Support Vector Machines

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Data Analytics – ITWS-4963/ITWS-6965

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Support Vector Machine

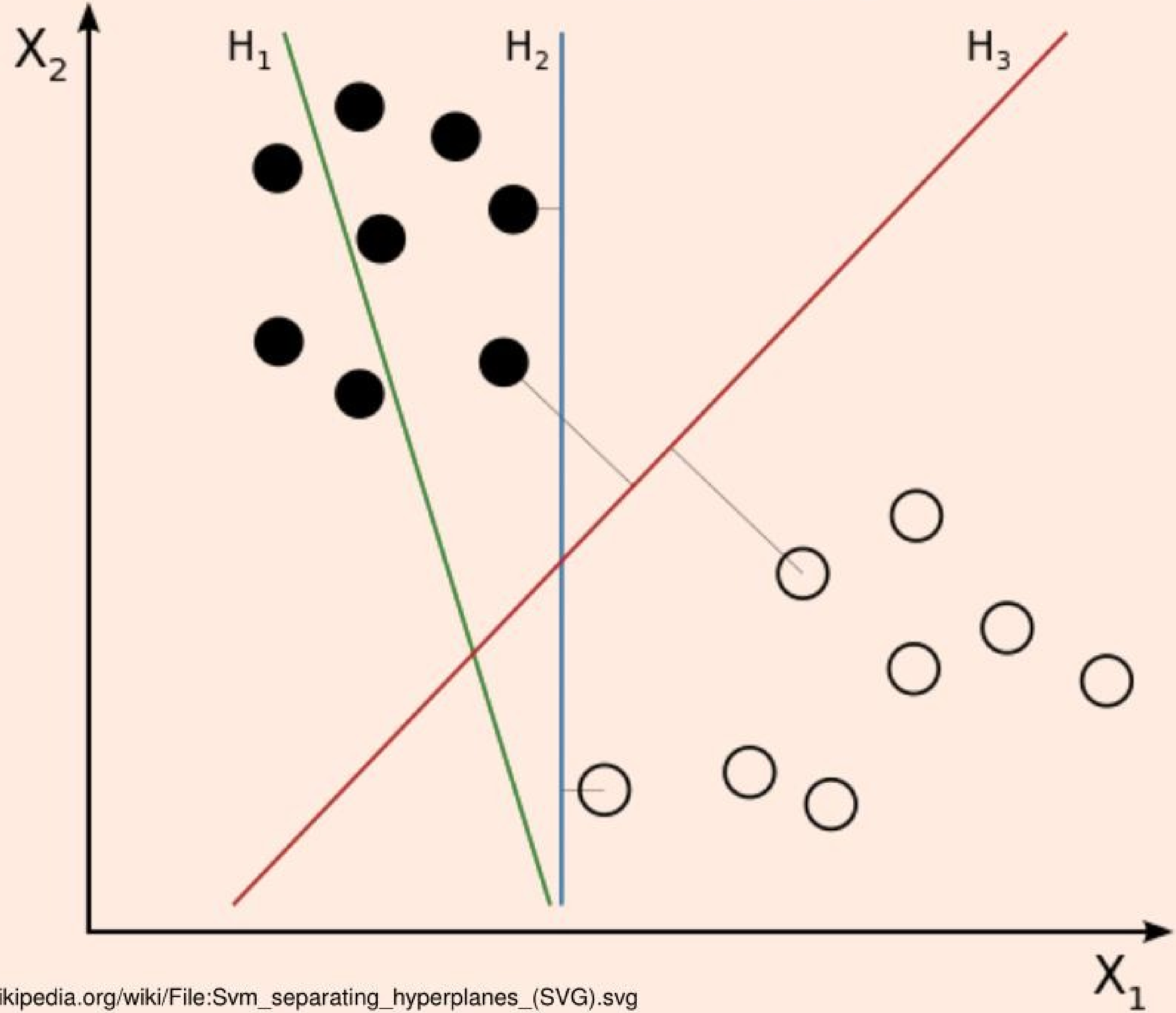
- Conceptual theory, formulae…

- SVM - general (nonlinear) classification, regression and outlier detection with an intuitive model representation

- Hyperplanes separate the classification spaces (can be multi-dimensional)

