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Our goal today

Understand Support Vector Machines on a deeper level!

Support vector machines

The statistical classification problem
Support Vector Classifier
The kernel trick

A short excursion to convex optimization

The kernel trick

Reproducing kernel Hilbert spaces

Kernel examples

MNIST - data: an example

Literature (incomplete, but growing):

- Ian Goodfellow, Yoshua Bengio und Aaron Courville (2016). Deep Learning. http://www.deeplearningbook.org. MIT Press
- D. Barber (2012). Bayesian Reasoning and Machine Learning.
 Cambridge University Press
- Richard S. Sutton und Andrew G. Barto (1998). Reinforcement Learning: An Introduction. MIT Press
- Gareth James u. a. (2014). An Introduction to Statistical Learning: With Applications in R. Springer Publishing Company, Incorporated. ISBN: 1461471370, 9781461471370
- T. Hastie, R. Tibshirani und J. Friedman (2009). **The Elements of Statistical Learning**. Springer Series in Statistics. Springer New York Inc. URL: https://statweb.stanford.edu/~tibs/ElemStatLearn/

Support vector machines

- The first example of a tool we visit but which is not typical for classical statistics is Support Vector Machines.
- For the introduction we mainly follow Hastie et. al. (2009) and Steinwart & Covel¹.

^{1|.} Steinwart und C. Scovel (2007). "Fast rates for support vector machines using Gaussian kernels". In: Ann. Statist, 35.2, S. 575–607.

- We start by formally introducing the **statistical classification problem**.
- We have a finite training set

$$T = ((x_1, y_1), \dots, (x_n, y_n)) \in (X \times Y)^n,$$

where $X \subset \mathbb{R}^d$ and $Y = \{-1, 1\}$.

- The standard **batch model** assumes that the samples $(x_i, y_i)_{1 \le i \le n}$ are i.i.d. according to an unknown probability measure P on $X \times Y$. Furthermore, a new sample (x, y) is drawn from P independently of T.
- A classifier \mathscr{C} assigns to every T a measurable function $f = f_T : X \to \mathbb{R}$.
- The prediction of \mathscr{C} for y is

with the convention sign(0) := 1.

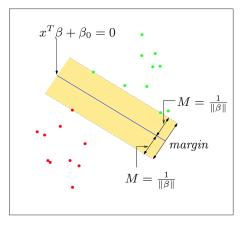
 \blacksquare We measure the quality of the classification f by the classification risk

$$\mathcal{R}(f) := P(\{(x, y) : \operatorname{sign} f(x) \neq y\}).$$

 Clearly, it is the goal to achieve the smallest possible risk, the so-called Bayes risk

$$\mathscr{R}_P := \inf \{ \mathscr{R}(f) | f : X \to \mathbb{R} \text{ measurable} \}.$$

- A function which attains this level is called a **Bayes decision function**.
- Let us start with an illustrative introduction to SVM (Pictures taken from Hastie et.al. (2009))



Consider the hyperplane described by $x^{\top}\beta + \beta_0 = 0$, with $\parallel \beta \parallel = 1$ and the classification \mathscr{G} :

$$\operatorname{sign}(x^{\top}\beta + \beta_0).$$

The maximal margin is obtained by the following optimization problem

$$\begin{aligned} & \max_{\beta,\beta_0:\|\beta\|=1} M \\ & \text{subject to } y_i(x_i^\top \beta + \beta_0) \geq M, \ i = 1,\dots,n \end{aligned}$$

- Such classifiers, computing a linear combination of the input and returning the sign were called **perceptrons** in the late 1950s (Rosenblatt, 1958) and set the foundations for later models of neural networks in the 80s and the 90s.
- We reformulate this criterion as follows: first, we get rid of $\parallel \beta \parallel = 1$ by considering

$$\frac{1}{\parallel \beta' \parallel} y_i(x_i^\top \beta' + \beta_0') \ge M$$

or, equivalently

$$y_i(x_i^{\top} \beta' + \beta_0') \ge M \| \beta' \|.$$

■ With β' , β'_0 satisfying these equations, any (positive) multiple will also satisfy these, we rescale to $\|\beta'\| = M^{-1}$ and arrive at

$$\min_{\beta,\beta_0} \frac{1}{2} \parallel \beta \parallel^2$$
subject to $y_i(x_i^\top \beta + \beta_0) > 1, i = 1, \dots, n.$

- This is a convex optimization problem and can be solved via the classical Karush-Kuhn-Tucker conditions.
- It should be noted that the solution does only depend on a small amount of the data, and hence has a certain kind of robustness. On the other side, it will possibly not be optimal under additional information on the underlying distribution.

