

Module 9: Support Vector Machines

TMA4268 Statistical Learning V2020

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Introduction

This field dates back to the 1990s in computer science, and in this presentation we put emphasis on the underlying motivation and connections to linear algebra, optimization theory and statistics.

We will only cover classification, and in particular two-class problems.

Learning material for this module

- James et al (2013): An Introduction to Statistical Learning. Chapter 9.
- [Classnotes 11.03.2019](#) (Todo: Replace this by saying there will be classnotes e.g. on the board)

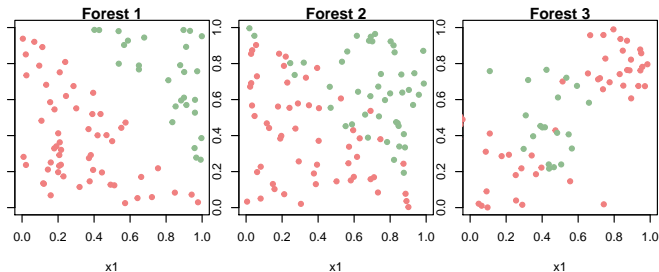
Some of the figures in this presentation are taken from (or are inspired by) James et al. (2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani.

Topics

- Motivation
- Maximal margin classifier
- Support vector classifier
- Support vector machines
- Extensions
- Comparisons
- Summing up

Motivating example

- Suppose that you are interested in the distribution of two tree types: redwood and pines.
- You have three different study areas in which these trees grow.
- Your study areas with the tree positions in three forests is visualized in the figures below. Orange: redwood tree; green: pine tree.



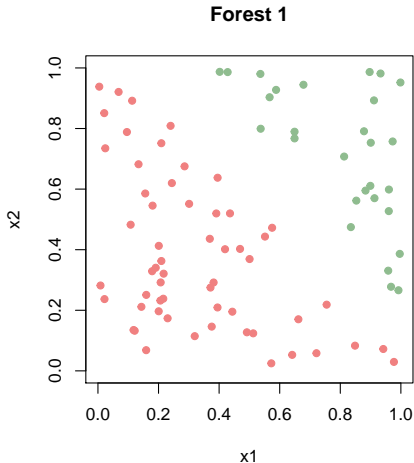
- You want to build one continuous fence to separate the two tree types in each of the three study areas. **Where should you build the fence?**

Three cases:

- Forest 1 seems easy: The orange and green points are clearly separated and the fence can be built anywhere inside the band that separates them. However, we can draw infinitely many straight lines that all separate the two tree types, and we should take into account that the trees reproduce and that we want future pines and future redwoods to grow up on the correct side of the fence.
- Forest 2 is a bit more complicated: A linear fence still seems like a good idea, but in this case the two tree types cannot be perfectly separated. You have to allow some of the trees to be on the wrong side of the fence.
- Forest 3 is the most complex: It is not possible to separate the two tree types by a straight line without getting a large number of misclassifications. Here, a circular fence around the pine trees seems like a reasonable choice.

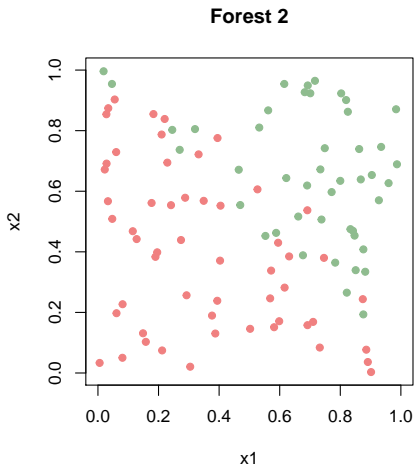
Forest 1 illustrates the problem of finding an **optimal separating hyperplane** for a dataset.

Topic: **Maximal Margin hyperplanes**



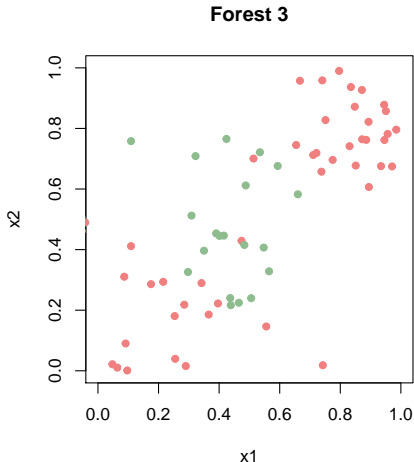
You are also going to learn how you can find an optimal separating hyperplane when your data cannot be perfectly separated by a straight line, as in Forest 2.

Topic: **Support Vector Classifier** or **Soft Margin Classifier**



The Support vector classifier can be generalised to an approach that produces non-linear decision boundaries. This is useful when the data is distributed as illustrated in Forest 3.

Topic: Support Vector Machines (SVMs)



Why are we interested in an optimal hyperplane or a separating curve?

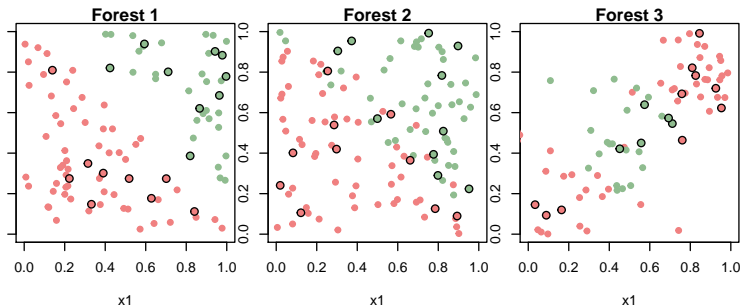
→ We want to use it for classification.

- In our example: Is it likely that a random seed found at location $(0.8, 0.4)$ becomes a redwood or a pine tree given the observed data?
- Classification of a new observation based on which side of the decision boundary it falls into.

Note: In this module we look at **binary classification**, but extensions to more than two classes are briefly mentioned.

- We will use the three forests example throughout this module.
- The two covaraites (x_1, x_2) are the coordinates of the trees.
- The response is either *pine* ($y = 1$) or *redwood* ($y = -1$).
- **Goal:** to make a classifier for random seeds that we find on the ground for each of the three forests. The locations of the seeds are shown in the figure below (black circles).

- The point patterns of the known locations can be thought of as the training set.
- The point pattern generated by the black circles can be thought of as the test set.



