

# **Big Data Analytics**

#### Session 8 Support Vector Machines

## So far



- Classifiers
  - Logistic regression
  - Decision trees
  - Ensemble learning: Bagging and Random Forests
  - SVM: Support Vector Machines
    - Developed in 1990s
    - Perform well on a variety of settings
    - Often considered one of the best "out of the box" classifiers

### Outline

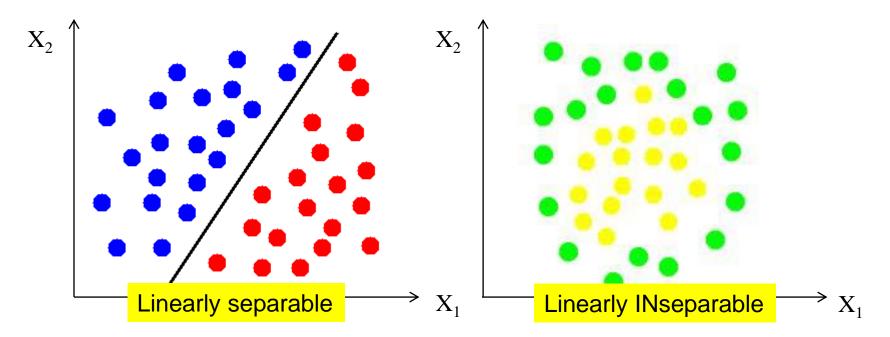


- Maximal Margin Classifier
- The Support Vector Classifier
- (A glance at) The Support Vector Machine Classifier

#### **Linearly Separable Classes**



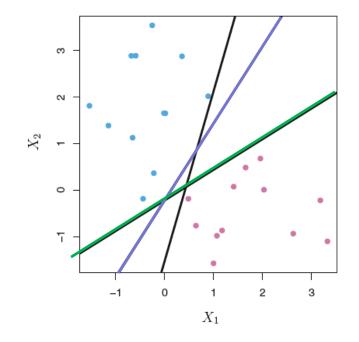
• Imagine a situation where you have a two-class classification problem with two predictors  $X_1$  and  $X_2$ .



• Suppose that the two classes are "linearly separable" i.e. one can draw a straight line in which all points on one side belong to the first class and points on the other side to the second class.

#### **Linearly Separable Classes**





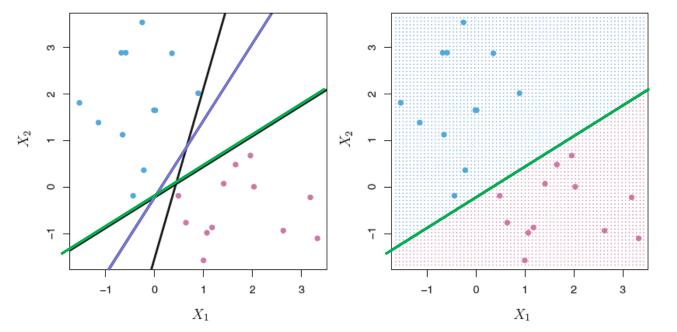
Recall: in linear regression Least squares line

The one with the least residual sum of squares

#### **Linearly Separable Classes**



• Then a natural approach is to find the straight line that gives the biggest separation between the classes i.e. the points are as far from the line as possible.



Recall: in linear regression Least squares line

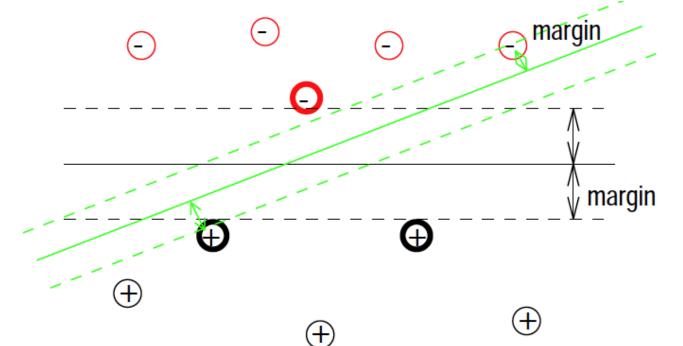
The one with the least residual sum of squares

→ This is the basic idea of a maximal margin classifier.

### **Maximal Margin Line**



- Margin: the minimal (perpendicular) distance from all the observations to the separation line
- Maximal margin line: the line for which the margin is largest
- We can then use maximal margin line to classify a test observation
  - The classification of a point depends on which side of the line it falls on.



### **Support Vectors**

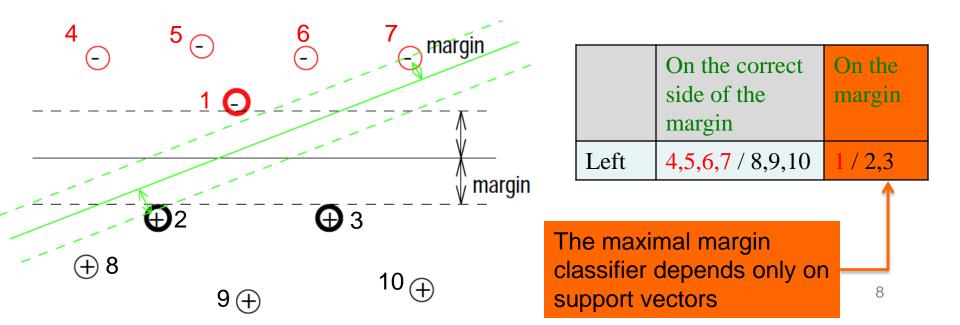
- Support vectors: observations 1,2,3
  - They are on the margin
  - They are vectors (here 2-dimensional)
  - They support the maximal margin line





Atlas supporting the sky

- If these three points were moved, then the maximal margin line would move
- The maximal margin line depends only on support vectors



#### **More Than Two Predictors**



- This idea works just as well with more than two predictors.
- For example, with three predictors you want to find the plane that produces the largest separation between the (two) classes.
- With more than three dimensions it becomes hard to visualise a plane but it still exists.
- In general they are called *hyper-planes*.
  - Two predictors: a line
  - Three predictors: a plane
  - More than three predictors: a hyper-plane

 $\rightarrow$  So we are looking for the maximal margin hyper-planes as maximal margin classifiers.