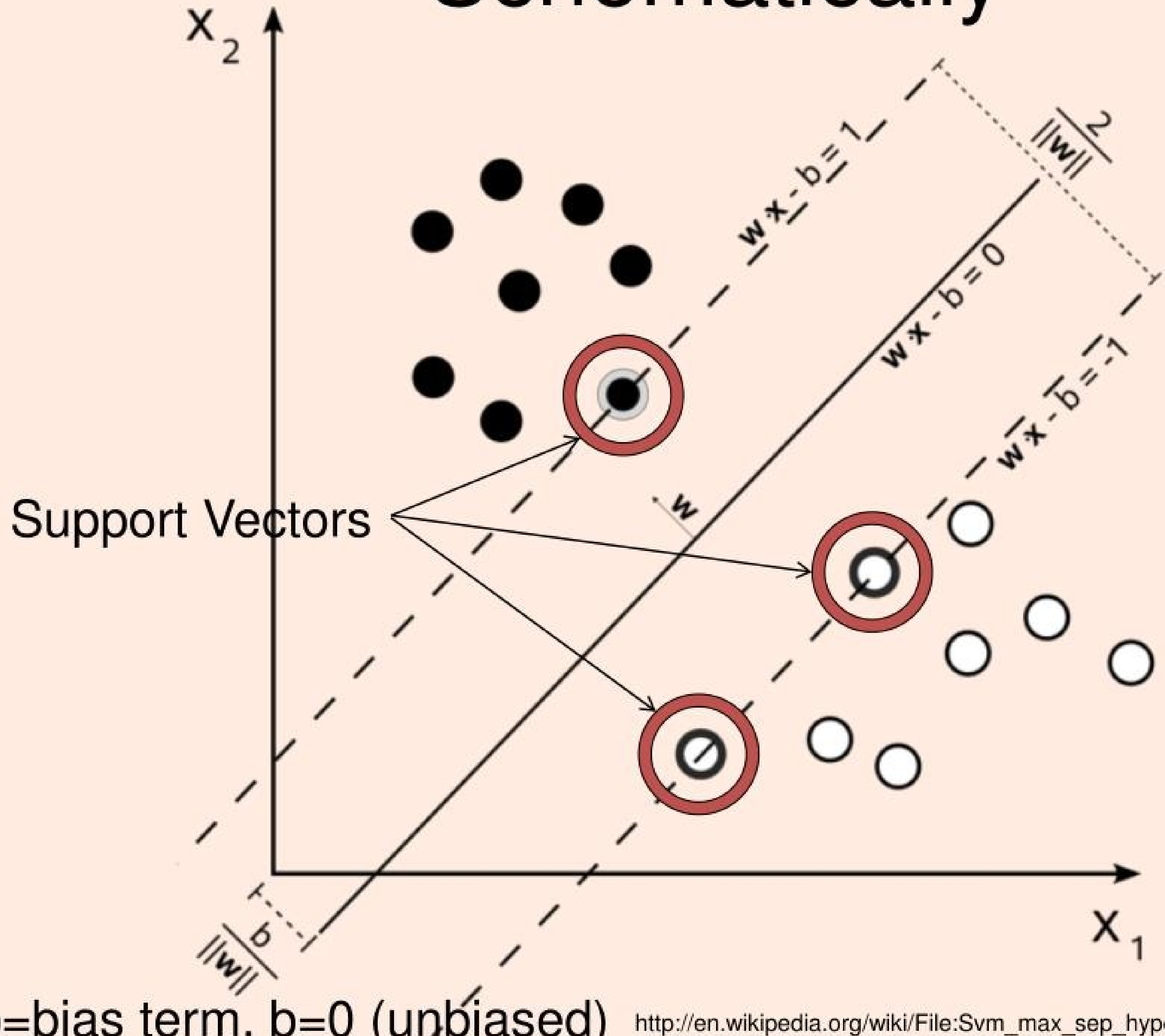
- Kernel functions can play a key role

Schematically



http://en.wikipedia.org/wiki/File:Svm_separating_hyperplanes_(SVG).svg

Schematically



b=bias term, b=0 (unbiased)

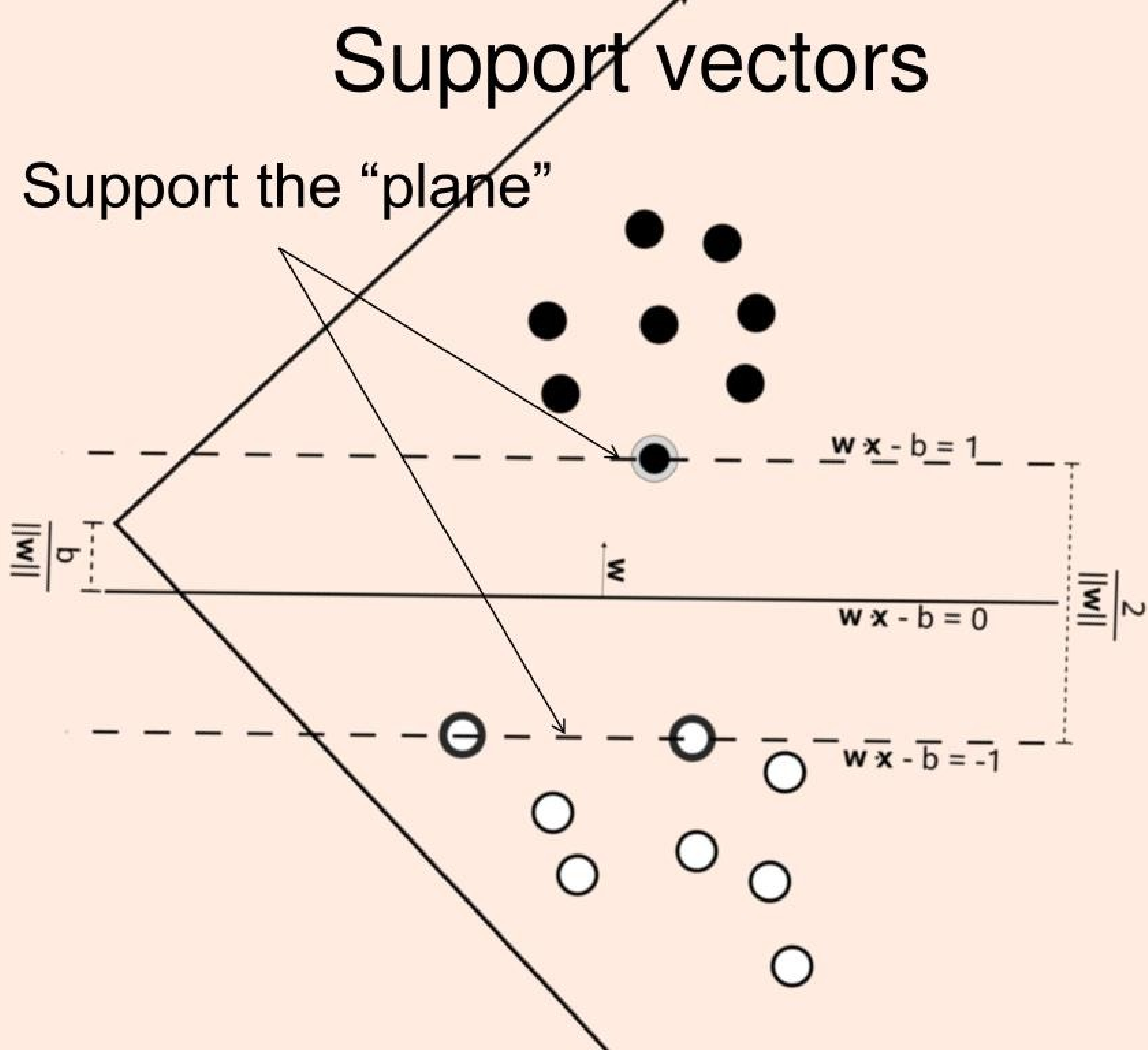
http://en.wikipedia.org/wiki/File:Svm_max_sep_hyperplane_with_margin.png

Construction

- Construct an optimization objective function that is inherently subject to some constraints
  - Like minimizing least square error (quadratic)
- Most important: the classifier gets the points right by “at least” the margin
- Support Vectors can then be defined as those points in the dataset that have "non zero” Lagrange multipliers*.
  - make a classification on a new point by using only the support vectors – why?

Support vectors

- Support the “plane”