Maximal Margin Classifier

Hyperplane

A **hyperplane** in p -dimensions is defined as

$$\beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p = \beta_0 + \mathbf{x}^T \boldsymbol{\beta} = 0.$$

and is a $p - 1$ dimensional subspace of \mathbb{R}^p .

Recap:

- If a point $\mathbf{x} = (x_1, x_2, \dots, x_p)^T$ satisfies the above equation, it lies on the hyperplane.
- If $\beta_0 = 0$ the hyperplane goes through the origin.
- The vector $\boldsymbol{\beta} = (\beta_1, \dots, \beta_p)$ (not including β_0) is called the normal vector and points in the direction orthogonal to the hyperplane.

If a point \mathbf{x} satisfies

- $\beta_0 + \boldsymbol{\beta}^\top \mathbf{x} > 0$ it lies on one side of the hyperplane
 - $\beta_0 + \boldsymbol{\beta}^\top \mathbf{x} < 0$ it lies on the opposite side of the hyperplane.
 - $\beta_0 + \boldsymbol{\beta}^\top \mathbf{x} = 0$ it lies on the hyperplane (by definition!).
-
- The signed distance of any point \mathbf{x} to the hyperplane is given by

$$\frac{1}{\|\boldsymbol{\beta}\|} (\beta_0 + \boldsymbol{\beta}^\top \mathbf{x}) ,$$

where $\|\boldsymbol{\beta}\|^2 = \sum_{j=1}^p \beta_j^2 = 1$ is the (squared) length of $\boldsymbol{\beta}$ (Euclidian norm).

- See board for a graphical description (todo).

Assumptions

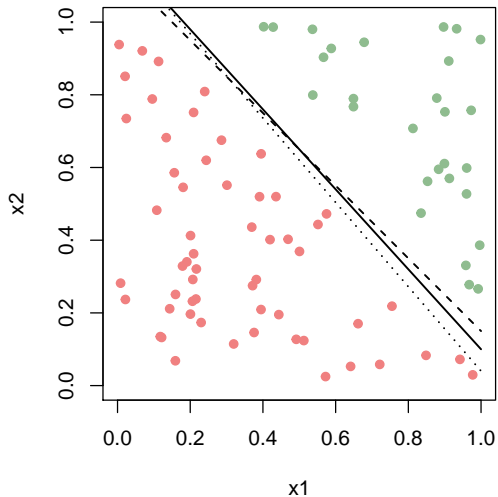
- Assume that we have n training observations with p predictors

$$\mathbf{x}_1 = \begin{pmatrix} x_{11} \\ \vdots \\ x_{1p} \end{pmatrix}, \dots, \mathbf{x}_n = \begin{pmatrix} x_{n1} \\ \vdots \\ x_{np} \end{pmatrix}$$

- The responses \mathbf{y} fall into two classes $y_1, \dots, y_n \in \{-1, 1\}$.
- It is possible to separate the training observations perfectly according to their class.

Possible hyperplanes (Forest 1)

Which is “best”?



Classification with a simple hyperplane

The three lines displayed in the figure are three possible separating hyperplanes for this dataset which contains two predictors x_1 and x_2 ($p = 2$). The hyperplanes have the property that

$$\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip} = \beta_0 + \mathbf{x}_i^T \boldsymbol{\beta} > 0$$

if $y_i = 1$ (green points) and

$$\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip} = \beta_0 + \mathbf{x}_i^T \boldsymbol{\beta} < 0$$

if $y_i = -1$ (orange points).

This means that for all observations (all are correctly classified)

$$y_i(\beta_0 + \mathbf{x}_i^T \boldsymbol{\beta}) > 0 .$$

The hyperplane thus leads to a *natural classifier*, depending on the side of the hyperplane where the new observation lies.

The class y^* of a new observation $x^* = (x_1^*, \dots, x_n^*)$ is assigned depending on the value $f(x^*) = \beta_0 + \beta_1 x_1^* + \beta_2 x_2^* + \dots + \beta_p x_p^*$

Hyperplane classifier:

$$y^* = \begin{cases} 1 , & \text{if } f(x^*) > 0 , \\ -1 , & \text{if } f(x^*) < 0 . \end{cases}$$

Which hyperplane is best?

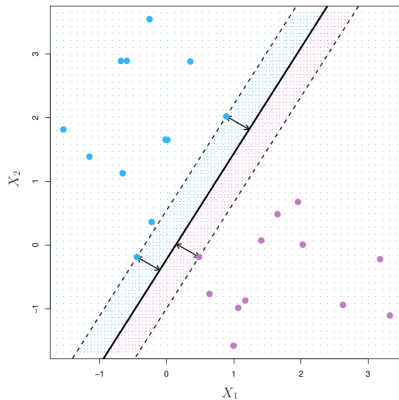
- In the above figure we plotted three possible hyperplanes.
- In general, if data are linearly separable, infinitely many possible separating hyperplanes exist.
- Natural choice: the **maximal margin hyperplane**, which maximises the distance from the training observations.

Procedure:

- Compute the perpendicular distance from each training observation to a given separating hyperplane.
- The smallest such distance is the minimal distance from the observations to the hyperplane (the **margin**).
- We want to maximize this margin.

(From a statistical point of view we might be afraid that we are overfitting the data now. Why?)

We have an **optimization problem** to maximize the width of the margin:



ISLR Figure 9.3

The process of finding the maximal margin hyperplane for a dataset with p covariates and n training observations can be formulated through the following **optimization problem**:

$$\text{maximize}_{\beta_0, \beta_1, \dots, \beta_p} M$$

$$\text{subject to } \sum_{j=1}^p \beta_j^2 = 1,$$

$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip}) \geq M \quad \forall i = 1, \dots, n$$

where M is the width of the margin.

Observe:

- $y_i(\beta_0 + \mathbf{x}^T \boldsymbol{\beta})$ is the (signed) distance from the i th point to the hyperplane defined by the β s ¹.
- We want to find the hyperplane, where each observation is at least M units away - on the correct side, where M is as big as possible.

¹(Todo: Perhaps add exercise about that, or make drawing)

- In the ISLR Figure 9.3, the three equidistant points are called **support vectors**.
- If one of the support vectors changes its position, the whole hyperplane will move.
- This is a property of the maximal margin hyperplane: It only depends on the support vectors, and not on the other observations.

