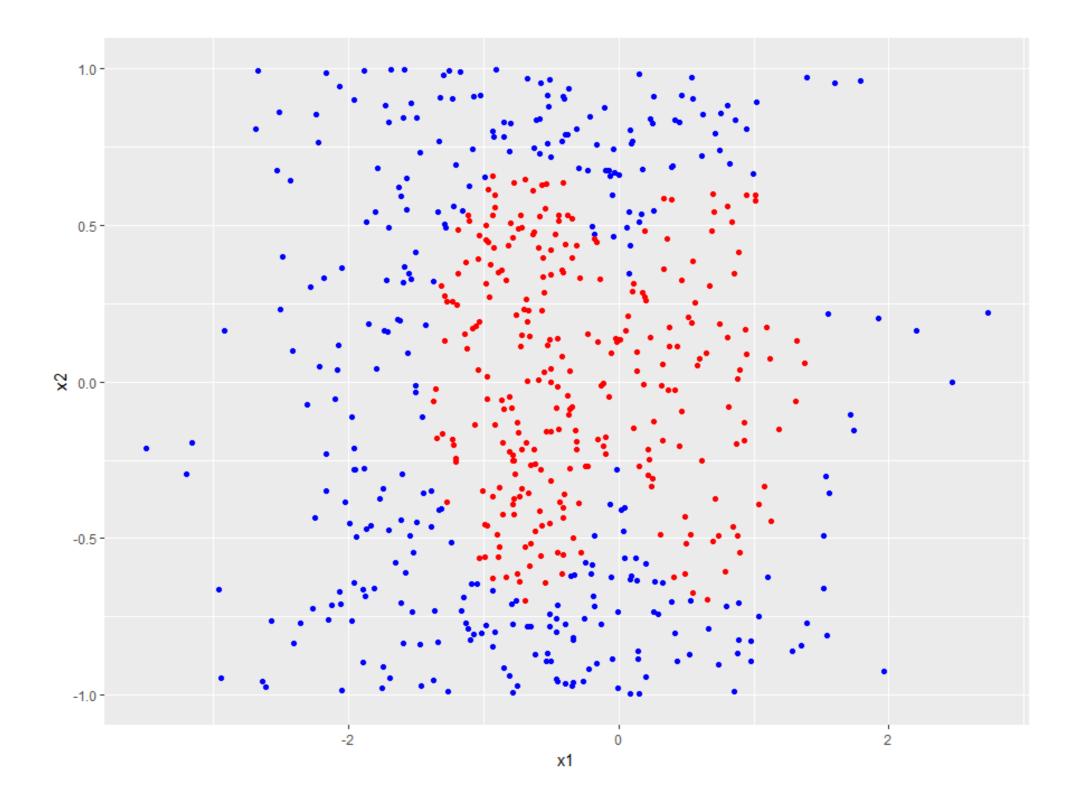
```
# Set radius and centers
radius <- 0.7
radius_squared <- radius ^ 2</pre>
center_1 <- c(-0.7, 0)
center_2 <- c(0.7, 0)
# Classify points
df$y <-
    factor(ifelse(
        (df$x1 - center_1[1]) ^ 2 + (df$x2 - center_1[2]) ^ 2 < radius_squared |
        (df$x1 - center_2[1]) ^ 2 + (df$x2 - center_2[2]) ^ 2 < radius_squared,
        -1, 1), levels = c(-1, 1))
```