Non-linearly separable data

- When the data does not separate fully we will allow some points to be on the wrong side.
- In this regard, define the **slack variables** $\xi_1, ..., \xi_n$ and consider

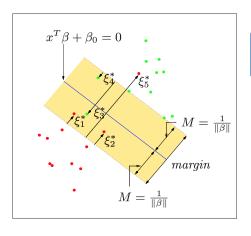
$$y_i(x_i^\top \beta + \beta_0) \ge M - \xi_i \tag{2}$$

or

$$y_i(x_i^{\top}\beta + \beta_0) \ge M(1 - \xi_i) \tag{3}$$

with $\xi_i \ge 0$, $\sum \xi_i \le K$ with a constant K.

■ The first conditions seems more natural, while the second choice measures the overlap in relative distance, which chances with the width of the margin, *M*. However, (2) leads to a non-convex optimization problem. The second problem is convex and is the "standard" support vector classifier.



The case for data which is not fully linearly separable. Misclassification occurs when $\xi_i > 1$.

Summarizing we arrive at the following minimization problem (again choosing $\parallel \beta \parallel = M^{-1}$) for the **support vector classifier**.

$$\min \parallel \beta \parallel \text{ subject to } \begin{cases} y_i(x_i^\top \beta + \beta_0) \geq (1 - \xi_i), \forall i \\ \xi_i \geq 0, \sum \xi_i \leq K. \end{cases}$$

■ For a detailed description we will revisit the Properties from Jungnickel (2014) in the following. Beforehand we illustrate the SVM with a small R example.

A toy example

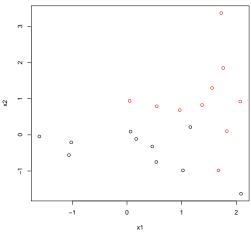
The classical statistical example is to consider two groups of normal distributions with different mean.

- Consider (X_i, Y_i) which are standard normal in group one and normal with mean (1,1) but same (identity) covariance matrix.
- The example is taken from Chapter 9 of James et al. (2013)

```
% N=20
% x=matrix(rnorm(N*2), ncol=2)  # data - x corresponds
% y=c(rep(-1,N/2), rep(1,N/2))  # data - y has the
% x[y==1,]=x[y==1,] + 1  # We shift the mean f
```

data - x corresponds to 2-dimensional data
 # data - y has the classifier
We shift the mean for the second class by (1,1)



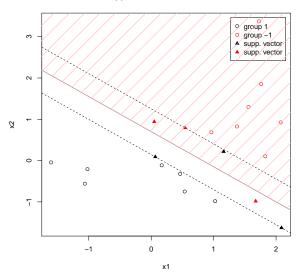


library(e1071)

plot(x, col=(3-y))

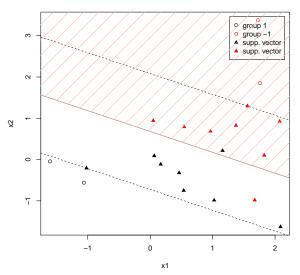
- This small code fits a linear SVM with cost factor 10 to the data.
- Its output is the number and identities of the support vectors (unfortunately not the classification rule)

Support Vector Classifier C=10



The summary plot: red / black decode the classes and the crosses are the support vectors. Note that we have four misclassifications.

Support Vector Classifier C=0.1



A smaller parameter C leads to more misclassfications. What could be an optimal choice ?

The library provides a connection to cross-validation for the choice of parameters.

```
tune.out=tune(svm,v ~.,data=dat,kernel="linear",ranges=list(
      cost=c(0.001, 0.01, 0.1, 1.5,10,100)))
summary(tune.out)
#Parameter tuning of 'svm':
#- sampling method: 10-fold cross validation
#- best parameters:
# cost
# 0.1
#- Detailed performance results:
    cost error dispersion
#1 1e-03 0.65 0.3374743
#2 1e-02 0.65 0.3374743
#3 1e-01 0.05 0.1581139
#4 1e+00 0.10 0.2108185
#5 5e+00 0.15 0.2415229
#6 1e+01 0.15 0.2415229
#7 1e+02 0.15 0.2415229
```

The kernel trick

- It seems quite restrictive to consider only linear classification rules. We have already seen that in linear regression we were able to overcome this problem by a suitable transformation of the data. This can also be achieved here and is often called the kernel trick.
- We first give a rather informative introduction and thereafter discuss the mathematical properties.