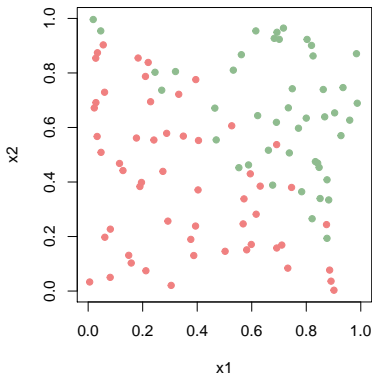
- It can be shown, see for example Friedman, Hastie, and Tibshirani (2001) Section 4.5.2 (*Optimal Separating Hyperplanes*), that the optimization problem can be reformulated using Lagrange multipliers (primal and dual problem) into a quadratic convex optimization problem that can be solved efficiently.
- However, we do of course have to solve the optimization problem to identify the support vectors and the unknown parameters for the separating hyperplane.
- Since we in TMA4268 Statistical learning do not require a course in optimization - we do not go into details here.

Questions

1. Explain briefly the idea behind the maximal margin classifier.
2. Is there any tuning parameters that needs to be chosen?

Support Vector Classifiers

For some data sets a separating hyperplane does not exist, the data set is *non-separable*. What then? Forest 2:



It is still possible to construct a hyperplane and use it for classification, but then we have to allow some misclassification in the training data.

- In some situations allowing for some misclassifications makes the class boundaries more robust to future observations (avoid overfitting).
- When there are more predictors than observations it is always possible to find a separating hyperplane in the predictor space, but the might not be the “best” hyperplane for us.
- We relax the maximal margin classifier to allow for a *soft margin classifier* (=support vector classifier).

Optimization problem

To obtain a support vector classifier we relax the conditions that we had for the maximal margin hyperplane by allowing for a “budget” C of misclassifications:

$$\text{maximize}_{\beta_0, \beta_1, \dots, \beta_p} M$$

$$\text{subject to } \sum_{j=1}^p \beta_j^2 = 1,$$

$$y_i(\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{ip}) \geq M(1 - \epsilon_i) \quad \forall i = 1, \dots, n.$$

$$\epsilon_i \geq 0, \quad \sum_{i=1}^n \epsilon_i \leq C.$$

- M is the width of the margin.
- $\epsilon_1, \dots, \epsilon_n$ are *slack variables*.
 - If $\epsilon_i = 0$ it means that observation i is on the correct side of the margin,
 - if $\epsilon_i > 0$ observation i is on the wrong side of the margin, and
 - if $\epsilon_i > 1$ observation i is on the wrong side of the hyperplane.
- C is a *tuning (regularization) parameter* (chosen by cross-validation) giving the *budget for slacks*. It restricts the number of the training observations that can be on the wrong side of the hyperplane. No more than C of the observations can be on the wrong side.

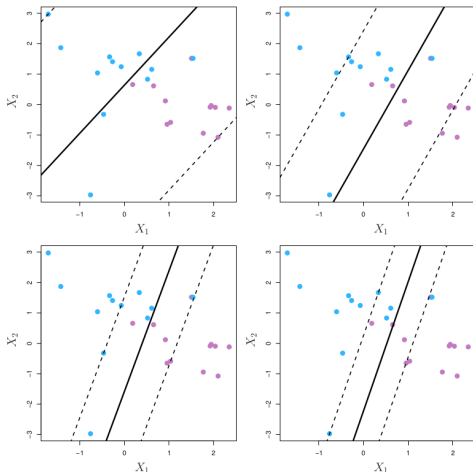
- The hyperplane has the property that it **only** depends on the observations that **either lie on the margin or on the wrong side of the margin**.
- These observations are called our **support vectors**.
- The observations on the correct side of the margin do not affect the support vectors. The length of distance for the support vectors to the class boundary is proportional to the slacks.

Classification rule: We classify a test observation \mathbf{x}^* based on the sign of $f(\mathbf{x}^*) = \beta_0 + \beta_1 x_1^* + \dots + \beta_p x_p^*$ as before:

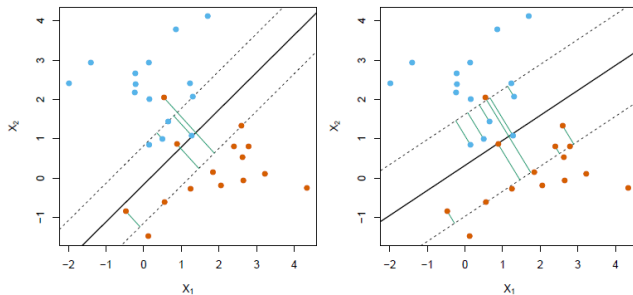
- If $f(\mathbf{x}^*) < 0$ then $y^* = -1$.
- If $f(\mathbf{x}^*) > 0$ then $y^* = 1$.

More on solving the optimization problem: Friedman, Hastie, and Tibshirani (2001) Section 12.2.1 (primal and dual Lagrange problem, quadratic convex problem).

ISLR Figure 9.7: From large C (top left) to small C (bottom right). As C decreases the tolerance for observations being on the wrong side of the margin decreases and the margin narrows.



See also Figure 19.3 in Efron and Hastie (2016):



Questions

- Should the variables be standardized before used with this method?
- The support vector classifier only depends on the observations that violate the margin. How does C affect the width of the margin?
- Discuss how the tuning parameter C affects the bias-variance trade-off of the method.

A: Yes, should be standardized because this method treats all variables equally. Same as for lasso and ridge.

If C is small then M must give narrow margin? C is our bias-variance trade-off tuning parameter: C large: allow many violations: more bias, less variance. C small: highly fit the data: less bias, more variance.

Example

We will now find a support vector classifier for the second training dataset (forest2) and use this to classify the observations in the second test set (seeds2).

- There are 100 observations of trees: 45 pines ($y_i = 1$) and 55 redwood trees ($y_i = -1$).
- In the test set there are 20 seeds: 10 pine seeds and 10 redwood seeds.

The function `svm` in the package `e1071` is used to find the maximal margin hyperplane. The response needs to be coded as a factor variable, and the data set has to be stored as a dataframe.

```
library(e1071)
forest2 = read.table(file = "https://www.math.ntnu.no/emner/TMA4268/2019v/data/
seeds2 = read.table(file = "https://www.math.ntnu.no/emner/TMA4268/2019v/data/s
train2 = data.frame(x = forest2[, 1:2], y = as.factor(forest2[, 3]))
test2 = data.frame(x = seeds2[, 1:2], y = as.factor(seeds2[, 3]))
```

The `svm` function uses a slightly different formulation from what we wrote above.