### Outline



- Maximal Margin Classifier
- The Support Vector Classifier
- The Support Vector Machine Classifier

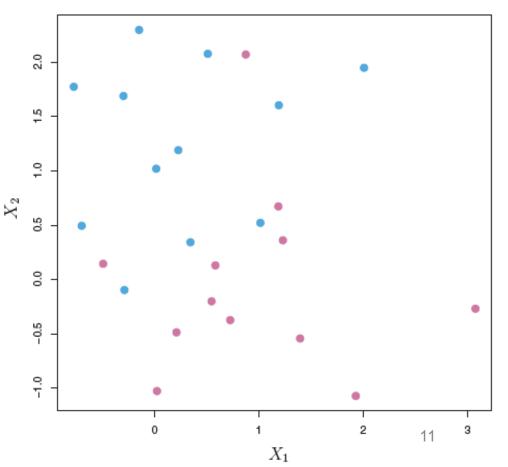
#### Why Maximal Margin Classifiers Are Not Ideal?



- Reason One:
  - Maximal margin hyperplanes may not exist.  $\rightarrow$  linearly inseparable classes

In practice it is not usually possible to find a hyper-plane that perfectly separates two classes.

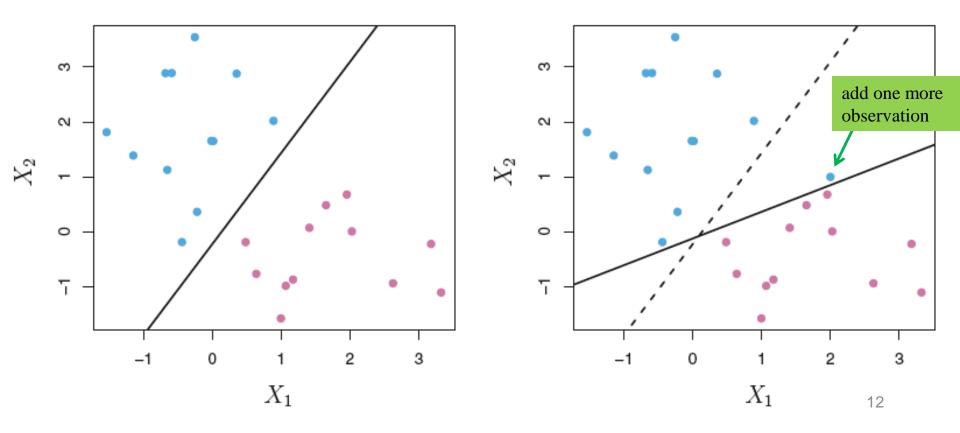
In other words, for any straight line one draws there will always be at least some points on the wrong side of the line.



#### Why Maximal Margin Classifiers Are Not Ideal?



- Reason Two:
  - Even if maximal margin hyperplanes exist, they are extremely sensitive to a change in a single observation.  $\rightarrow$  easy to overfit



#### Support Vector Classifiers (SVC)



- SVCs are based on a hyperplane that does not perfectly separate the two classes, in the interest of
  - Greater robustness to individual observations, and
  - <u>Better classification</u> of most of the training observations.
  - At the cost of <u>worse classification</u> of a few training observations.



- Soft margin
  - We allow some observations to be on the incorrect side of the margin, or even the incorrect side of the hyperplane.

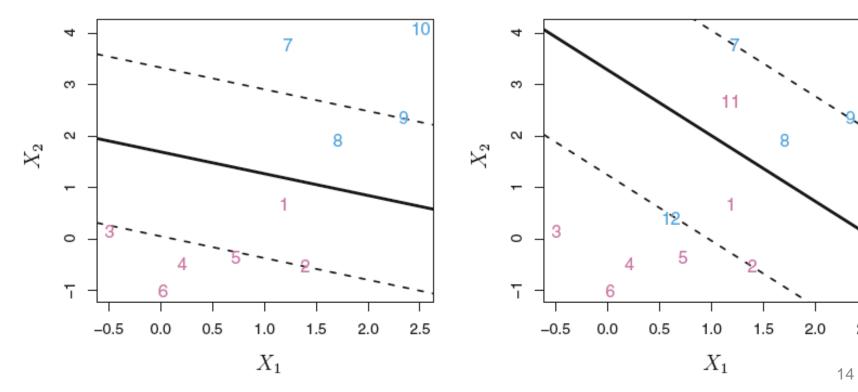
#### **SVC Examples**

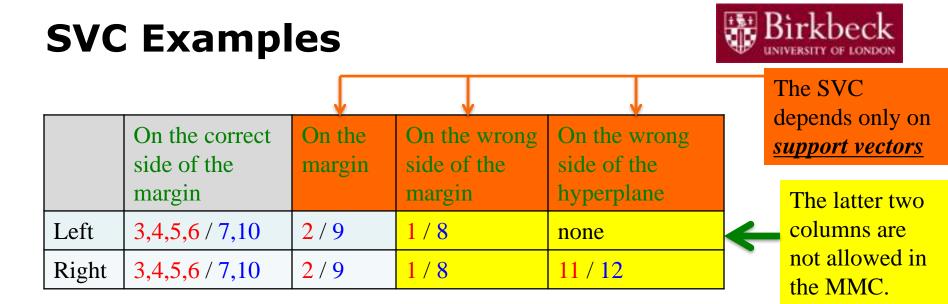


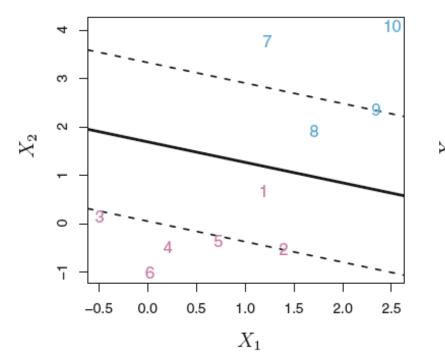
10

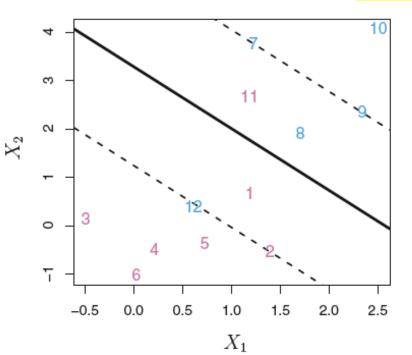
2.5

	On the correct side of the margin	On the margin	On the wrong side of the margin	On the wrong side of the hyperplane
Left				
Right				









#### Cost



• A Cost allows us to specify the cost of a violation to the margin.



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3) Classifier highly

fit to the data or not?