Visualizing the dataset

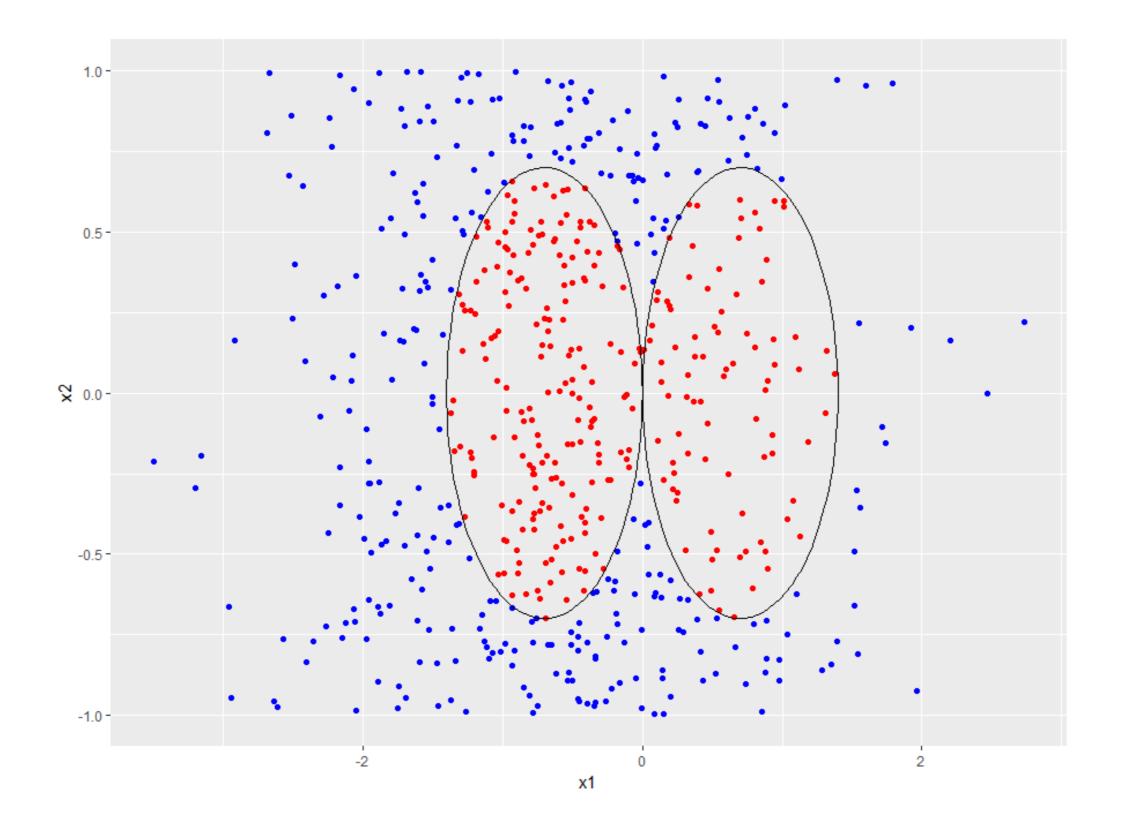
Visualize the dataset using ggplot; distinguish classes by color

```
library(ggplot2)

p <- ggplot(data = df, aes(x = x1, y = x2, color = y)) +
    geom_point() +
    guides(color = "none") +
    scale_color_manual(values = c("red", "blue"))</pre>
```



```
# Function to generate points on a circle
circle <- function(x1_center, x2_center, r, npoint = 100) {
   theta \leftarrow seq(0, 2 * pi, length.out = npoint)
   x1_circ <- x1_center + r * cos(theta)
   x2_circ <- x2_center + r * sin(theta)
   data.frame(x1c = x1_circ, x2c = x2_circ)
# Generate boundary and plot it
boundary_1 <- circle(x1_center = center_1[\frac{1}{1}], x2_center = center_1[\frac{2}{1}], r = radius)
p <- p +
     geom_path(data = boundary_1,
               aes(x = x1c, y = x2c),
               inherit.aes = FALSE)
boundary_2 <- circle(x1_center = center_2[1], x2_center = center_2[2], r = radius)
p <- p +
     geom_path(data = boundary_2,
               aes(x = x1c, y = x2c),
               inherit.aes = FALSE)
```



Time to practice!

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Motivating the RBF kernel

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Quadratic kernel (default parameters)