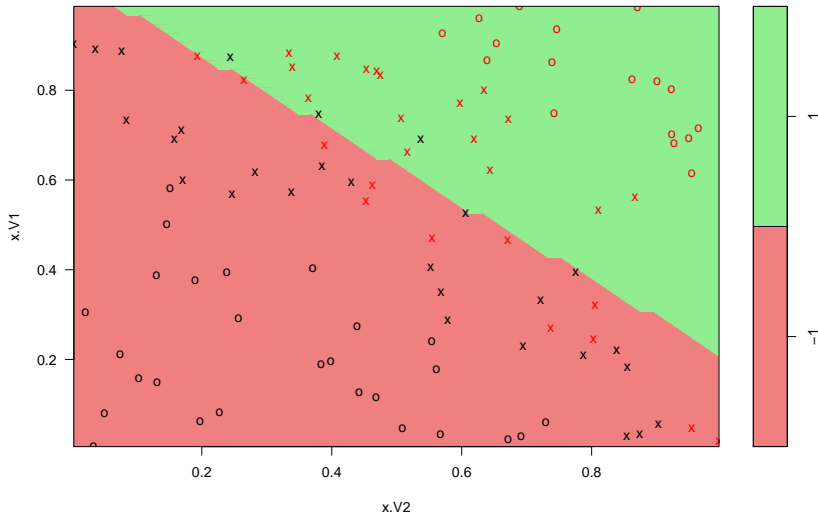
We had in our presentation a budget for errors C , but in `svm` we instead have an argument `cost` that allows us to specify the cost of violating the margin.

- When `cost` is set to a low value, the margin will be wider than if set to a large value.

We first try with `cost=1`. We set `kernel='linear'` as we are interested in a linear decision boundary. `scale=TRUE` scales the predictors to have mean 0 and standard deviation 1. We choose not to scale.

```
svmfit_linear1 = svm(y ~ ., data = train2, kernel = "linear", cost = 1,  
  scale = FALSE)  
plot(svmfit_linear1, train2, col = c("lightcoral", "lightgreen"))
```

SVM classification plot



```
summary(svmfit_linear1)
```

```
##
```

```
## Call:
```

```
## svm(formula = y ~ ., data = train2, kernel = "linear", cost =
```

```
##     scale = FALSE)
```

```
##
```

```
##
```

```
## Parameters:
```

```
##   SVM-Type:  C-classification
```

```
## SVM-Kernel:  linear
```

```
##       cost:  1
```

```
##
```

```
## Number of Support Vectors:  56
```

```
##
```

```
##   ( 28 28 )
```

```
##
```

```
##
```

```
## Number of Classes:  2
```

```
##
```

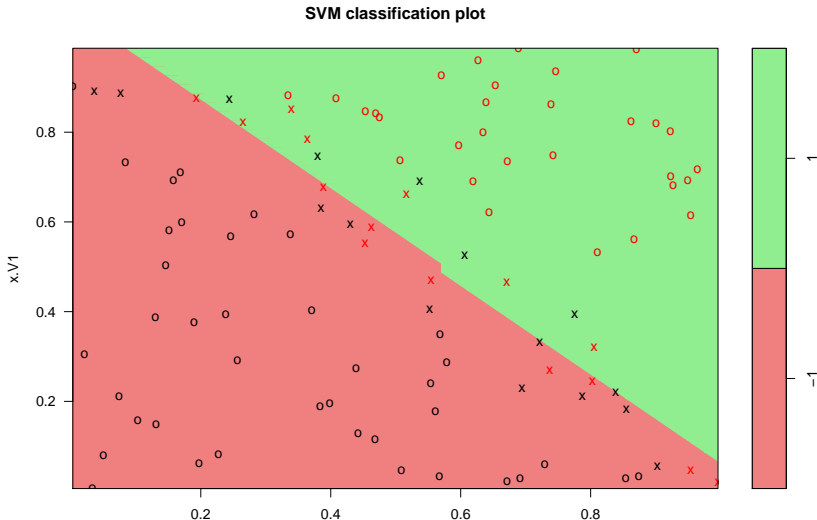
```
## Levels:
```

Observations

- Remark that the x_1 is plotted on the vertical axis, and the the implementation of the plotting function is made in a way that the linear boundary looks jagged.
- The crosses in the plot indicate the support vectors. With $cost = 1$, we have 56 support vectors, 28 in each class.
- All other observations are shown as circles.

Next, we set $cost = 100$:

```
svmfit_linear2 = svm(y ~ ., data = train2, kernel = "linear", cost = 100,  
  scale = FALSE)  
plot(svmfit_linear2, train2, col = c("lightcoral", "lightgreen"))
```



```
summary(svmfit_linear2)
```

```
##
```

```
## Call:
```

```
## svm(formula = y ~ ., data = train2, kernel = "linear", cost =
```

```
##     scale = FALSE)
```

```
##
```

```
##
```

```
## Parameters:
```

```
##   SVM-Type:  C-classification
```

```
## SVM-Kernel:  linear
```

```
##         cost:  100
```

```
##
```

```
## Number of Support Vectors:  31
```

```
##
```

```
##   ( 15 16 )
```

```
##
```

```
##
```

```
## Number of Classes:  2
```

```
##
```

```
## Levels:
```


With $cost = 100$ we have 31 support vectors, i.e the width of the margin is decreased.

How do we find an optimal $cost$ parameter? By using the `tune()` function we can perform ten-fold cross-validation and find the cost-parameter that gives the lowest cross-validation error:

```
set.seed(1)
CV_linear = tune(svm, y ~ ., data = train2, kernel = "linear", ranges = list(cost =
  0.01, 0.1, 1, 5, 10, 100)))
summary(CV_linear)
```

```
##
## Parameter tuning of 'svm':
##
## - sampling method: 10-fold cross validation
##
## - best parameters:
##   cost
##     5
##
## - best performance: 0.14
##
## - Detailed performance results:
##   cost error dispersion
## 1 1e-03  0.45 0.10801234
```

According to the *tune()* function we should set the cost parameter to 0.1. The function also stores the best model obtained and we can access it as follows:

```
bestmod_linear = CV_linear$best.model
```

Next, we want to predict the class label of the seeds in the test set. We use the `predict` function and make a confusion table:

```
ypred_linear = predict(bestmod_linear, test2)
table(predict = ypred_linear, truth = test2[, 3])
```