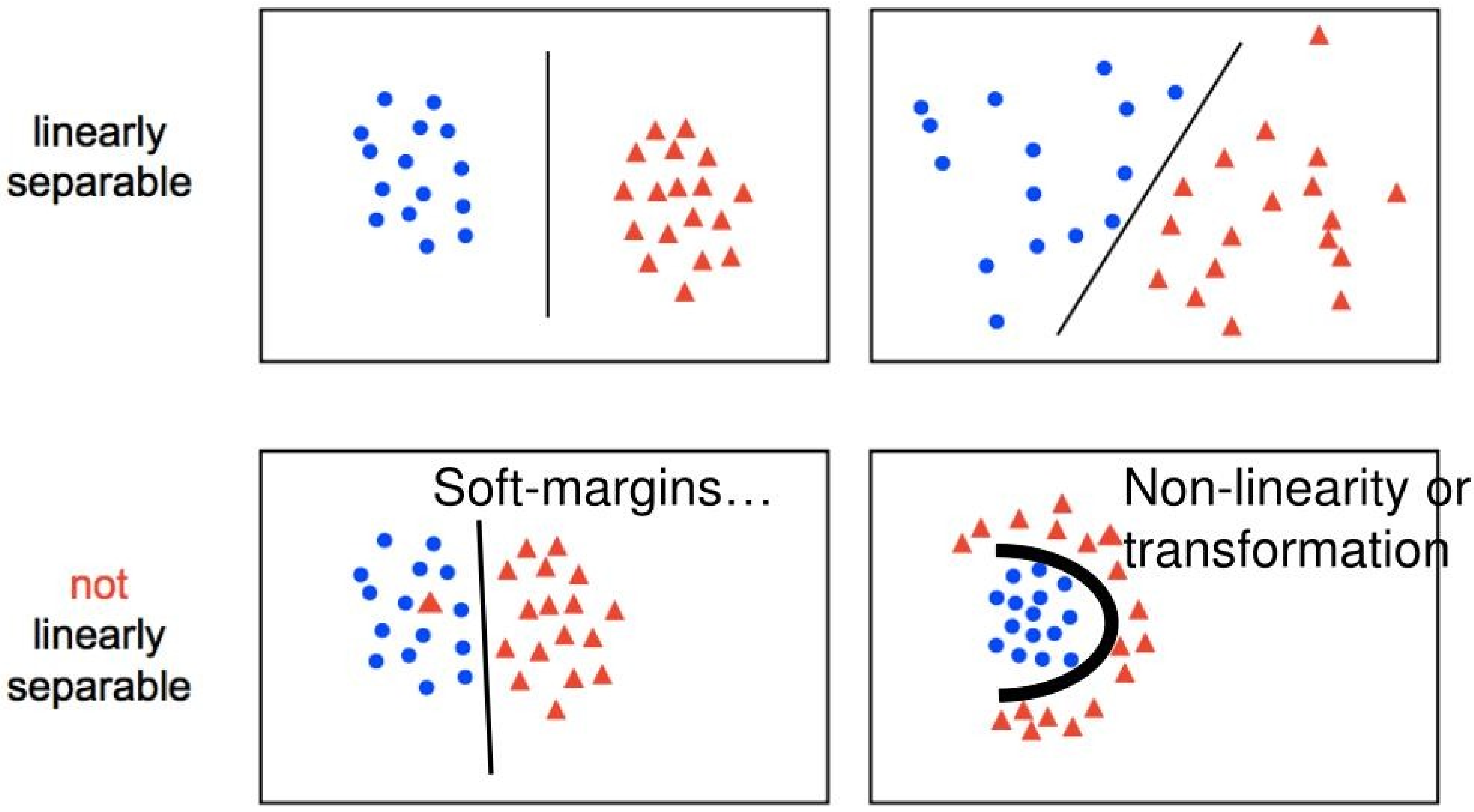


What about the “machine” part

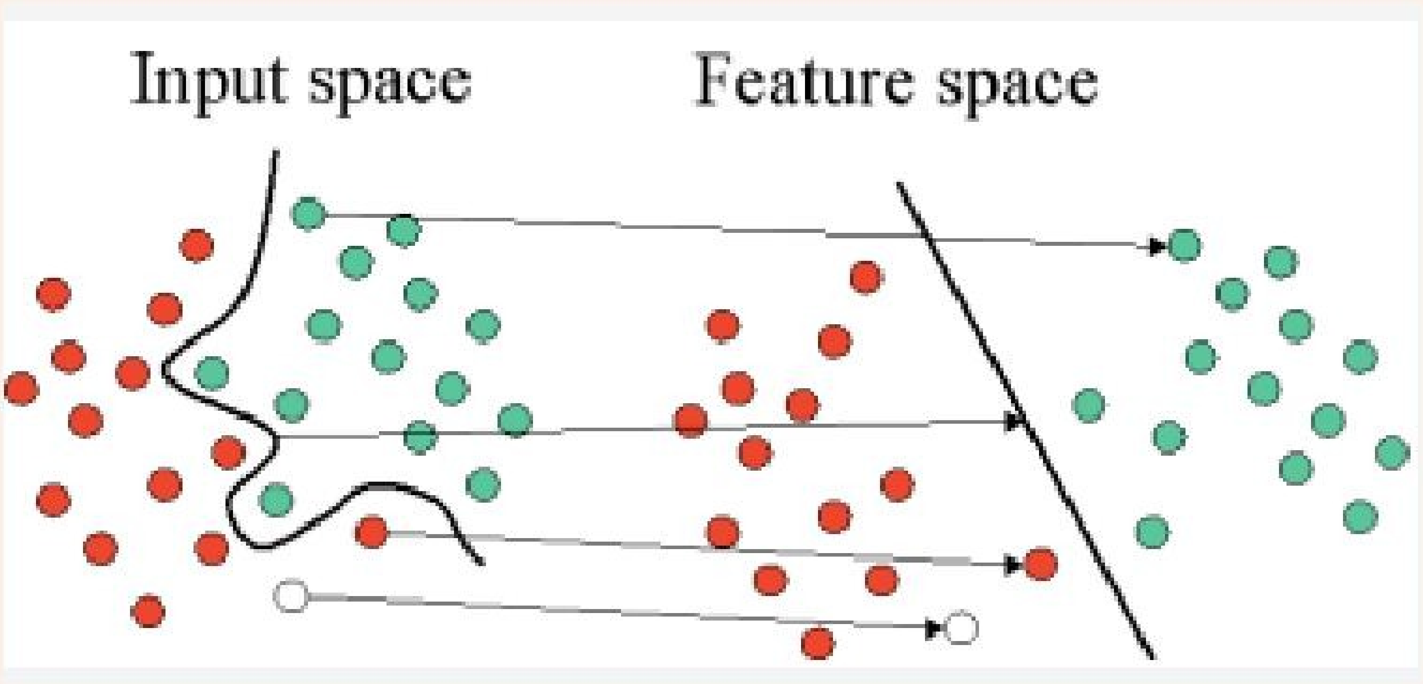
- Ignore it – somewhat leftover from the “machine learning” era
  - It is trained and then
  - Classifies

No clear separation = no hyperplane?