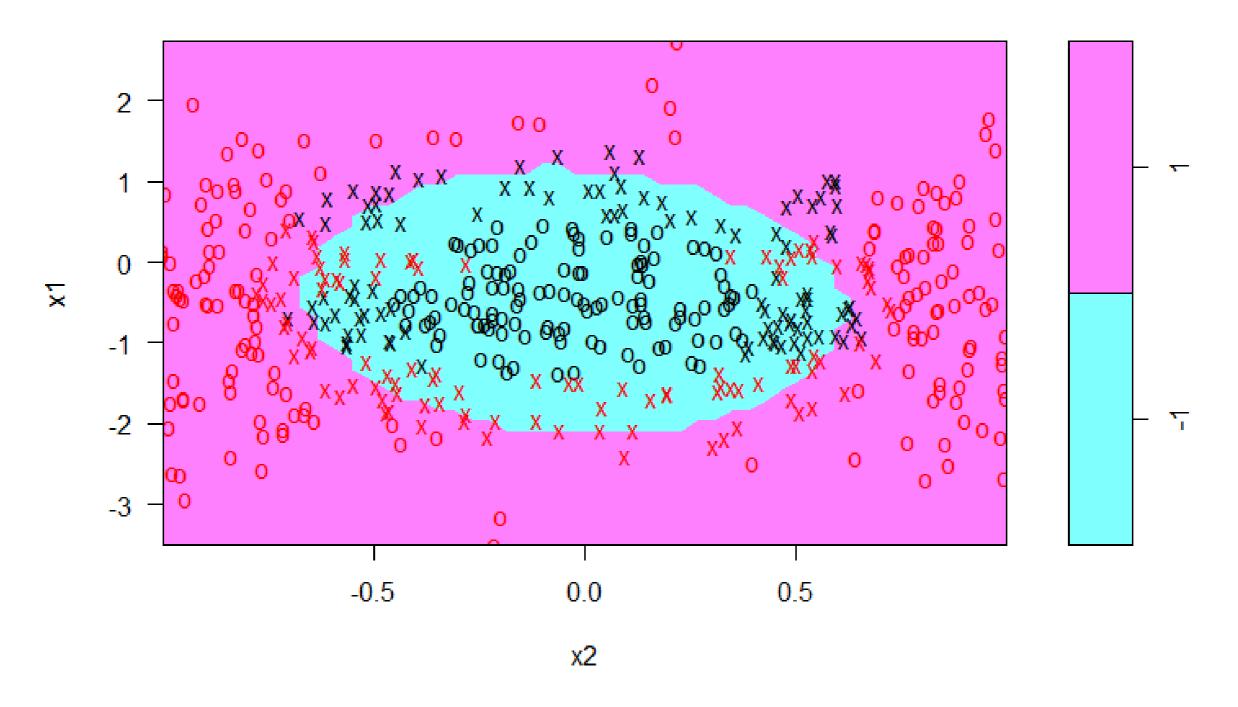
- Partition data into test/train (not shown)
- Use degree 2 polynomial kernel (default params)

```
Number of Support Vectors: 204
```

```
# Predictions
pred_test <- predict(svm_model, testset)
mean(pred_test == testset$y)</pre>
```

0.8666667

```
plot(svm_model, trainset)
```



Try higher degree polynomial

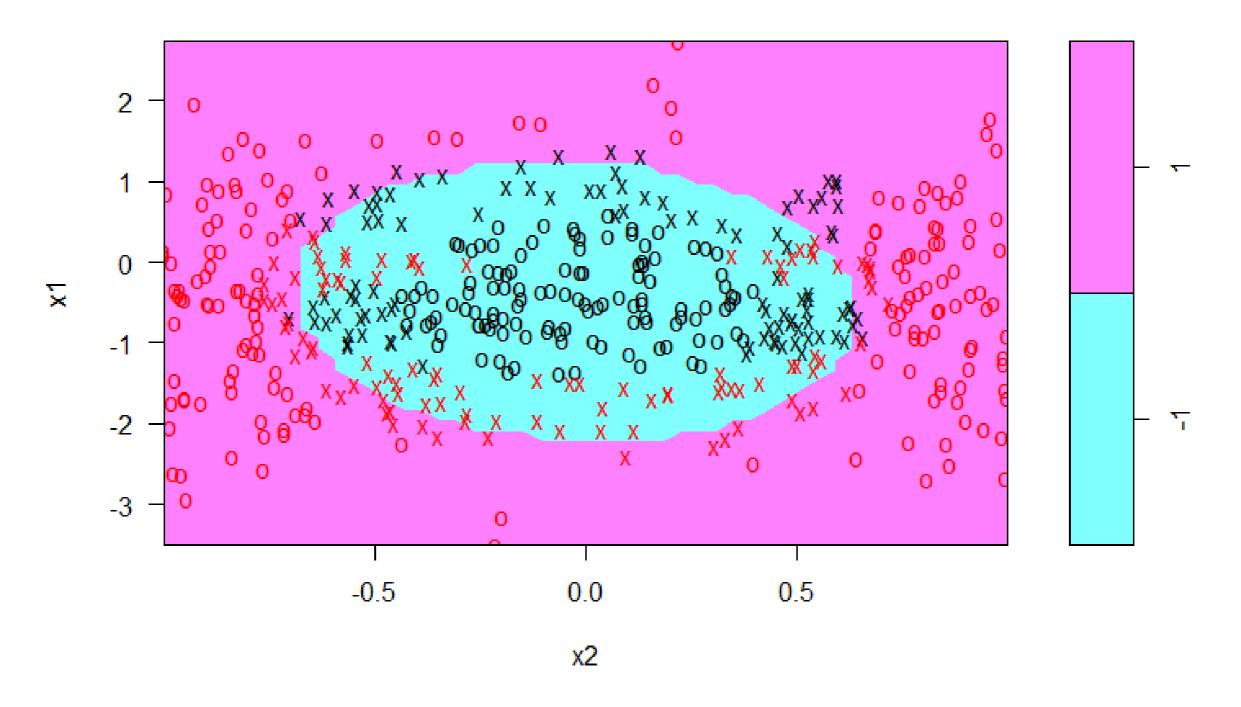
- Rule out odd degrees -3,5,9 etc.
- Try degree 4

```
Number of Support Vectors: 203
```

```
# Predictions
pred_test <- predict(svm_model, testset)
mean(pred_test == testset$y)</pre>
```

```
0.8583333
```

```
plot(svm_model, trainset)
```