#### Cost

- A Cost allows us to specify the cost of a violation to the margin.
  - Cost is a tuning parameter and is generally chosen via cross validation
    - The choice of cost is very important
    - It determines the extent to which the model underfits or overfits the data. ٠
  - When cost is large, then —
    - The margin will be narrow
      - There will be few support vectors involved in determining the hyperplane
      - Amounts to a classifier that is highly fit to the data
      - Low bias and high variance • 4) Bias? Variance?
  - When cost is small, then \_\_\_\_
    - The margin will be wide
    - Many support vectors will be involved in determining the hyperplane ٠
    - Amounts to fitting the data less hard •
    - High bias and low variance

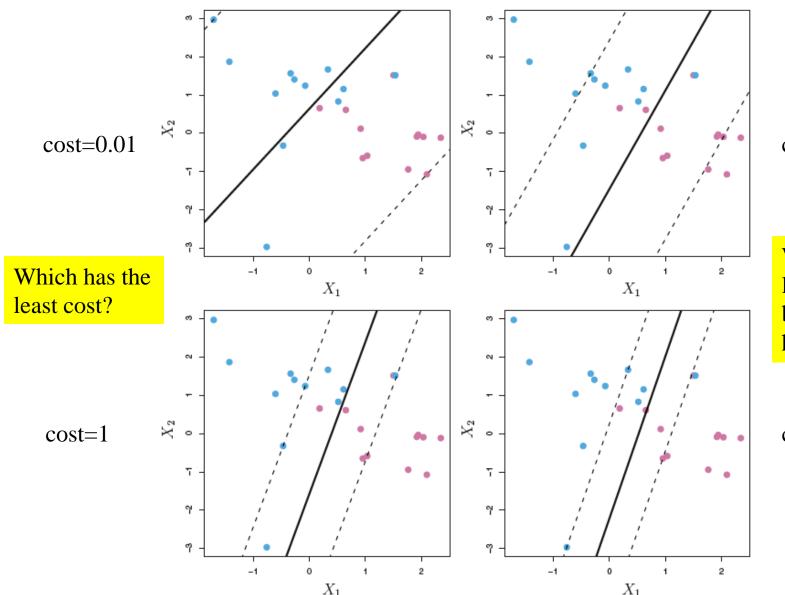
or more support vectors?

2) Fewer

1) Margin narrow or wide?

#### **Cost Examples**





cost=0.1

Which has low variance, but potentially high bias?

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cost=10

#### Some Remarks



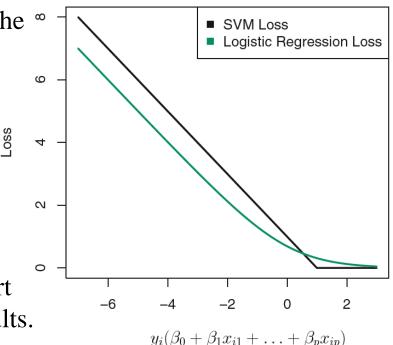
- In the book, "budget C" is used to explain the concept rather than "cost". Budget and cost are dual.
  - The higher the budget is, the smaller the cost is.
  - The lower the budget is, the bigger the cost is.
- Which points should influence optimality?
  - All points
    - Linear regression
    - Naïve Bayes
    - Linear discriminant analysis
  - Only "difficult points" close to decision boundary
    - Support vector machines
    - Logistic regression (kind of) [See section 9.5 for more details]

 $\rightarrow$  These models are robust to the behaviour of observations that are far away from the hyperplane.

## **SVM and Logistic Regression**



- Loss functions
  - SVM's hinge loss function is exactly zero for observations that are on the correct side of the ∞ margin.
  - Logistic regression's loss function is very small for observations that are far from the decision boundary.
- Comparison
  - Due to the similarities between their loss functions, logistic regression and the support vector classifier often give very similar results.
  - When the classes are well separated, SVMs tend to behave better than logistic regression.
  - In more overlapping regimes, logistic regression is often preferred.



### **Support Vector Classifier**



- To demonstrate the SVC (and SVM), we use
  - e1071 library or
  - LiblineaR library (useful for very large linear problems)
- Use svm() function to fit a support vector classifier/machine
  - With kernel="linear" to fit a SVC, otherwise a SVM
  - With cost argument: specify the cost of a violation to the margin
    - cost is small: wide margins
      - many support vectors will be on the margin or will violate the margin
    - cost is large: narrow margins
      - Few support vectors will be on the margin or will violate the margin



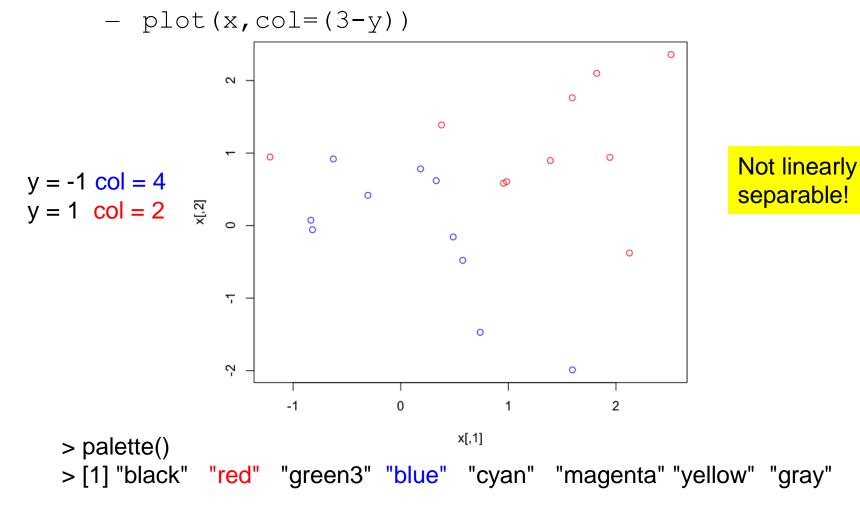
	> X	> X
set.seed(1)	[,1] [,2]	[,1] [,2]
7	[1,] -0.62645381 0.91897737	
	[2,] 0.18364332 0.78213630	[2,] 0.1836433 0.78213630
x <- matrix(rnorm(20*2),ncol=2)	[3,] -0.83562861 0.07456498	[3,] -0.8356286 0.07456498
······································	[4,] 1.59528080 -1.98935170	[4,] 1.5952808 -1.98935170
X	[5,] 0.32950777 0.61982575	[5,] 0.3295078 0.61982575
	[6,] -0.82046828 -0.05612874	[6,] -0.8204684 -0.05612874
	[7,] 0.48742905 -0.15579551	[7,] 0.4874291 -0.15579551
y <- c(rep(-1,10),rep(1,10))	[8,] 0.73832471 -1.47075238	[8,] 0.7383247 -1.47075238
<u> </u>	[9,] 0.57578135 -0.47815006	[9,] 0.5757814 -0.47815006
У	[10,]-0.30538839 0.41794156	[10,] -0.3053884 0.41794156
[1] -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1	[11,] 1.51178117 1.35867955	[11,] 2.5117812 2.35867955
1 1 1 1 1 1 1 1 1 /	[12,] 0.38984324 -0.10278773	[12,] 1.3898432 0.89721227
	[13,] -0.62124058 0.38767161	[13,] 0.3787594 1.38767161
	[14,] -2.21469989 -0.05380504	[14,] -1.2146999 0.94619496
	[15,] 1.12493092 -1.37705956	[15,] 2.1249309 -0.37705956
x[y==1,] <- x[y==1,]+1	[16,] -0.04493361 -0.41499456	[16,] 0.9550664 0.58500544
	[17,] -0.01619026 -0.39428995	[17,] 0.9838097 0.60571005
X	[18,] 0.94383621 -0.05931340	[18,] 1.9438362 0.94068660
	[19,] 0.82122120 1.10002537	[19,] 1.8212212 2.10002537
	[20,] 0.59390132 0.76317575	[20,] 1.5939013 1.76317575