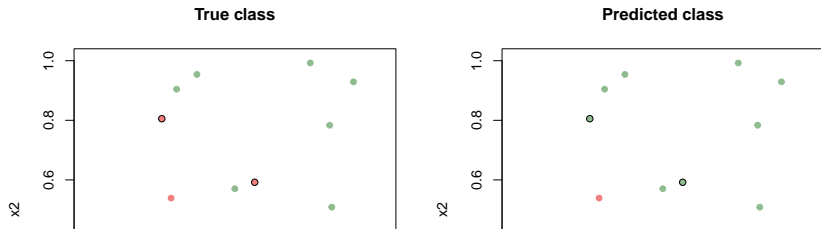
```
##          truth
## predict -1  1
##        -1  8  0
##         1  2 10
```

```

par(mfrow = c(1, 2))
par(pty = "s")
plot(NA, xlab = "x1", ylab = "x2", xlim = c(0, 1), ylim = c(0, 1))
title("True class")
points(seeds2[seeds2[, 3] == -1, 1:2], pch = 19, col = "lightcoral",
       cex = 0.9)
points(seeds2[seeds2[, 3] == 1, 1:2], pch = 19, col = "darkseagreen",
       cex = 0.9)
points(seeds2[which(ypred_linear != seeds2[, 3]), 1:2], pch = 21) #Mark miscla

plot(NA, xlab = "x1", ylab = "x2", xlim = c(0, 1), ylim = c(0, 1))
title("Predicted class")
points(seeds2[ypred_linear == -1, 1:2], pch = 19, col = "lightcoral",
       cex = 0.9)
points(seeds2[ypred_linear == 1, 1:2], pch = 19, col = "darkseagreen",
       cex = 0.9)
points(seeds2[which(ypred_linear != seeds2[, 3]), 1:2], pch = 21) #Mark miscla

```

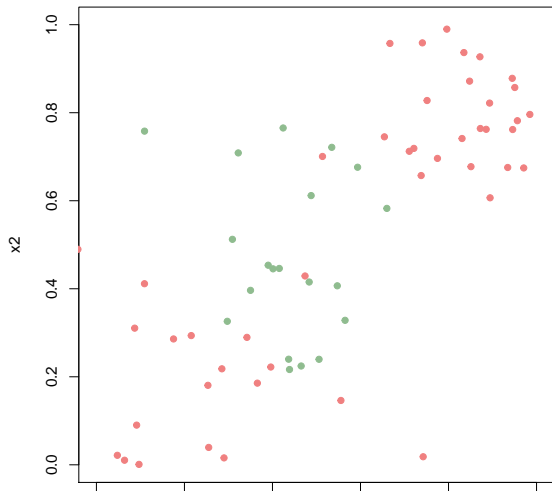


In this case three of the test observations are misclassified: These three observations are marked with a black circle in the plot, and we observe that they lie on the border between the green and the orange points which is reasonable: The test observations located on the border between green and orange are hardest to predict.

Missing: the `svm` function is not (directly) outputting the equation for the class boundary, and not the value for the width of the margin. Want to see how to find this? See the recommended exercises.

Support Vector Machines

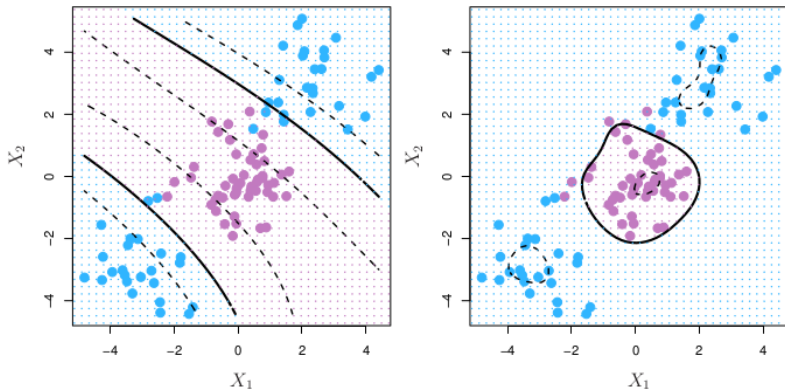
For some datasets a non-linear decision boundary between the classes is more suitable than a linear decision boundary. In such cases you can use a **Support Vector Machine** (SVM). This is an extension of the support vector classifier.



Expanding the feature space

We saw in Module 7 that in regression we could fit non-linear curves by using a polynomial basis - adding polynomials of different order as covariates. This was a linear regression in the transformed variables, but non-linear in the original variables. Maybe we may add many such extra features and find a nice linear boundary in that high-dimensional space?

Efron and Hastie (2016) (page 377): *If $n \leq p + 1$ we can always find a separating hyperplane, unless there are exact features ties across the class barrier.* (Two observations with equal covariate vector, but different classes.)



Left: expanding feature space to include cubic polynomials ($x_1, x_2, x_1x_2, x_1^2, x_2^2, x_1^2x_2, x_1x_2^2x_1^3, x_2^3$, 9 parameters to estimate in addition to intercept), and also observe the margins. (Right: radial basis function kernel - wait a bit.)

Next: replace polynomials with *kernels* for elegance and computational issues.

Inner products

We have not focused on how to solve the optimisation problem of finding the support vector classifier hyperplane, because this is outside the scope of this course.

Remember that we classify a new observation \mathbf{x}^* by first calculating a numerical value for the estimated $f(\mathbf{x}^*)$ and then if $f(\mathbf{x}^*) < 0$ classify as -1 and if $f(\mathbf{x}^*) > 0$ classify as 1 .

It can be *shown* (using optimization theory) that the solution to the support vector classifier problem at a new observation \mathbf{x}^* , can be expressed as

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

where α_i is some parameter and $i = 1, \dots, n$.

A term of the form $\langle \mathbf{x}_i, \mathbf{x}_{i'} \rangle$ denotes the inner product between two observations i and i' and is defined as:

$$\langle \mathbf{x}_i, \mathbf{x}_{i'} \rangle = \sum_{j=1}^p x_{ij} x_{i'j}.$$

This means that we need (in addition to the intercept) to estimate n parameters (α_i s) instead of p (β_j s) (and for our expanded feature space then p might be larger than n). (For the interested reader: See Eq. 19.22 and 19.23 of Efron and Hastie (2016).)

Further, it then turns out that to estimate the parameters $\beta_0, \alpha_1, \dots, \alpha_n$ this can be based on the *nchoose2* inner products $\langle \mathbf{x}_i, \mathbf{x}_i' \rangle$ between all pair of training observations (the class of the training observations is also included).