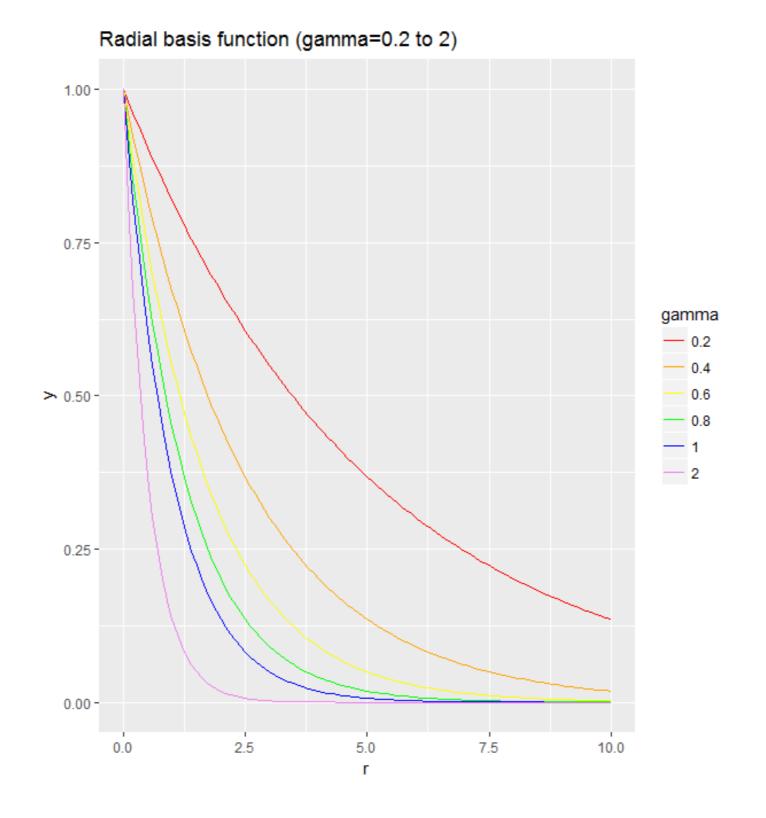


Another approach

- Heuristic: points close to each other have the same classification:
 - Akin to K-Nearest Neighbors algorithm.
- For a given point in the dataset, say X1 = (a, b):
 - The kernel should have a maximum at (a, b)
 - Should decay as one moves away from (a, b)
 - The rate of decay should be the same in all directions
 - The rate of decay should be tunable
- A simple function with this property is exp(-gamma * r), where r is the distance between
 X1 and any other point X