rnorm() generates a vector of random normal variables matrix(rnorm(20\*2), ncol=2) generates a 20\*2 matrix of 40 random normal variables By default, byrow=FALSE. In other words, fill the matrix column-wise.



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• Check whether the classes are linearly separable





5

2

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SVM classification plot

-1

0

x.2

Encode the response as a factor variable by creating a data frame:
 dat <- data.frame(x=x,y=as.factor(y))</li>
 library(e1071)

svmfit <- svm(y ~ ., data=dat, kernel="linear", cost=10, scale=FALSE)</pre>

2.5 plot(svmfit,dat) 0 2.0 - y = -1 blue; y = +1 purple 0 – linear boundary 1.5 One misclassification 1.0 -Support vectors: cross; remaining: circle 0 ×. 0 0.5 7 support vectors: \_ > svmfit\$index 0.0 -1 2 5 7 14 16 17 [1] 0 -0.5 00 -1.0 -

as.factor coerces its argument to a factor.



> summary(svmfit)

#### Call:

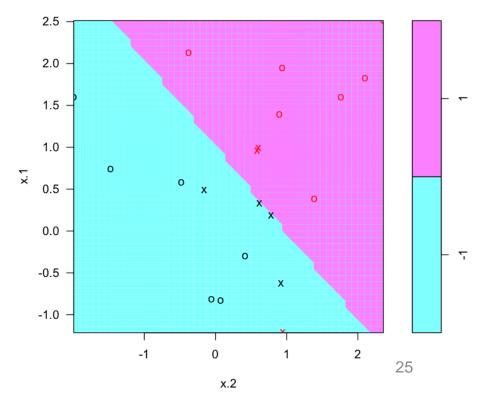
svm(formula = y ~ ., data = dat, kernel = "linear", cost = 10, scale = FALSE)

#### Parameters:

SVM-Type: C-classification SVM-Kernel: linear cost: 10 gamma: 0.5

Number of Support Vectors: 7

SVM classification plot

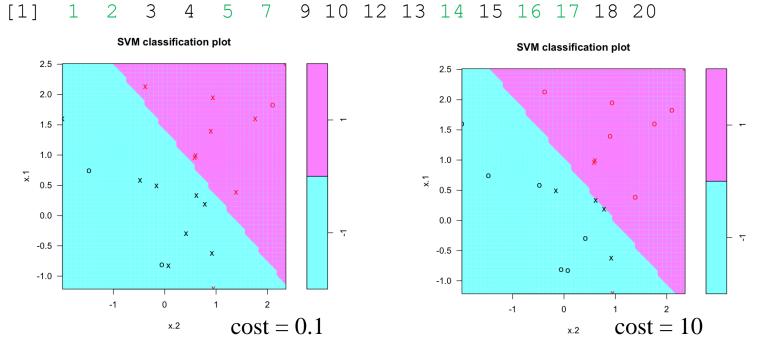




#### • Try a smaller cost:

svmfit <- svm(y~.,data=dat,kernel="linear",cost=0.1,scale=FALSE)
plot(svmfit,dat)</pre>

svmfit\$index



• Smaller cost  $\rightarrow$  a larger number of support vectors, a wider margin

### **Try Another Function**



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- tune() in e1071 library
  - Perform 10-fold cross-validation
- Compare SVMs with a linear kernel, using a range of values of the <code>cost</code> parameter  $_{\tt set.seed(1)}$

```
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)</pre>
```

```
Parameter tuning of 'svm':
```

- sampling method:
   10-fold cross validation
- best parameters: cost 0.1
- best performance: 0.1

```
- Detailed performance results:
cost error dispersion
```

```
11e-030.700.421637021e-020.700.421637031e-010.100.210818541e+000.150.241522955e+000.150.241522961e+010.150.241522971e+020.150.2415229
```

```
bestmod <- tune.out$best.model
summary(bestmod)
Call:
best.tune(method = svm, train.x = y ~ ., data = dat,
ranges = list(cost = c(0.001, 0.01, 0.1, 1, 5, 10, 100)),
kernel = "linear")</pre>
```

```
Parameters:

SVM-Type: C-classification

SVM-Kernel: linear

cost: 0.1

gamma: 0.5

Number of Support Vectors: 16 (88)

Number of Classes: 2

Another

example of

using CV to

compare and

select model
```

#### **Predict Class Labels**



#### • First generate a test data set

xtest <- matrix(rnorm(20\*2),ncol=2)</pre>

ytest <- sample(c(-1,1),20,rep=TRUE)</pre>

#rep: Should sampling be with replacement?

ytest # The number of 1 and -1 in ytest might be different.