A short excursion to convex optimization

We follow Jungnickel 2 . Consider the **linear optimization problem**, also called **linear programm**

$$2x_1 + 2x_2 \ge 5 \tag{2}$$

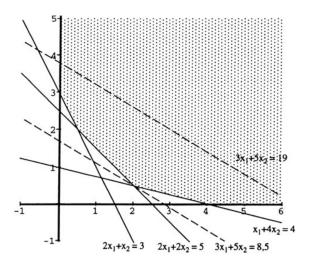
$$x_1 + 4x_2 \ge 4 \tag{3}$$

$$x_1 \ge 0 \tag{4}$$

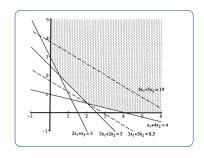
$$x_2 \ge 0 \tag{5}$$

We illustrate the setting in the following picture. Besides this, we plot the target function.

$$3x_1 + 5x_2 = 19$$
.



The optimal solution can be found by moving $3x_1 + 5x_2 = 19$ towards the origin (0,0).



- We realize that the optimal solution will be on one of the intersection points (this important observation leads to the Simplex algorithm)
- The optimal solution is $x^* = (2,0.5)$ representing $3x_1 + 5x_2 = 8.5$
- As we obtained this geometrically, are we able to prove that this solution is optimal?

$$\begin{array}{ccc} & \min & 3x_1 + 5x_2 \\ \text{subject to} & 2x_1 + x_2 \geq 3 & (1) \\ & 2x_1 + 2x_2 \geq 5 & (2) \\ & x_1 + 4x_2 \geq 4 & (3) \\ & x_1 \geq 0 & (4) \\ & x_2 \geq 0 & (5) \end{array}$$

- Observe, that such an equation might not always have a finite solution (eg. if one of the coefficients is negative)
- Any of the boundary conditions can be multiplied with positive constants. The boundary conditions can also be added. We could, for example look at 1.5·(2) and obtain

$$3x_1 + 3x_2 \ge 7.5$$

- As, moreover $x_2 \ge 0$, we obtain necessarily $3x_1 + 5x_2 \ge 7.5$
- Can we do better? Are we able to reach, e.g. 8.5??

The dual problem

■ Multiplying the inequalities with y_i , we arrive at the following scheme: let us find multipliers y_1 , y_2 , $y_3 \ge 0$, such that

$$2y_1 + 2y_2 + y_3 \le 3$$
$$y_1 + 2y_2 + 4y_2 \le 5$$
$$y_1, y_2, y_3 \ge 0.$$

■ The r.h.s. should be **maximized**, to be as close to x^* as possible, such that the objective function is

max
$$3y_1 + 5y_2 + 4y_3$$
.

■ This is the so-called dual problem. We can easily verify that $x^* = (2, 0.5)$ verifies the dual problem, hence is optimal.

Arguing similar, but more general we arrive at the following result.

Proposition (Weak duality)

Consider $c \in \mathbb{R}^n$, $b \in \mathbb{R}^m$ and $A \in \mathbb{R}^{m \times n}$ and the two problems

$$\min c^{\top} x$$
, subject to $Ax \ge b, x \ge 0$ (P)

$$\max y^{\top} b$$
, subject to $y^{\top} A \le c^{\top}, y \ge 0$. (D)

Then, for any x_0 satisfying the constraints in (P) and y_0 the ones in (D) it holds that

$$y_0^{\top} b \le c^{\top} x_0.$$

The proof is fairly easy:

$$y_0^{\top} b \le y_0^{\top} (Ax_0) = (y_0^{\rightarrow} A) x_0 \le c^{\top} x_0.$$

It can even be shown that in this case $y^{*\top} = c^{\top}x^*$, see Satz 2.9.17 in Jungnickel (2014).

Convex optimization

Actually we are interested in convex optimization problems. More precisely, we consider the following **minimization problem (MP)**

$$\begin{aligned} & & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

where $x \in X \subset \mathbb{R}^n$ and $g: X \to \mathbb{R}^m$, $h: X \to \mathbb{R}^p$. We denote by S the set where the constraints in (MP) are satisfied. Define the **Lagrange function**

$$\ell(x, \lambda, \mu) := f(x) + \lambda^{\top} h(x) + \mu^{\top} g(x).$$

Define the dual function $\theta(\lambda,\mu) := \inf\{\ell(x,\lambda,\mu) : x \in X\}$. Then the dual problem to (MP) is

$$\begin{array}{ll} \max & \theta(\lambda,\mu) & \text{(DP)} \\ \text{subject to} & \mu \geq 0. & \end{array}$$

Again, we have strong duality under additional assumptions, see Satz 6.5.10 in Jungnickel (2014).