How does the RBF kernel vary with gamma (code)

```
#rhf function
rbf <- function(r, gamma) exp(-gamma * r)</pre>
ggplot(data.frame(r = c(-0, 10)), aes(r)) +
  stat_function(fun = rbf, args = list(gamma = 0.2), aes(color = "0.2")) +
  stat_function(fun = rbf, args = list(gamma = 0.4), aes(color = "0.4")) +
  stat_function(fun = rbf, args = list(gamma = 0.6), aes(color = "0.6")) +
  stat_function(fun = rbf, args = list(gamma = 0.8), aes(color = "0.8")) +
  stat_function(fun = rbf, args = list(gamma = 1), aes(color = "1")) +
  stat_function(fun = rbf, args = list(gamma = 2), aes(color = "2")) +
  scale_color_manual("gamma",
                     values = c("red", "orange", "yellow",
                                "green", "blue", "violet")) +
  ggtitle("Radial basis function (gamma = 0.2 to 2)")
```





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The RBF Kernel

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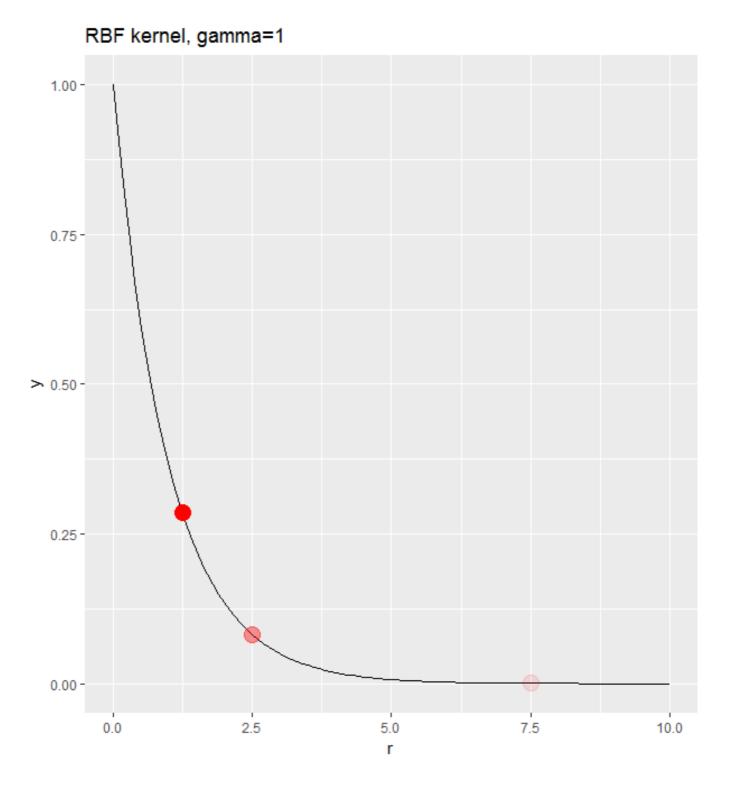


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RBF Kernel in a nutshell

- Decreasing function of distance between two points in dataset.
- Simulates k-NN algorithm.



Building an SVM using the RBF kernel

Build RBF kernel SVM for complex dataset

 Calculate training/test accuracy and plot against training dataset.