Linear separability



Feature space



Mapping (transformation) using a function, i.e. a kernel

- goal is – linear separability

Kernels or “non-linearity”…

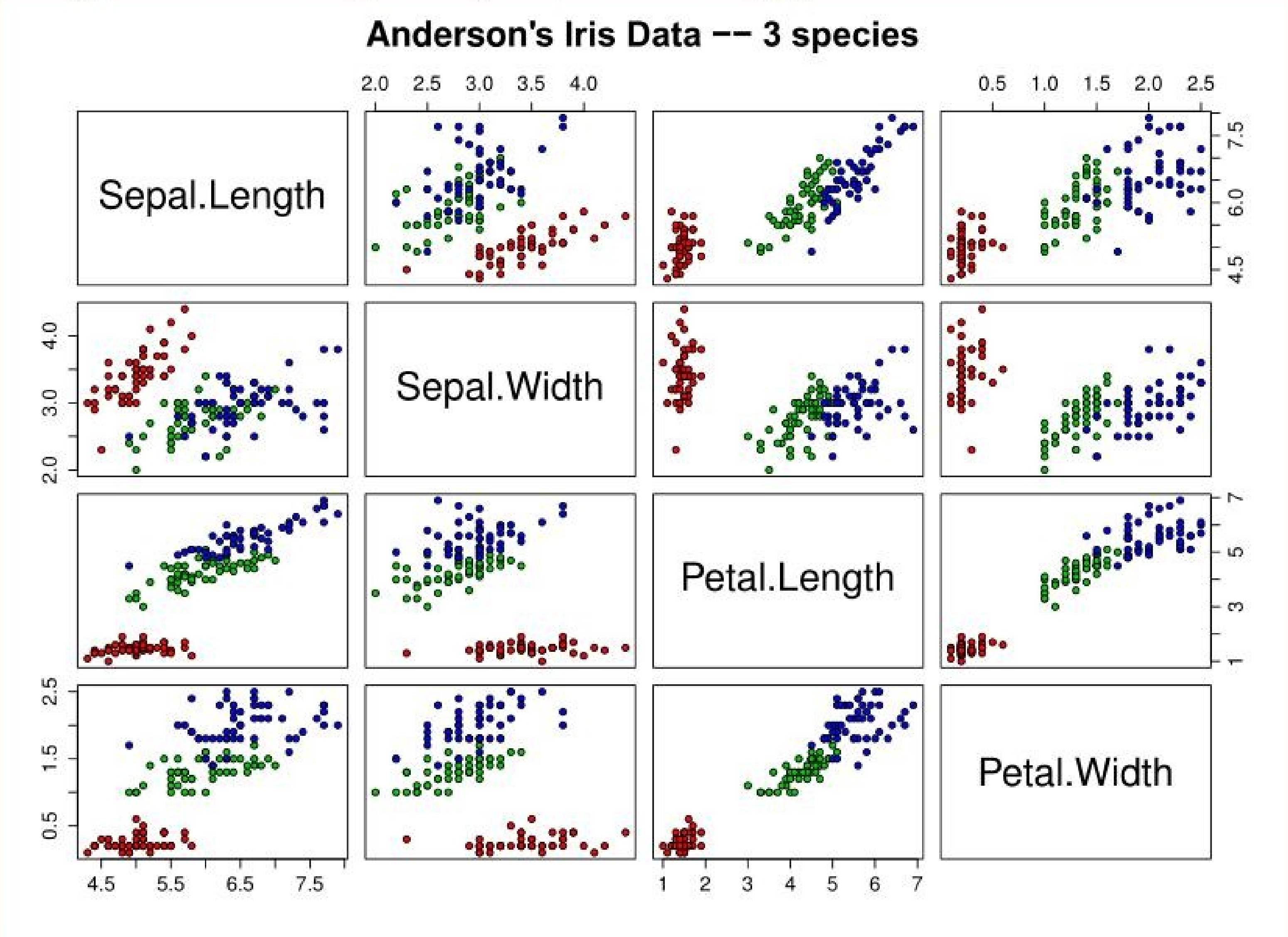
$$K(\mathbf{X}_i, \mathbf{X}_j) = \begin{cases} \mathbf{X}_i \cdot \mathbf{X}_j & \text{Linear} \\ (\gamma \mathbf{X}_i \cdot \mathbf{X}_j + \mathrm{C})^d & \text{Polynomial} \\ \exp(-\gamma |\mathbf{X}_i - \mathbf{X}_j|^2) & \text{RBF} \\ \tanh(\gamma \mathbf{X}_i \cdot \mathbf{X}_j + \mathrm{C}) & \text{Sigmoid} \end{cases}$$

where $K(\mathbf{X}_i, \mathbf{X}_j) = \phi(\mathbf{X}_i) \bullet \phi(\mathbf{X}_j)$

http://www.statsoft.com/Textbook/Support-Vector-Machines

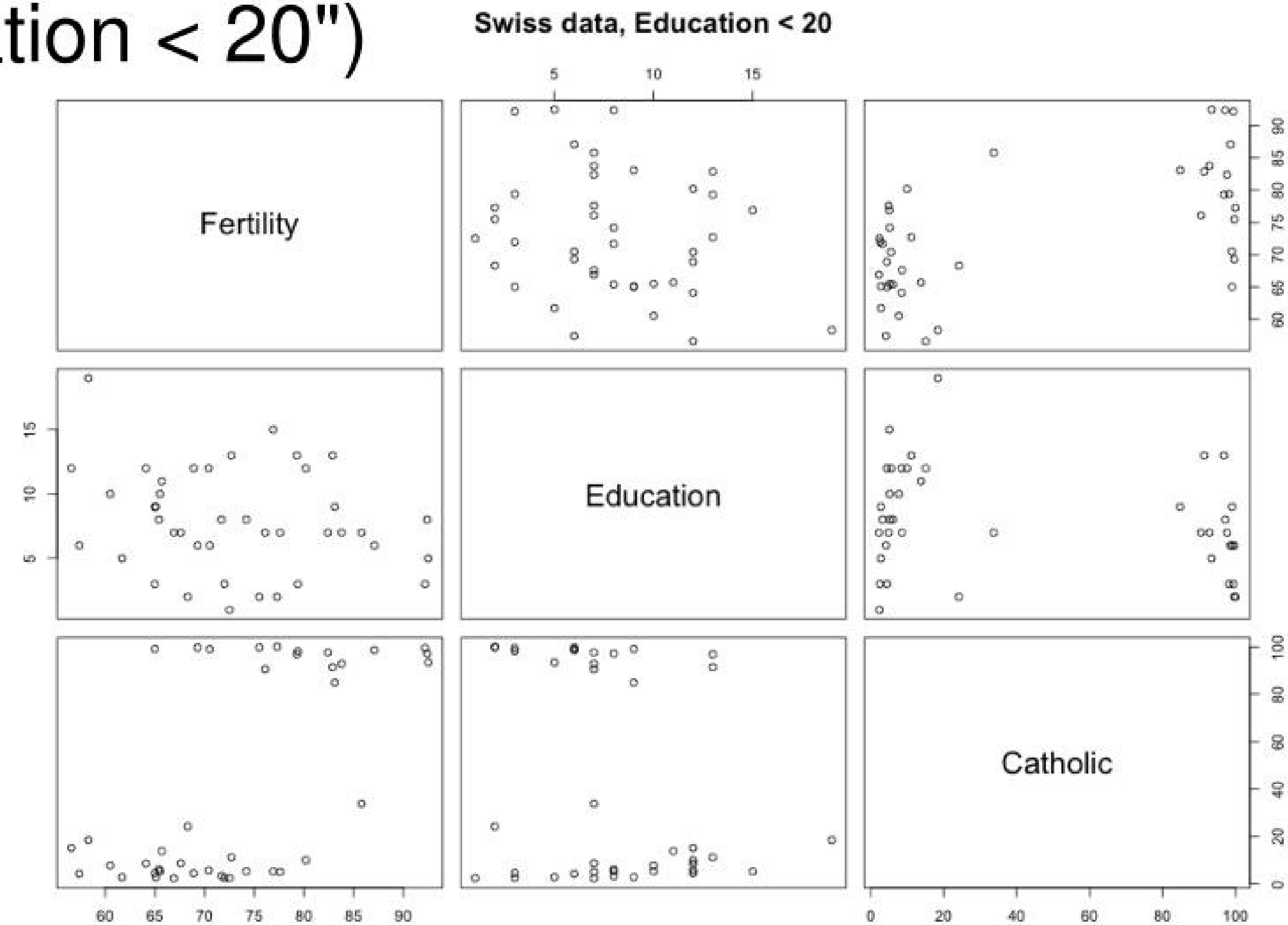
the kernel function, represents a dot product of input data points mapped into the higher dimensional feature space by transformation phi + note presence of “gamma” parameter

```
pairs(iris[1:4], main = "Anderson's Iris Data -- 3 species", pch = 21, bg = c("red", "green3", "blue")[unclass(iris$Species)])
```