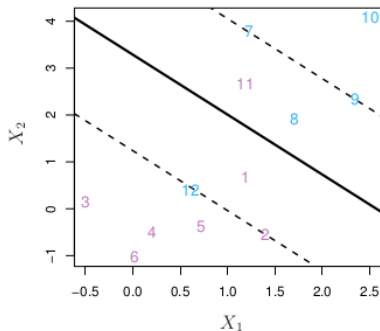
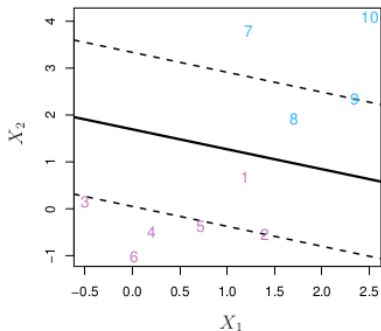
Also, $\alpha_i = 0$ for the observations i that are *not* the support vectors.
Remark: we could alternatively say that $\alpha_i \neq 0$ define the support vectors.

Thus, we only need the inner product between the new observation and the observations corresponding to support vectors to classify a new observation, and

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

where \mathcal{S} contains the indices of the support points. So, we have sparsity in the observations (but not in the predictors).

Q: Find the support vectors



Observe: we need all observations (both x and y values) to decide on which observations are the support vectors.

Kernels

(we now use x to denote a new observation)

The next step is now to *replace the inner product* $\langle \mathbf{x}, \mathbf{x}_i \rangle$ with a function $K(\mathbf{x}_i, \mathbf{x}_{i'})$ referred to as the **kernel**:

$$f(\mathbf{x}) = \beta_0 + \sum_{i \in \mathcal{S}} \alpha_i K(\mathbf{x}, \mathbf{x}_i).$$

For the linear case (which is what we have considered so far), the kernel is simply the inner product $K(\mathbf{x}_i, \mathbf{x}'_i) = \sum_{j=1}^p x_{ij} x'_{ij}$.

The two arguments to the kernel are two p -vectors.

If we want a more flexible decision boundary we could instead use a **polynomial kernel**. This polynomial kernel of degree $d > 1$ is given by:

$$K(\mathbf{x}_i, \mathbf{x}'_i) = (1 + \sum_{j=1}^p x_{ij} x'_{ij})^d.$$

(This kernel is not so much used in practice, but is popular for proofs.)

Using these kernels our solution for the class boundary can be written of the form

$$f(\mathbf{x}) = \beta_0 + \sum_{i \in \mathcal{S}} \alpha_i K(\mathbf{x}, \mathbf{x}_i)$$

The nice thing here is that we only need to calculate the kernels, not the basis functions (what we in Module 7 did as extra columns of the design matrix).

A very popular choice is the radial kernel,

$$K(\mathbf{x}_i, \mathbf{x}'_i) = \exp(-\gamma \sum_{j=1}^p (x_{ij} - x'_{ij})^2),$$

where γ is a positive constant (a tuning parameter).

Observe the connection to a multivariate normal density, where $\gamma \propto 1/\sigma^2$ (σ^2 variance in normal distribution). If γ is small (similar to large variance in the normal distribution) the decision boundaries are smoother than for larger γ .

It turns out that this computes the inner product in a very high (infinite) dimensional feature space. But, this does not give overfitting because some of the dimensions are “squashed down” (but we have the parameter γ and the budget parameter that we have to decide on).

The radial kernel is convenient if we want a circular decision boundary, and γ and our budget can be chosen by cross-validation.

Remark: the mathematics behind this is based on *reproducing-kernel Hilbert spaces* (see page 384 of Efron and Hastie (2016) for a glimpse of the theory).

Study Figures 19.5 and 19.6 (page 383) in Efron and Hastie (2016) to see how the radial kernel can make smooth functions.

Computer Age Statistical Inference

Kernels and our optimization

We now merge our optimization problem (from our support vector classifier) with our kernel representation $f(\mathbf{x})$ to get the Support Vector Machine (SVM).

$$\begin{aligned} & \text{maximize}_{\beta_0, \alpha_1, \dots, \alpha_n, \epsilon_1, \dots, \epsilon_n} \quad M \\ & y_i(f(\mathbf{x}_i)) \geq M(1 - \epsilon_i) \quad \forall i = 1, \dots, n. \\ & \epsilon_i \geq 0, \quad \sum_{i=1}^n \epsilon_i \leq C. \end{aligned}$$

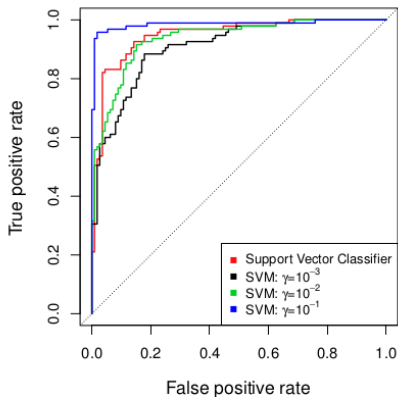
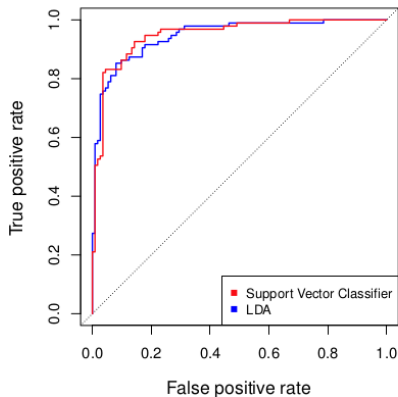
where

$$f(\mathbf{x}_i) = \beta_0 + \sum_{l \in \mathcal{S}} \alpha_l K(\mathbf{x}_i, \mathbf{x}_l)$$

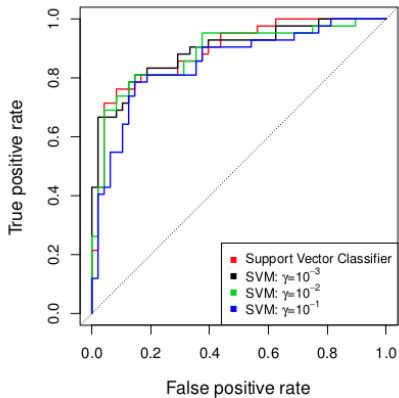
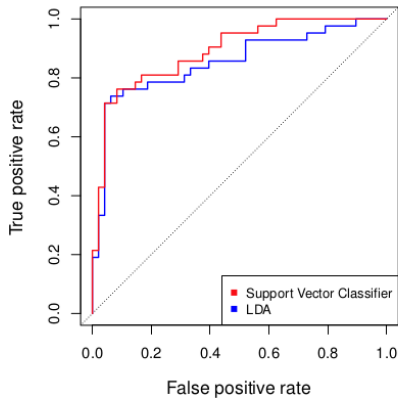
Tuning parameter example

Heart data - predict heart disease from $p = 13$ predictors.