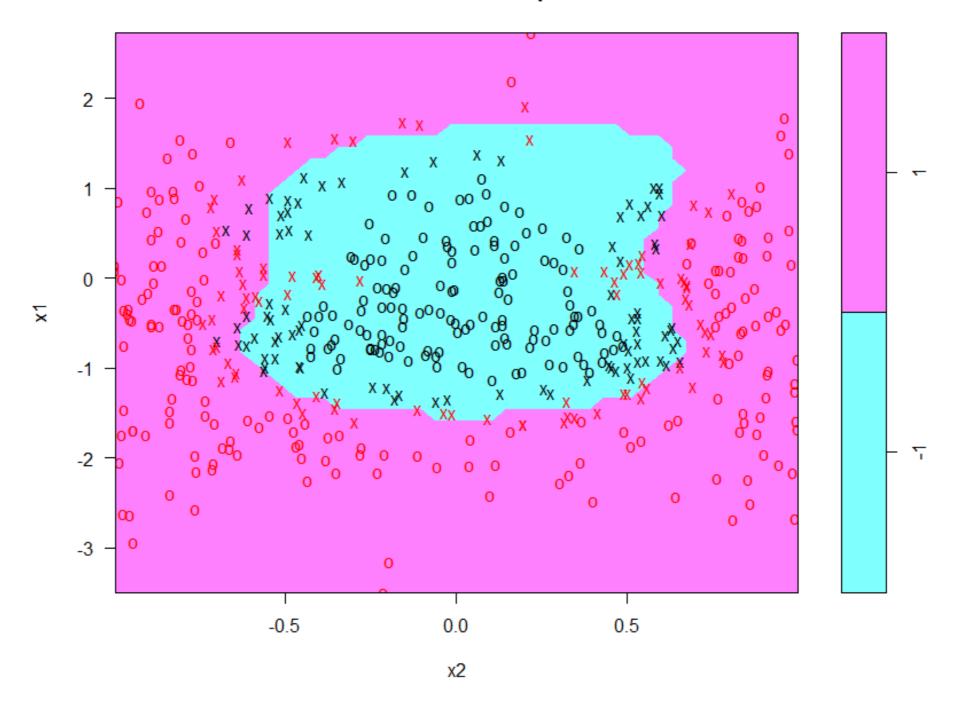
```
pred_train <- predict(svm_model, trainset)
mean(pred_train == trainset$y)</pre>
```

0.93125

```
pred_test <- predict(svm_model, testset)
mean(pred_test == testset$y)</pre>
```

0.9416667

```
#plot decision boundary
plot(svm_model, trainset)
```



Refining the decision boundary

Tune gamma and cost using tune.svm()

Print best parameters

```
# Print best values of cost and gamma
tune_out$best.parameters$cost
```

1

```
tune_out$best.parameters$gamma
```

5

The tuned model

Build tuned model using best.parameters

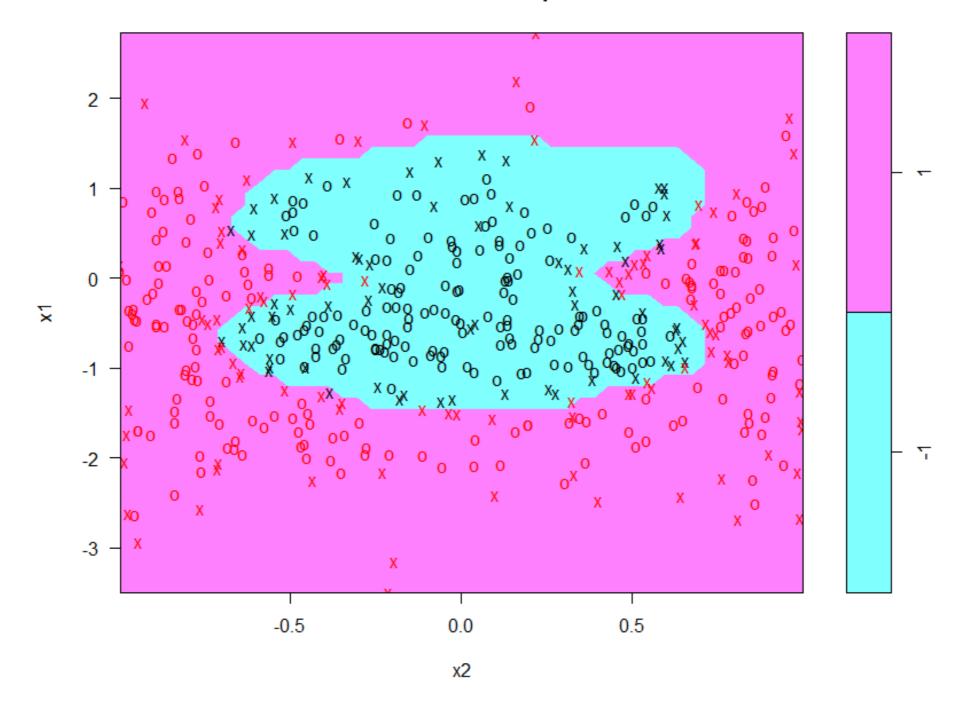
Calculate test accuracy

```
mean(pred_test == testset$y)
```

0.95

Plot decision boundary

```
plot(svm_model, trainset)
```



Time to practice!

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