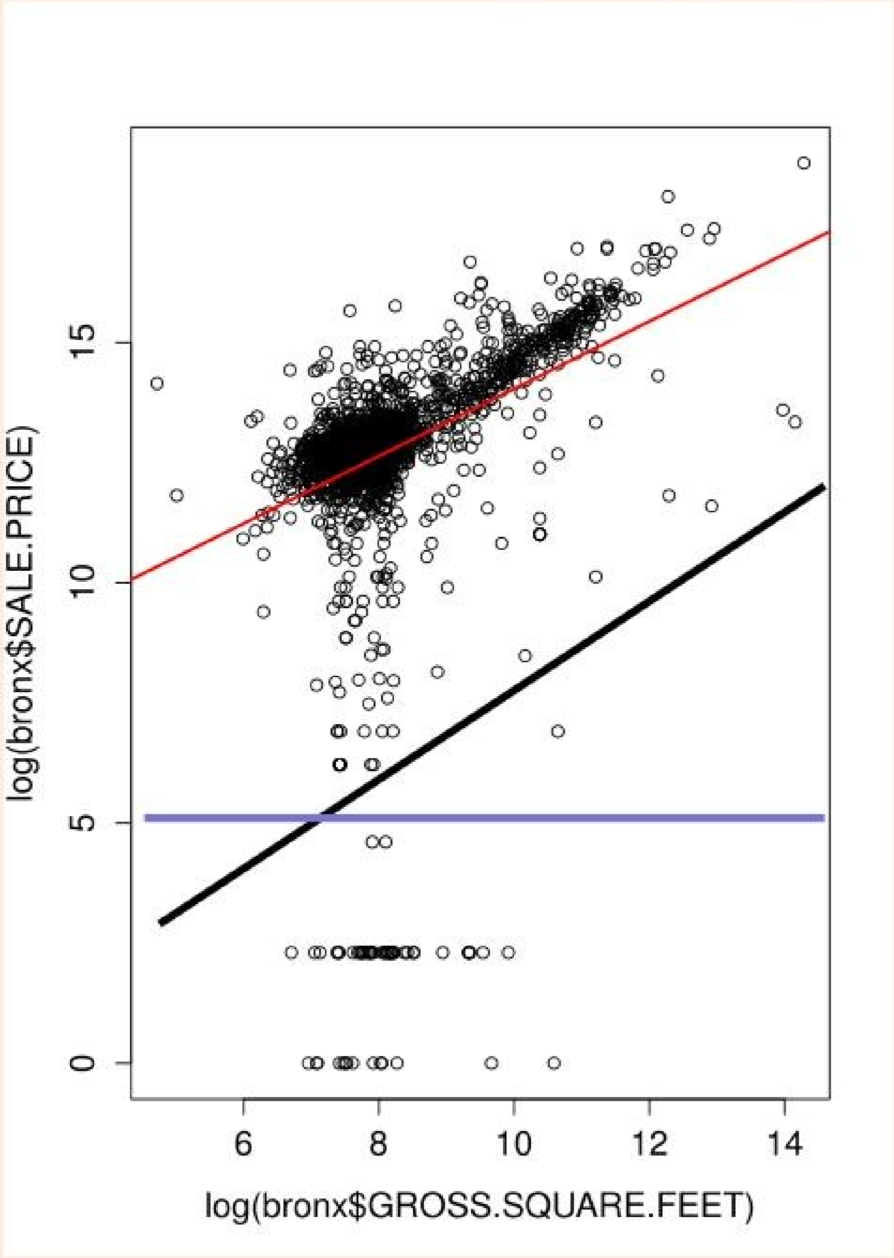


Swiss - pairs

pairs(~ Fertility + Education + Catholic, data = swiss, subset = Education < 20, main = "Swiss data, Education < 20")



Remember this one?



How would you apply SVM here?

Outlier detection

- SVMs have also been extended to deal with the problem of novelty detection (or one-class classification)
- Detection works by creating a spherical decision boundary around a set of data points by a set of support vectors describing the sphere's boundary

Multiple classification

- In addition to these heuristics for extending a binary SVM to the multi-class problem, there have been reformulations of the support vector quadratic problem that deal with more than two classes
- One of the many approaches for native support vector multi-class classification works by solving a single optimization problem including the data from all classes (spoc-svc)

Iris – svm -

Karatzoglou et al. 2006

Karatzoglou et al. 2006

kernlab, svmpath and klaR

- http://escience.rpi.edu/data/DA/v15i09.pdf

Karatzoglou et al. 2006

- Work through the examples – how did these go?
  - Familiar datasets and samples procedures from 4 libraries (these are the most used)
  - kernlab
  - e1071
  - svmpath
  - klaR

Application of SVM

- Classification, outlier, regression…
- Can produce labels or probabilities (and when used with tree partitioning can produce decision values)

- Different minimizations functions subject to different constraints (Lagrange multipliers)

See Karatzoglou et al. 2006

- Observe the effect of changing the *C* parameter and the kernel

Types of SVM (names)

- Classification SVM Type 1 (also known as C-SVM classification)
- Classification SVM Type 2 (also known as nu-SVM classification)
- Regression SVM Type 1 (also known as epsilon-SVM regression)
- Regression SVM Type 2 (also known as nu-SVM regression)