[1] 1 -1 -1 1 1 -1 -1 -1 1 1 1 1 -1 -1 -1 -1 1 1 -1 1 vtoot

#### xtest

	[,1]	[,2]
[1,]	1.51178117	1.35867955
[2,]	0.38984324	-0.10278773
[3,]	-0.62124058	0.38767161
[4,]	-2.21469989	-0.05380504
[5,]	1.12493092	-1.37705956
[6,]	-0.04493361	-0.41499456
[7,]	-0.01619026	-0.39428995
[8,]	0.94383621	-0.05931340
[9,]	0.82122120	1.10002537
[10,]	0.59390132	0.76317575
[11,]	0.91897737	-0.16452360
[18,]	-1.47075238	0.76853292
[19,]	-0.47815006	-0.11234621
[20,]	0.41794156	0.88110773

```
xtest[ytest==1,] <- xtest[ytest==1,]+1
testdat <- data.frame(x=xtest,y=as.factor(ytest))
testdat</pre>
```

	x.1	x.2	У
1	2.51178117	2.3586796	1
2	0.38984324	-0.1027877	-1
3	-0.62124058	0.3876716	-1
4	-1.21469989	0.9461950	1
5	2.12493092	-0.3770596	1
6	-0.04493361	-0.4149946	-1
7	-0.01619026	-0.3942900	-1
8	0.94383621	-0.0593134	-1
9	1.82122120	2.1000254	1
10	1.59390132	1.7631757	1
11	1.91897737	0.8354764	1
•			
18	-1.47075238	0.7685329	-1
19	-0.47815006	-0.1123462	-1
20	1.41794156	1.8811077	1

#### **Predict Class Labels**

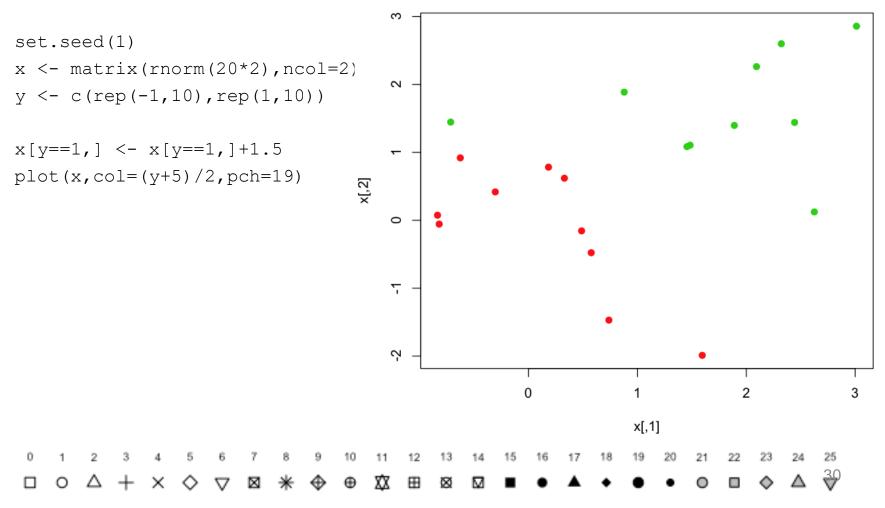


- Then predict the class labels of these test observations
  - First using the best model (with cost=0.1)

#### - What if cost=0.01?



• First generate a linearly separable training set





• We fit the SVC and plot the resulting hyperplane, using a very large value of cost so that no observations are misclassified

```
dat <- data.frame(x=x,y=as.factor(y))</pre>
svmfit <- svm(y ~ ., data=dat, kernel="linear", cost=1e5)</pre>
summary(svmfit)
Call:
svm(formula = y \sim ., data = dat, kernel = "linear", cost = 1e+05)
Parameters:
   SVM-Type: C-classification
 SVM-Kernel: linear
       cost: 1e+05
      gamma: 0.5
Number of Support Vectors: 3 (12)
Number of Classes: 2
Levels:
 -1 1
```

plot(svmfit,dat)



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Only 3 support vectors were used.

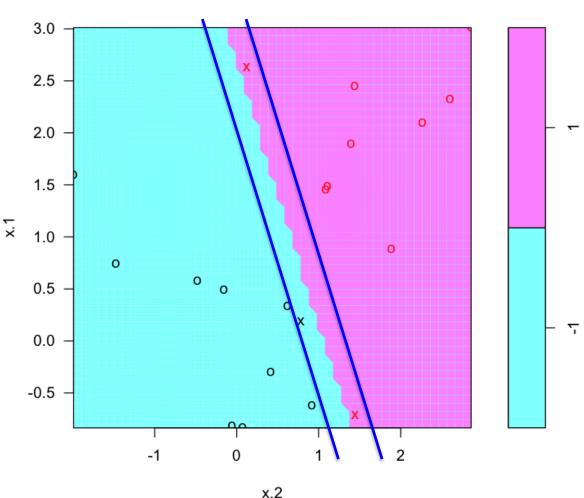
The margin is very narrow.

However, some circle observations are very close to the decision boundary.

It seems that this model will perform poorly on test data.

Your task: generate a test dataset and calculate the test error rate.

#### SVM classification plot



• Now try a smaller value of cost:

```
svmfit <- svm(y~.,data=dat,kernel="linear",cost=1)
summary(svmfit)</pre>
```

```
Call:
```

svm(formula = y ~ ., data = dat, kernel = "linear", cost = 1)

#### Parameters:

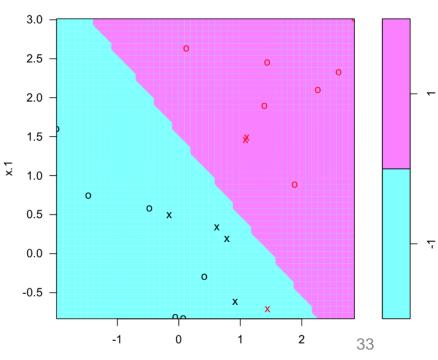
```
SVM-Type: C-classification
SVM-Kernel: linear
cost: 1
gamma: 0.5
```

```
Number of Support Vectors: 7 (43)
Number of Classes: 2
Levels:
-1 1
```

```
plot(svmfit,dat)
```

Misclassify one training observation, but a much wider margin and 7 support vectors May perform better than the previous one

Your task: To use the same test dataset and calculate the test error rate. Compare the error rate with the one on the previous slide.



x.2

#### SVM classification plot

### Outline

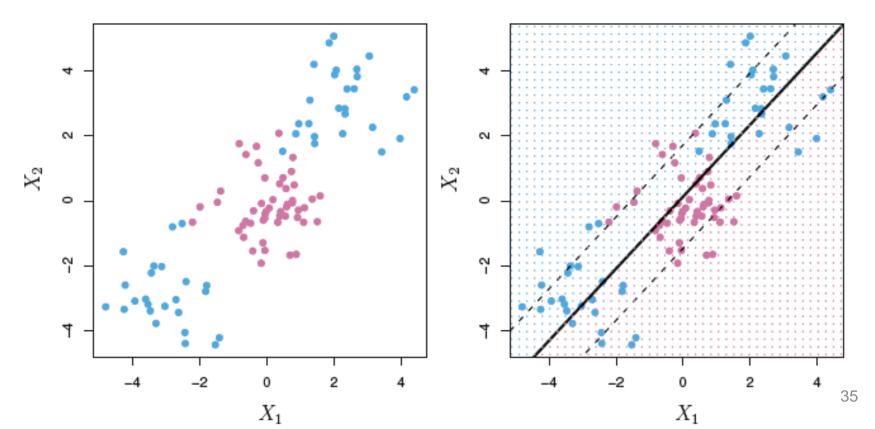


- Maximal Margin Classifier
- The Support Vector Classifier
- The Support Vector Machine Classifier