Training errors as ROC and AUC.



Heart data - test error.



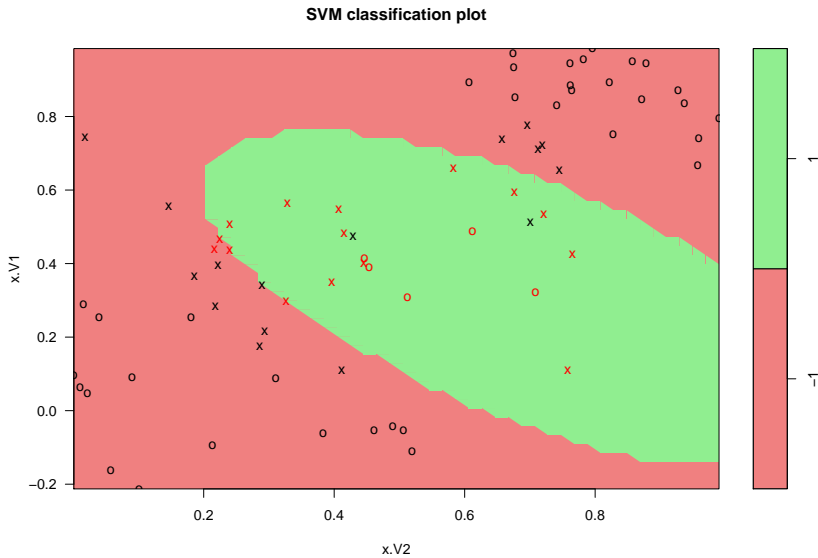
Example: forest 3

To illustrate the SVM we use the third training dataset (forest3) and the third test set (seeds3). We use the `svm` function as before.

However, we now set `kernel='radial'` as we want a non-linear decision boundary:

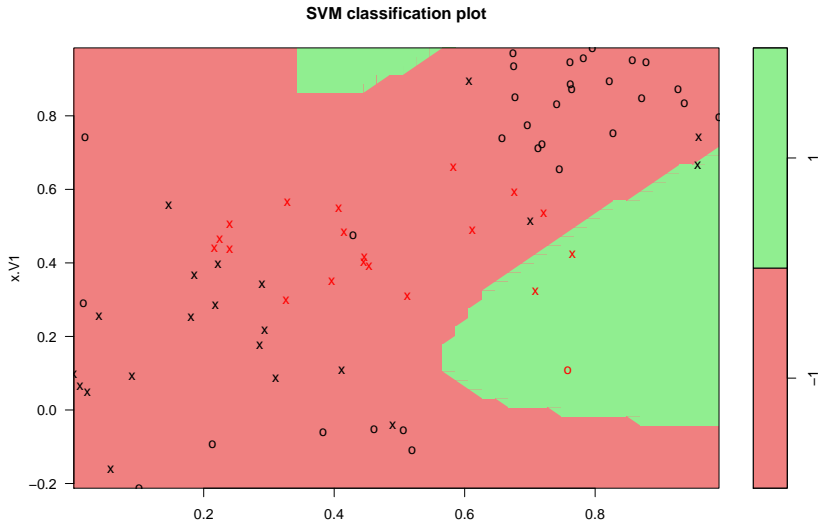
```
library(e1071)
forest3 = read.table(file = "forest3.txt")
seeds3 = read.table(file = "seeds3.txt")
train3 = data.frame(x = forest3[, 1:2], y = as.factor(forest3[, 3]))
test3 = data.frame(x = seeds3[, 1:2], y = as.factor(seeds3[, 3]))
```

```
svmfit_kernel1 = svm(y ~ ., data = train3, kernel = "radial", gamma = 0.01,  
  cost = 10, scale = FALSE)  
plot(svmfit_kernel1, train3, col = c("lightcoral", "lightgreen"))
```



We could also try with a polynomial kernel with degree 4 as follows:

```
svmfit_kernel2 = svm(y ~ ., data = train3, kernel = "polynomial",  
  degree = 4, cost = 1e+05, scale = FALSE)  
plot(svmfit_kernel2, train3, col = c("lightcoral", "lightgreen"))
```



```
summary(svmfit_kernel2)
```

```
##
```

```
## Call:
```

```
## svm(formula = y ~ ., data = train3, kernel = "polynomial", de
```

```
##      cost = 1e+05, scale = FALSE)
```

```
##
```

```
##
```

```
## Parameters:
```

```
##      SVM-Type:  C-classification
```

```
##      SVM-Kernel: polynomial
```

```
##          cost:  1e+05
```

```
##          degree: 4
```

```
##          coef.0: 0
```

```
##
```

```
## Number of Support Vectors: 40
```

```
##
```

```
##      ( 21 19 )
```

```
##
```

```
##
```

```
## Number of Classes: 2
```


For this dataset a radial kernel is a natural choice: A circular decision boundary seems like a good idea. Thus, we proceed with `kernel='radial'`, and use the `tune()` function to find the optimal tuning parameter C :

```
set.seed(1)
CV_kernel = tune(svm, y ~ ., data = train3, kernel = "radial", gamma = 1,
  ranges = list(cost = c(0.001, 0.01, 0.1, 1, 5, 10, 100)))
summary(CV_kernel)
```

```
##
## Parameter tuning of 'svm':
##
## - sampling method: 10-fold cross validation
##
## - best parameters:
##   cost
##   100
##
## - best performance: 0.1089286
##
## - Detailed performance results:
##   cost      error dispersion
## 1 1e-03 0.2732143 0.1472658
## 2 1e-02 0.2732143 0.1472658
## 3 1e-01 0.2732143 0.1472658
```

The optimal C is 10. Next, we predict the class label of the seeds in the test set with a model with $C=10$, make a confusion table and plot the results:

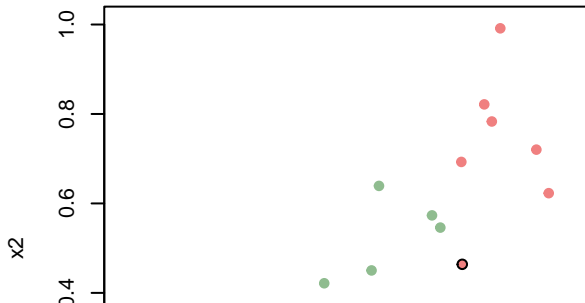
```
bestmod_kernel = CV_kernel$best.model  
ypred_kernel = predict(bestmod_kernel, test3)
```

```

par(mfrow = c(1, 3))
par(pty = "s")
plot(NA, xlab = "x1", ylab = "x2", xlim = c(0, 1), ylim = c(0, 1),
title("True class")
points(seeds3[seeds3[, 3] == -1, 1:2], pch = 19, col = "lightcoral",
      cex = 0.9)
points(seeds3[seeds3[, 3] == 1, 1:2], pch = 19, col = "darkseagreen",
      cex = 0.9)
points(seeds3[which(ypred_kernel != seeds3[, 3]), 1:2], pch = 21,

```

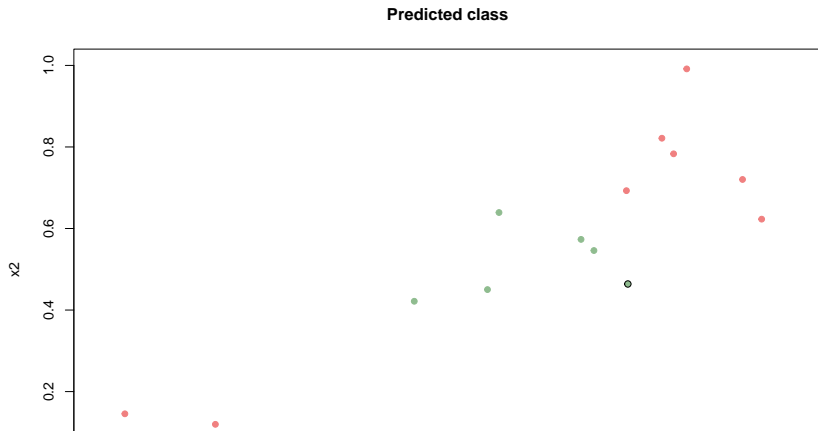
True class



```

plot(NA, xlab = "x1", ylab = "x2", xlim = c(0, 1), ylim = c(0, 1),
title("Predicted class"))
points(seeds3[ypred_kernel == -1, 1:2], pch = 19, col = "lightcoral",
       cex = 0.9)
points(seeds3[ypred_kernel == 1, 1:2], pch = 19, col = "darkseagreen",
       cex = 0.9)
points(seeds3[which(ypred_kernel != seeds3[, 3]), 1:2], pch = 21,

```



Extensions

More than two classes

What if we have k classes?

- OVA: one-versus-all. Fit k different two-class SVMs $f_k(\mathbf{x})$ where one class is compared to all other classes. Classify a test observation to the class where $f_k(\mathbf{x}^*)$ is largest.
- OVO: one-versus-one. `libsvm` uses this approach, in which $k(k-1)/2$ binary classifiers are trained; the appropriate class is found by a voting scheme (the class that wins the most pairwise competitions are chosen).

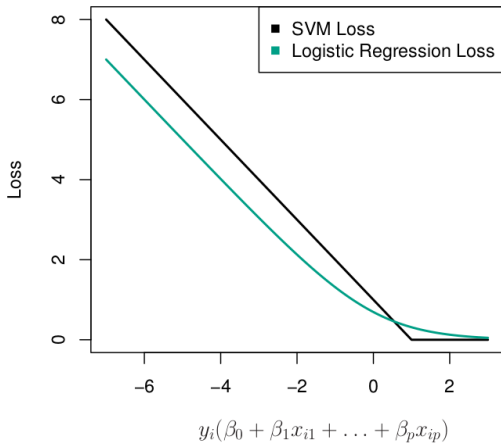
Comparisons

Focus is comparing the support vector classifier and logistic regression

It is possible to write the optimization problem for the support vector classifier as a “loss”+“penalty”:

$$\text{minimize}_{\beta} \left\{ \sum_{i=1}^n \max(0, 1 - y_i f(\mathbf{x}_i)) + \lambda \sum_{j=1}^p \beta_j^2 \right\}$$

- the loss is called *hinge loss* - observe the max and 0 to explain why only support vectors contribute
- the penalty is a ridge penalty
- large λ gives β s small and more violations=high bias, but low variance
- small λ gives β s large and less violations=low bias, but high variance



Hinge loss:

$$\max(0, 1 - y_i f(\mathbf{x}_i))$$

For comparison a logistic regression (with ridge penalty) would be (binomial deviance with -1,1 coding of y)

$$\log(1 + \exp(-y_i f(\mathbf{x}_i)))$$

It can be shown that in logistic regression all observations contribute weighted by $p_i(1 - p_i)$ (where p_i is probability for class 1), that fade smoothly with distance to the decision boundary

It is possible to extend the logistic regression to include non-linear terms, and ridge penalty.

When to use SVM?

- If classes are nearly separable SVM will perform better than logistic regression. (LDA will also perform better than logistic regression.)
- and if not, then a ridge penalty version of logistic regression are very similar to SVM, and logistic regression will also give you probabilities for each class.
- If class boundaries are non-linear then SVM is more popular, but kernel versions of logistic regression is possible, but more computationally expensive.

Summing up

- We use methods from computer science, not probability models - but looks for a separating hyperplane in (an extended) feature space in the classification setting.
- SVM is a widely successful and a “must have tool”
- Interpretation of SVM: all features are included and maybe not so easy to interpret (remember ridge-type penalty does not shrink to zero).
- The budget must be chosen wisely, and a bad choice can lead to overfitting.
- Not so easy to get class probabilities from SVM (what is done is actually to fit a logistic regression after fitting SVM).

References

- Videos on YouTube by the authors of ISL, Chapter 9, and corresponding slides
- Solutions to exercises in the book, chapter 9

Efron, Bradley, and Trevor Hastie. 2016. *Computer Age Statistical Inference - Algorithms, Evidence, and Data Science*. Cambridge University Press.

Friedman, Jerome, Trevor Hastie, and Robert Tibshirani. 2001. *The Elements of Statistical Learning*. Vol. 1. Springer series in statistics New York.

James, Gareth, Daniela Witten, Trevor Hastie, and Robert Tibshirani. 2013. *An Introduction to Statistical Learning*. Vol. 112. Springer.