More kernels

- the linear kernel implementing the simplest of all kernel functions

$$k(\mathbf{x}, \mathbf{x}') = \langle \mathbf{x}, \mathbf{x}' \rangle$$

- the Gaussian Radial Basis Function (RBF) kernel

$$k(\mathbf{x}, \mathbf{x}') = \exp(-\sigma \|\mathbf{x} - \mathbf{x}'\|^2)$$

- the polynomial kernel

$$k(\mathbf{x}, \mathbf{x}') = \left(\text{scale} \cdot \langle \mathbf{x}, \mathbf{x}' \rangle + \text{offset}\right)^{\text{degree}}$$

- the hyperbolic tangent kernel

$$k(\mathbf{x}, \mathbf{x}') = \tanh\left(\text{scale} \cdot \langle \mathbf{x}, \mathbf{x}' \rangle + \text{offset}\right)$$

- the Bessel function of the first kind kernel

$$k(\mathbf{x}, \mathbf{x}') = \frac{\text{Bessel}^n_{(\nu+1)}(\sigma \|\mathbf{x} - \mathbf{x}'\|)}{(\|x - x'\|)^{-n(\nu+1)}}$$

- the Laplace Radial Basis Function (RBF) kenrel

$$k(\mathbf{x}, \mathbf{x}') = \exp(-\sigma \|\mathbf{x} - \mathbf{x}'\|)$$

- the ANOVA radial basis kernel

$$k(\mathbf{x}, \mathbf{x}') = \left(\sum_{k=1}^{n} \exp(-\sigma(x^k - x'^k)^2)\right)^d$$

- the linear splines kernel in one dimension

$$k(x, x') = 1 + xx' \min(x, x') - \frac{x + x'}{2}(\min(x, x')^2 + \frac{(\min(x, x')^3)}{3}$$

and for the multidimensional case $k(\mathbf{x}, \mathbf{x}') = \prod_{k=1}^{n} k(x^k, x'^k)$.

Karatzoglou et al. 2006

Timing

	ksvm() (kernlab)	svm() (e1071)	svmlight() (klaR)	svmpath() (svmpath)
spam	18.50	17.90	34.80	34.00
musk	1.40	1.30	4.65	13.80
Vowel	1.30	0.30	21.46	NA
DNA	22.40	23.30	116.30	NA
BreastCancer	0.47	0.36	1.32	11.55
BostonHousing	0.72	0.41	92.30	NA

Table 2: The training times for the SVM implementations on different datasets in seconds. Timings where done on an AMD Athlon 1400 Mhz computer running Linux.

Karatzoglou et al. 2006

Library capabilities

	`ksvm()` (**kernlab**)	`svm()` (**e1071**)	`svmlight()` (**klaR**)	`svmpath()` (**svmpath**)
Formulations	C-SVC, ν-SVC, C-BSVC, spoc-SVC, one-SVC, ϵ-SVR, ν-SVR, ϵ-BSVR	C-SVC, ν-SVC, one-SVC, ϵ-SVR, ν-SVR	C-SVC, ϵ-SVR	binary C-SVC
Kernels	Gaussian, polynomial, linear, sigmoid, Laplace, Bessel, Anova, Spline	Gaussian, polynomial, linear, sigmoid	Gaussian, polynomial, linear, sigmoid	Gaussian, polynomial
Optimizer	SMO, TRON	SMO	chunking	NA
Model Selection	hyper-parameter estimation for Gaussian kernels	grid-search function	NA	NA
Data	formula, matrix	formula, matrix, sparse matrix	formula, matrix	matrix
Interfaces	`.Call`	`.C`	temporary files	`.C`
Class System	S4	S3	none	S3
Extensibility	custom kernel functions	NA	NA	custom kernel functions
Add-ons	plot function	plot functions, accuracy	NA	plot function
License	GPL	GPL	non-commercial	GPL

Karatzoglou et al. 2006

Ozone

```
> library(e1071)
> library(rpart)
> data(Ozone, package="mlbench")
> ## split data into a train and test set
> index <- 1:nrow(Ozone)
> testindex <- sample(index, trunc(length(index)/3))
> testset <- na.omit(Ozone[testindex,-3])
> trainset <- na.omit(Ozone[-testindex,-3])
> svm.model <- svm(V4 ~ ., data = trainset, cost = 1000,
gamma = 0.0001)
> svm.pred <- predict(svm.model, testset[,-3])
> crossprod(svm.pred - testset[,3]) / length(testindex)
```

See: http://cran.r-project.org/web/packages/e1071/vignettes/svmdoc.pdf

Glass

```
library(e1071)
library(rpart)
data(Glass, package="mlbench")
index <- 1:nrow(Glass)
testindex <- sample(index, trunc(length(index)/3))
testset <- Glass[testindex,]
trainset <- Glass[-testindex,]
svm.model <- svm(Type ~ ., data = trainset, cost = 100, gamma
= 1)
svm.pred <- predict(svm.model, testset[,-10])
rpart.model <- rpart(Type ~ ., data = trainset)
rpart.pred <- predict(rpart.model, testset[,-10], type = "class")
```

```
> table(pred = svm.pred, true = testset[,10])
      true
pred  1  2  3  5  6  7
   1 12  9  1  0  0  0
   2  6 19  6  5  2  2
   3  1  0  2  0  0  0
   5  0  0  0  0  0  0
   6  0  0  0  0  1  0
   7  0  1  0  0  0  4
```