#### **Non-Linear Classifier**



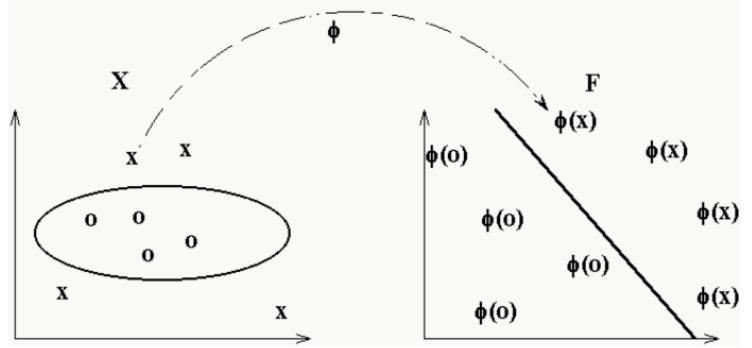
• The support vector classifier is fairly easy to think about. However, because it only allows for a linear decision boundary it may not be all that powerful.



#### **Support Vector Machines**



• SVM maps data into a high-dimensional feature space including non-linear features, then use a linear classifier there



In the original feature space: Polynomial boundary In the high-dimensional feature space: Linear boundary

#### **SVM Visualisation**



https://www.youtube.com/watch?v=3liCbRZPrZA

# SVM with a polynomial Kernel visualization

Created by: Udi Aharoni

#### How SVM Works – An Example



- In the original feature space:
  - Two features:  $X_1, X_2$
  - Quadratic function:  $f(X_1, X_2) = 2X_1^2 3X_2^2 + X_1 + 5X_2 8$
- In the high-dimensional feature space:
  Four features: Z<sub>1</sub>, Z<sub>2</sub>, Z<sub>3</sub>, Z<sub>4</sub>

  - Linear function:  $f(Z_1, Z_2, Z_3, Z_4) = 2Z_1 3Z_2 + Z_3 + 5Z_4 8$
- Transformations
  - The function  $f(Z_1, Z_2, Z_3, Z_4) = 2Z_1 3Z_2 + Z_3 + 5Z_4 8$  is
    - the optimal linear separating hyperplane obtained in the high-dimensional feature space
  - The transformations (or a basis) are as follows:
    - $Z_1 = X_1^2, Z_2 = X_2^2, Z_3 = X_1, Z_4 = X_2$
    - You don't have to preserve the dimensionality of the original dataset when doing transformation
  - If we know the basis, then we can easily obtain
    - the <u>optimal non-linear separating hyperplane</u> in the <u>original feature space</u>
  - This is basically how SVM works. ٠

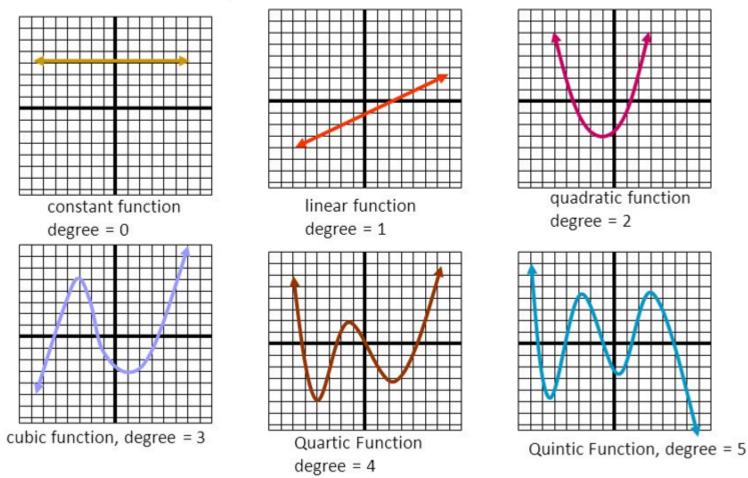
# In Reality



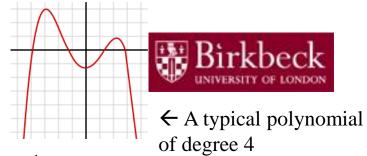
- While conceptually the basis approach is how the support vector machine works, there is some complicated maths (which I will spare you) which means that we don't actually choose the basis function.
- Instead we choose something called a kernel function which takes the place of the basis.
- Common kernel functions include
  - Linear
  - Polynomial
  - Radial Basis Function (Gaussian)
  - Sigmoid
- Pick a Kernel that represents your prior knowledge about the problem.

# Graphs of Polynomial Functions

#### **Common Graphs**

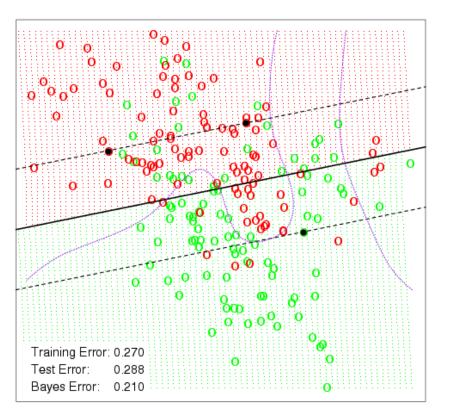


# **A Simulation Example**

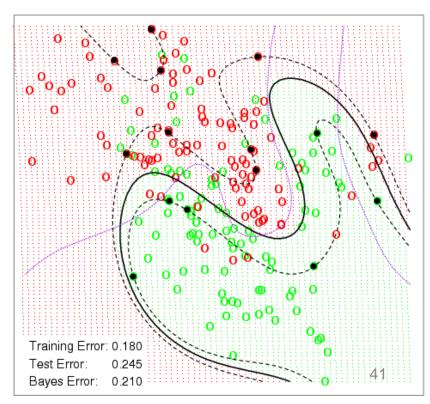


- This is the simulation example from Chapter 1.
- Using a polynomial kernel we now allow SVM to produce a non-linear decision boundary with a much lower test error rate.