Proposition (Strong duality)

Let X be a convex set and $f: X \to \mathbb{R}$, $g: X \to \mathbb{R}^p$ be convex functions and $h: X \to \mathbb{R}^m$ be an affine function.

If there exists $x_0 \in X$, s.t. $g(x_0) < 0$, $h(x_0) = 0$ and $0 \in \text{int } h(X)$, then

$$\sup\{\theta(\lambda,\mu): \mu \ge 0\} = \inf\{f(x): x \in S\}.$$

The following necessary conditions are found in Satz 2.9.9. in Jungnickel (2014).

It is also very useful to obtain necessary conditions, however in the simpler optimization problem where we only have inequality constraints. Set $I(x) = \{i : g_i(x) = 0\}$. We consider

$$\begin{array}{ll} & \min & f(x) \\ & \text{subject to} & g(x) \leq 0, \quad x \in X. \end{array} \tag{MPIC}$$

Proposition (Karush-Kuhn-Tucker conditions)

Let X be open and x an admissible point and g_i differentiable in x for all $i \in I(x)$ and continuous for $i \notin I(x)$. Moreover, let

$$\nabla g_i(x), i \in I(x)$$
 be linearly independent. (LICQ)

If *x* is a local minimum, then there exist μ_i , $i \in I(x)$, s.t.

$$\nabla f(x) + \sum_{i \in I(X)} \mu_i \nabla g_i(x) = 0.$$

If g_i are differentiable for all i, we obtain

$$\begin{split} \nabla f(x) + \sum_i \mu_i \nabla g_i(x) &= 0, \\ \mu_i \geq 0, \text{ and } \mu_i g_i(x) &= 0, \quad i = 1, \dots, p. \end{split}$$

Back to the kernel trick

We are interested in the following convex problem:

$$\begin{aligned} \min_{\beta,\beta_0,\xi} & & \frac{1}{2} \parallel \beta \parallel^2 + C \sum_{i=1}^N \xi_i \\ \text{subject to} & & y_i(x_i^\top \beta + \beta_0) \geq (1 - \xi_i), \forall i \\ & & \xi_i \geq 0. \end{aligned} \tag{MP}$$

The Lagrange function is

$$\frac{1}{2} \| \beta \|^2 + C \sum_{i=1}^{N} \xi_i - \sum_{i=1}^{N} \alpha_i (y_i (x_i^{\top} \beta + \beta_0) - (1 - \xi_i)) - \sum_{i=1}^{N} \mu_i \xi_i$$

with positivity constraints $\alpha, \mu, \xi \geq 0$.

The Lagrange function is

$$\frac{1}{2} \parallel \beta \parallel^2 + C \sum_{i=1}^{N} \xi_i - \sum_{i=1}^{N} \alpha_i (y_i (x_i^{\top} \beta + \beta_0) - (1 - \xi_i)) - \sum_{i=1}^{N} \mu_i \xi_i.$$

We see that this function is differentiable in β , β_0 and ξ . Setting the respective derivatives to zero, we obtain

$$\beta = \sum_{i=1}^{N} \alpha_i y_i x_i, \quad 0 = \sum_{i=1}^{N} \alpha_i y_i, \quad \alpha_i = C - \mu_i.$$
 (4)

Inserting this into the Lagrangian we obtain the Wolfe dual objective function

$$\ell_D = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j x_i^{\top} x_j,$$

giving a lower bound of the objective function of (MP).

$$\nabla f(x) + \sum_i \mu_i \nabla g_i(x) = 0,$$

$$\mu_i \geq 0, \text{ and } \mu_i g_i(x) = 0, \quad i = 1, \dots, p,$$

$$x \text{ admissible}.$$

In addition, we obtain the conditions

$$\alpha_i \left(y_i (x_i^\top \beta + \beta_0) - (1 - \xi_i) \right) = 0,$$

$$\mu_i \xi_i = 0,$$

$$y_i (x_i^\top \beta + \beta_0) - (1 - \xi_i) \ge 0.$$

■ We can also make a further observation: from (4), we see that the solution for β has the form

$$\beta^* = \sum_{i=1}^N \alpha_i^* y_i x_i,$$

with nonzero coefficients α_i^* for those observations i which lie on the margin (the **support vectors**).

$$\hat{G}(x) = \operatorname{sign}[x^{\top} \beta^* + \beta_0^*].$$

 An important observation is that the optimization problem now only depends on the scalar product

$$x_i^{\top} x_j$$

which opens the scenery for reproducing kernel Hilbert spaces.