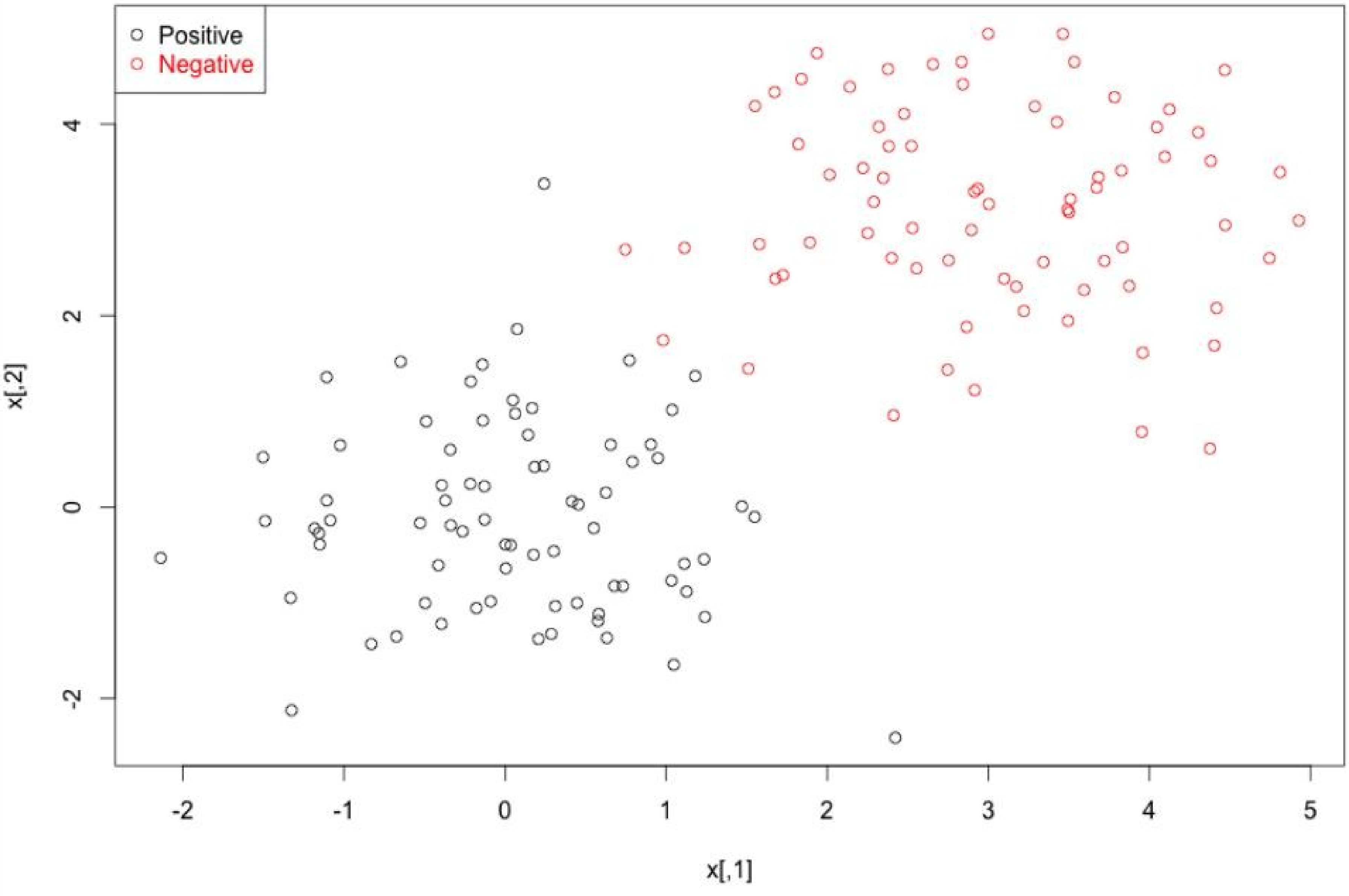
kernlab

- http://escience.rpi.edu/data/DA/svmbasic_notes.pdf
- Some scripts: Lab9b_<n>_2014.R

Example 1

```
n <- 150 # number of data points
p <- 2 # dimension
sigma <- 1 # variance of the distribution
meanpos <- 0 # centre of the distribution of positive examples
meanneg <- 3 # centre of the distribution of negative examples
npos <- round(n/2) # number of positive examples
nneg <- n-npos # number of negative examples
# Generate the positive and negative examples
xpos <- matrix(rnorm(npos*p,mean=meanpos,sd=sigma),npos,p)
xneg <- matrix(rnorm(nneg*p,mean=meanneg,sd=sigma),npos,p)
x <- rbind(xpos,xneg)
# Generate the labels
y <- matrix(c(rep(1,npos),rep(-1,nneg)))
# Visualize the data
plot(x,col=ifelse(y>0,1,2))
legend("topleft",c('Positive','Negative'),col=seq(2),pch=1,text.col=seq(2))
```

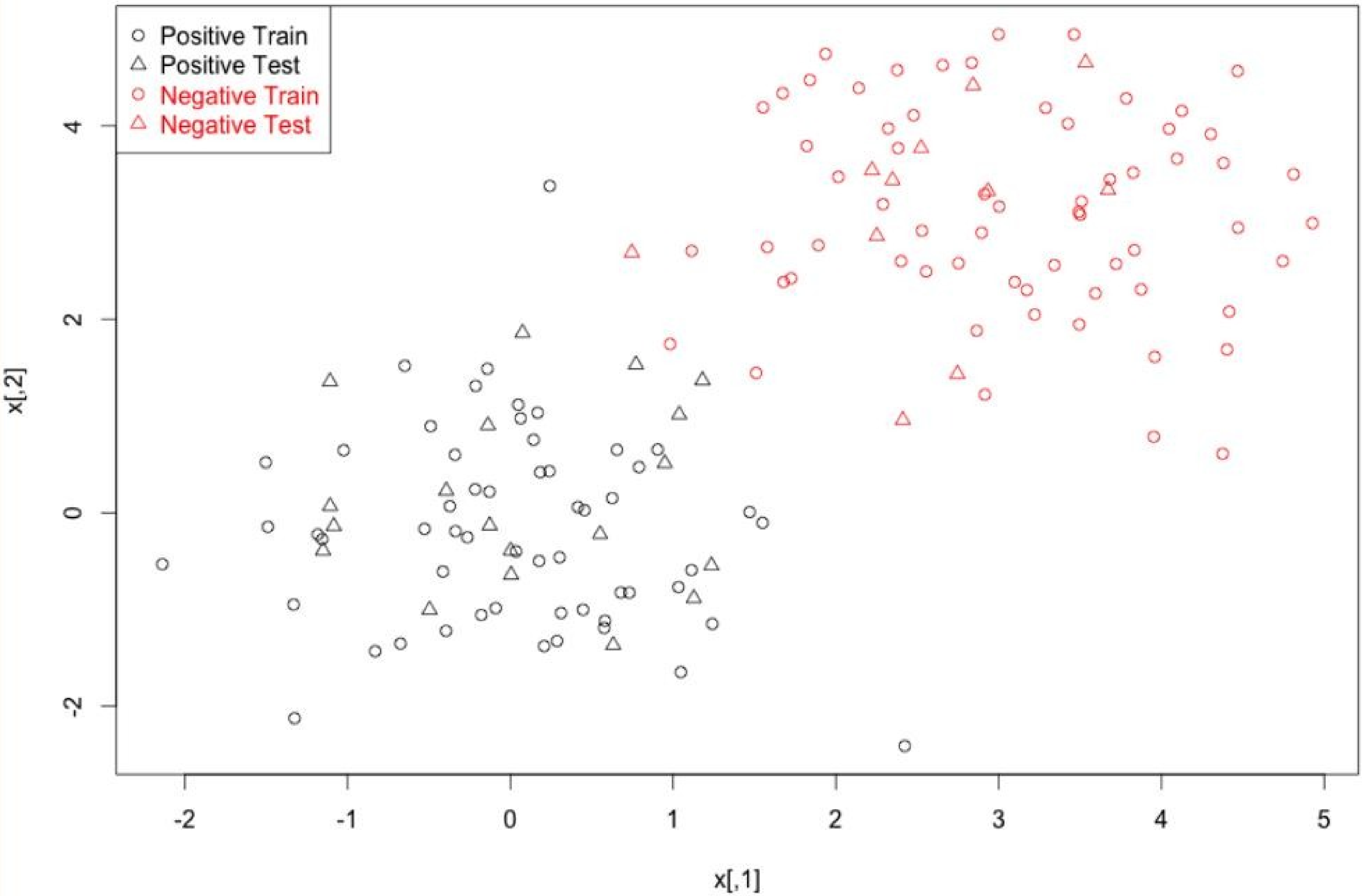
Example 1a



Train/ test

```
ntrain <- round(n*0.8) # number of training examples
tindex <- sample(n,ntrain) # indices of training samples
xtrain <- x[tindex,]
xtest <- x[-tindex,]
ytrain <- y[tindex]
ytest <- y[-tindex]
istrain=rep(0,n)
istrain[tindex]=1
# Visualize
plot(x,col=ifelse(y>0,1,2),pch=ifelse(istrain==1,1,2))
legend("topleft",c('Positive Train','Positive Test','Negative
Train','Negative Test'),col=c(1,1,2,2), pch=c(1,2,1,2),
text.col=c(1,1,2,2))
```