(The purple lines represent the Bayes decision boundaries)



SVM - Degree-4 Polynomial in Feature Space



#### SVM with Radial Kernel Visualisation



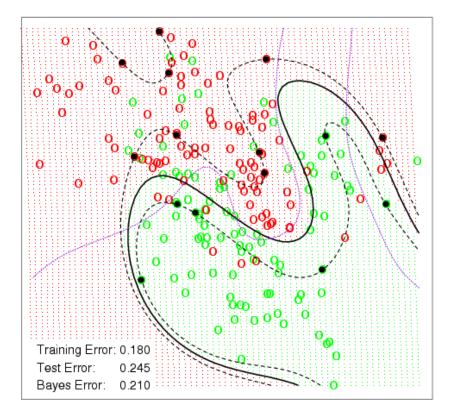


#### **Radial Basis Kernel**

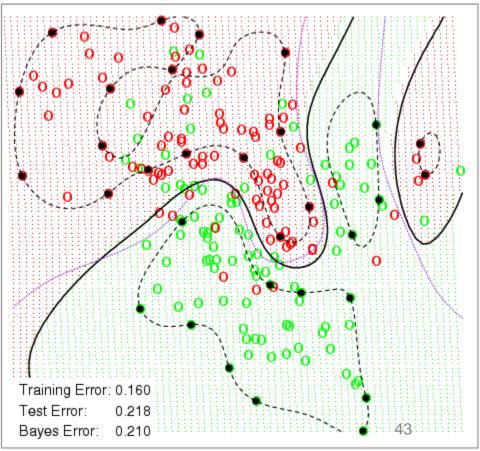


• Using a Radial Basis Kernel you get an even lower error rate.

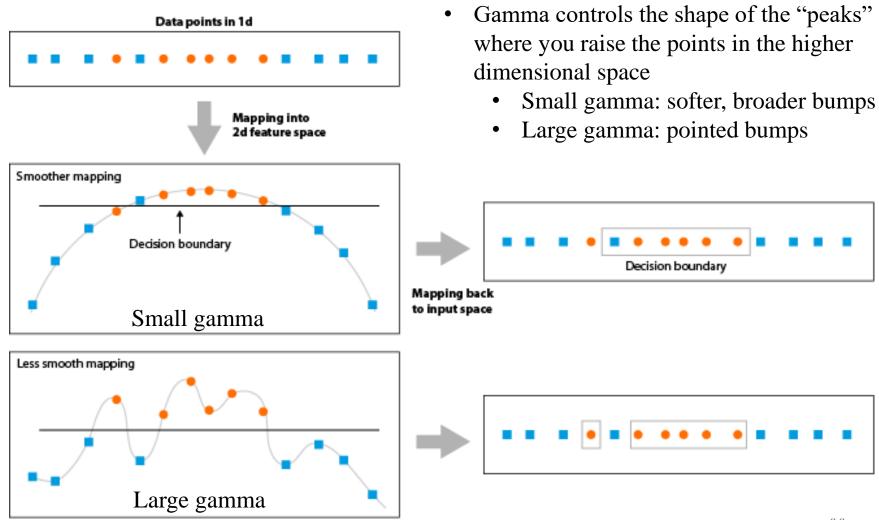
SVM - Degree-4 Polynomial in Feature Space



SVM - Radial Kernel in Feature Space



# **Gamma in RBF Kernel**



Raise green points to separate them from the red.

# **Gamma in RBF Kernel**

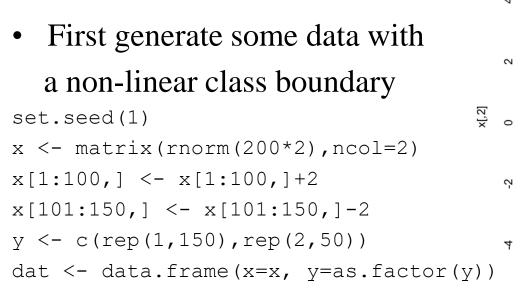


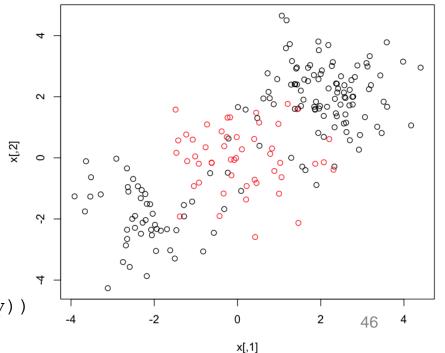
- Gamma defines how far the influence of a single training example reaches
- It determines which points can determine the decision boundary
  - Large gamma:
    - The decision boundary is only dependent on the points that are very close to it.
    - Wiggly, jagged boundary (A lot of weight carried by the nearby points)
    - Low bias and high variance  $\rightarrow$  overfitting
  - Small gamma:
    - The decision boundary is dependent even on the points that are quite far to it.
    - Smooth boundary
    - High bias and low variance

### **Support Vector Machine**



- Change the value of kernel in the svm () function
  - Polynomial kernel: kernel="polynomial"
    - Use degree argument to specify a degree for the polynomial kernel
  - Radial kernel: kernel="radial"
    - Use gamma argument to specify a value of  $\gamma$  for the radial basis kernel





#### **Support Vector Machine Example**



train <- sample(200,100) #randomly split into training and testing groups
svmfit <- svm(y~., data=dat[train,], kernel="radial", gamma=1, cost=1)
plot(svmfit, dat[train,]) #gamma is the value of γ for the radial basis kernel
summary(svmfit)</pre>

```
Call:
svm(formula = y ~ ., data = dat[train, ], kernel = "radial", gamma = 1, cost = 1)
SVM classification plot
```

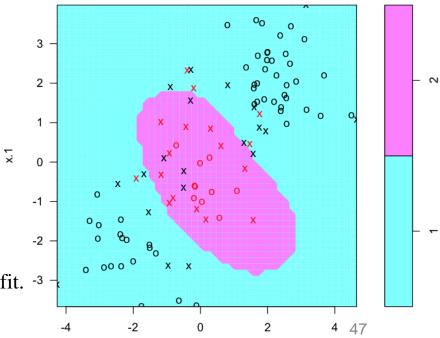
```
Parameters:
```

```
SVM-Type: C-classification
SVM-Kernel: radial
cost: 1
gamma: 1
```

```
Number of Support Vectors: 37 ( 17 20 )
```

```
Number of Classes: 2
Levels:
1 2
```

There are a fair number of training errors in this SVM fit. -3 -



#### **Support Vector Machine Example**



x.2

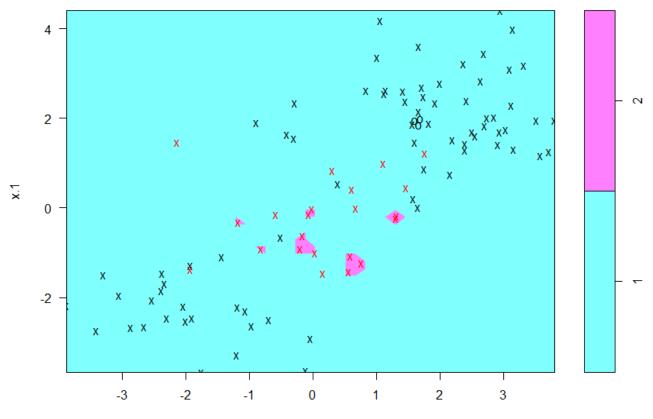
- What will happen if we increase the value of cost?
  - Reduce the number of training errors
  - More irregular boundary  $\rightarrow$  risk of overfitting the data

```
svmfit <- svm(y ~ ., data=dat[train,], kernel="radial", gamma=1, cost=1e5)</pre>
                                                           SVM classification plot
plot(svmfit,dat[train,])
summary(svmfit)
                                                  3
Parameters:
                                                  2
   SVM-Type: C-classification
 SVM-Kernel: radial
                                                  1
       cost: 1e+05
                                               ×.1
                                                  0
      gamma:
               1
                                                  -1
Number of Support Vectors: 26 (12 14)
                                                  -2
Number of Classes: 2
                                                  -3
Levels:
 1 2
                                                           -2
                                                                 0
                                                                        2
                                                                                 48
```

#### **Support Vector Machine Example**



• Gamma = 100, cost = 1



#### **Choosing Best Parameter Values**



#### • Choose the best choice of $\gamma$ and cost for an SVM with a radial kernel

```
Parameter tuning of 'svm':
```

- sampling method: 10-fold cross validation

```
- best parameters:
```

```
cost gamma
```

. . . . . .

```
1 2
```

- best performance: 0.12
- Detailed performance results: cost gamma error dispersion
- 1 1e-01 0.5 0.27 0.11595018
- 2 1e+00 0.5 0.13 0.08232726
- 3 1e+01 0.5 0.15 0.07071068

# **Predicting Class Labels**



• We can view the test set predictions for this model by applying the predict() function to the data

We take the subset of the data frame using -train as an index set.

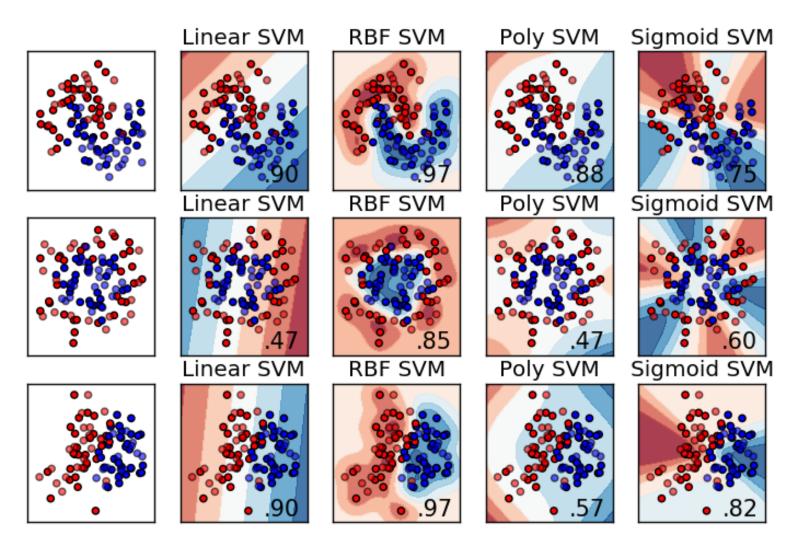
table(true=dat[-train,"y"], pred=predict(tune.out\$best.model,newdata=dat[-train,]))
 pred
true 1 2
 1 74 3
 2 7 16 10% of test observations are misclassified by this SVM.

#### The following code calculates the training error.

table(true=dat[train,"y"], pred=predict(tune.out\$best.model,newdata=dat[train,]))
 pred
true 1 2
 1 69 4
 2 5 22 9% of training observations are misclassified by this SVM. 51

#### **Which Kernel to Choose**





https://scikit-learn.org/stable/auto\_examples/classification/plot\_classifier\_comparison.html 52

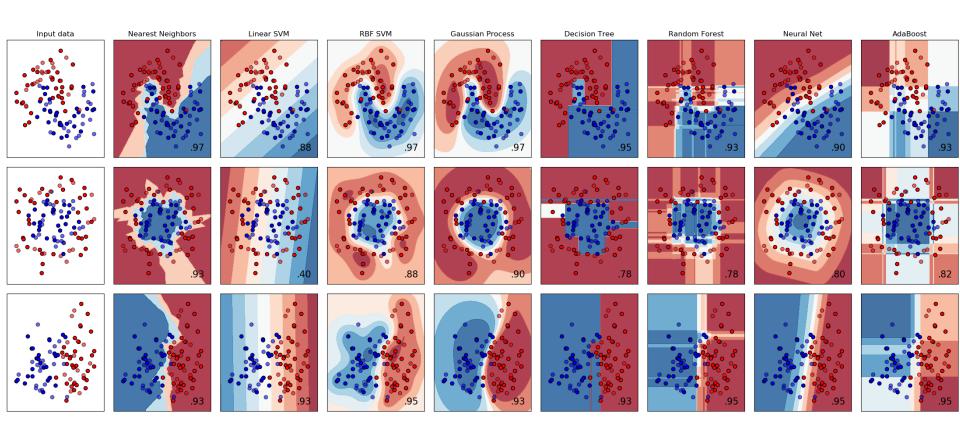
# **Which Kernel to Use**



- While reflecting on what a kernel is "good for" or when it should be used, there are no hard and fast rules.
- In the absence of expert knowledge, the Radial Basis Function kernel makes a good default kernel (once you have established it is a problem requiring a non-linear model).
- Use CV to help you decide, but be careful of overfitting

#### **More Classifiers to Compare**





#### **SVM With More than Two Classes**



- One versus one (all-pair) classification
  - svm () function in e1071 library uses this approach
  - Suppose there are K classes
  - Construct  $\frac{K(K-1)}{2}$  2-class SVMs (pairwise)
  - Apply all those 2-class SVMs to classify the same test observation
  - Tally the number of times that the test observation is assigned to each of the K classes
  - The most frequently assigned class is the final class



## LAB

- 404+405
  - One teacher Tingting + two TAs (Cosmin, Ylli)
  - Will go through each question
- 414+415
  - One teacher Nicos + one TA (Delik)
  - Moderate teaching
- 403
  - One TA (Pavel) answering questions
  - Work alone or in a group
  - May have group discussions