Comparison of test classifier



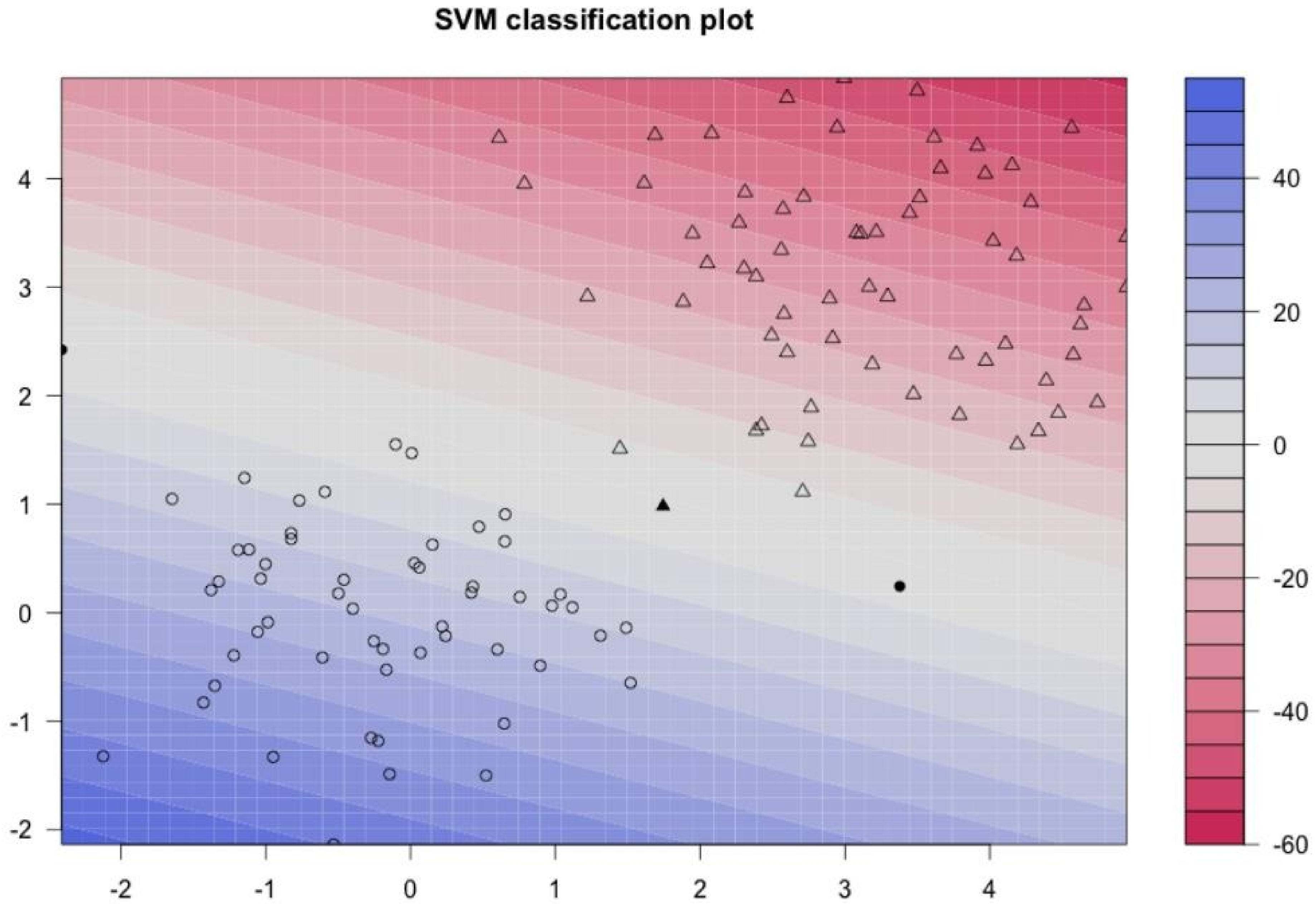
Example 2

```
svp <- ksvm(xtrain,ytrain,type="C-svc", kernel='vanilladot',
C=100,scaled=c())
# General summary
svp
# Attributes that you can access
attributes(svp) # did you look?
# For example, the support vectors
alpha(svp)
alphaindex(svp)
b(svp)          # remember b?
# Use the built-in function to pretty-plot the classifier
plot(svp,data=xtrain)
```

```
> # For example, the support vectors
> alpha(svp)
[[1]]
[1]  71.05875  28.94125 100.00000

> alphaindex(svp)
[[1]]
[1] 10 74 93

> b(svp)
[1] -17.3651
```


SVM classification plot
4
3
2
1
0
-1
-2
-2
-1
0
1
2
3
4
40
20
0
-20
-40
-60

ALL dataset (was dropped)

- http://www.stjuderesearch.org/site/data/ALL1/

R-SVM

- http://www.stanford.edu/group/wonglab/RSVMpage/r-svm.tar.gz
- http://www.stanford.edu/group/wonglab/RSVMpage/R-SVM.html
  - Read/ skim the paper
  - Explore this method on a dataset of your choice, e.g. one of the R built-in datasets

Reading some papers…

- They provide a guide to the type of project report you may prepare…

Assignment to come…

- Assignment 7: Predictive and Prescriptive Analytics. Due ~ week ~11. 20%..

Admin info (keep/ print this slide)

- Class: ITWS-4963/ITWS 6965
- Hours: 12:00pm-1:50pm Tuesday/ Friday
- Location: SAGE 3101
- Instructor: Peter Fox
- Instructor contact: pfox@cs.rpi.edu, 518.276.4862 (do not leave a msg)
- Contact hours: Monday** 3:00-4:00pm (or by email appt)
- Contact location: Winslow 2120 (sometimes Lally 207A announced by email)
- TA: Lakshmi Chenicheri chenil@rpi.edu
- Web site: http://tw.rpi.edu/web/courses/DataAnalytics/2014
  - Schedule, lectures, syllabus, reading, assignments, etc.