Reproducing kernel Hilbert spaces

For details on this subject, consider C. Berg, J. P. R. Christensen und P. Ressel (1984). **Harmonic analysis on semigroups**. Springer-Verlag.

Definition

Let X be a nonemtpy set. A function $K: X \times X \to \mathbb{C}$ is called a **kernel**, if

$$\sum_{i,j=1}^{n} c_i \bar{c}_j K(x_i, x_j) \ge 0$$

for all $n \in \mathbb{N}$, $\{x_1, \ldots, x_n\} \subset X$ and $\{c_1, \ldots, c_n\} \subset \mathbb{C}$. If we replace \mathbb{C} by \mathbb{R} , we call the kernel real-valued.

Example

Let $\phi: X \to \mathbb{C}$ be arbitrary. The $K(x_1, x_2) := \phi(x_1)\phi(x_2)$ is positive definite:

$$\sum_{i,j=1}^{n} c_i \bar{c}_j K(x_i, x_j) = \big| \sum_{i=1}^{n} c_i f(x_i) \big|^2 \ge 0.$$

There are also negative definite kernels (which is not of interest here), and more precisely one calls the above kernel a positive definite kernel.

Now consider such a kernel K and the linear subspace $H_0\subset\mathbb{C}^X$ generated by the functions

$$\{K_x:x\in X\},$$

where $K_x(y) = K(x,y)$.

We introduce a (well-defined) scalar product for $f = \sum a_i K_{x_i}$, $g = \sum b_j K_{x_j}$ by

$$\langle f,g\rangle := \sum_{i,j} a_i \bar{b}_j K(x_i,x_j).$$

Then, H_0 is a pre-Hilbert space and its completion H is a Hilbert space.

Most importantly, the scalar product has the reproducing property

$$\langle f, K_x \rangle = \sum_i a_i K(x_i, x) = f(x)$$

for all $f \in H_0$ and $x \in X$. This is why the space H is called **reproducing kernel Hilbert space**.

Mercer's theorem allows to obtain a different view on the kernel $\it K$. Associate the integral operator

$$T_K f := \int_X K(.,x) f(x) dv(x)$$

to the kernel K (in $L^2(X)$). The the spectracl decomposition of T_K yields

$$K(x_1, x_2) = \sum_{n} \lambda_n \phi_n(x_1) \bar{\phi}_n(x_2).$$
 (5)

The RKHS is given by

$$H = \{ f \in L_2(X) : \sum_n \lambda_n^{-1} \langle f, \phi_n \rangle^2 < \infty \}.$$

This yields in turn the representation

$$f(x) = \sum_{n} a_n \phi_n(x).$$

On the other side, any kernel satisfying (5) is non-negative definite and thus leads to a RKHS.

Summarizing, we obtain the following:

A RKHS allows a representation

$$f(x) = \sum_{n} a_n \phi_n(x)$$

with an associated kernel K satisfying

$$K(x_1,x_2) = \sum_n \lambda_n \phi_n(x_1) \bar{\phi}_n(x_2).$$

■ One can think of transforming x to $\phi_n(x)$ such that

$$\{(\phi_n(x))_{n=1}^\infty: x \in X\}$$

is called the feature space. This can in principle be an infinite dimensional space.

Kernel examples

From T. Evgeniou, M. Pontil und T. Poggio (2000). "Regularization networks and support vector machines". In: **Advances in computational mathematics** 13.1, S. 1–50 we cite the following list of kernels:

Table 1

Some possible kernel functions. The first four are radial kernels. The multiquadric and thin plate splines are positive semidefinite and thus require an extension of the simple RKHS theory of this paper. The last three kernels were proposed by Vapnik [96], originally for SVM. The last two kernels are one-dimensional: multidimensional kernels can be built by tensor products of one-dimensional ones. The functions B_n are piecewise polynomials of degree n_n whose exact definition can be found in [85].

degree 72, whose exact definition can be round in [65].	
Regularization Network	
Gaussian RBF	
Inverse multiquadric	
Multiquadric	
Thin plate splines	
(only for some values of θ)	
Multi-Layer Perceptron	
Polynomial of degree d	
B-splines	
Trigonometric polynomial of degree d	

- The choice of the kernel should be adapted to the question and influences the performance massively!
- Most important are probably: Gaussian (RBF), polynomial and splines. But there are many other choices, for example in speech recognition (where one uses string kernels...)

MNIST dataset with SVM

Lets look at an example: our aim is to classify handwritten digits with SVM.

- We will use (parts of) the MNIST dataset, available at http://yann.lecun.com/exdb/mnist/.
- This includes 60.000 images of handwritten digits (0-9) with classification. (→ wich learning?)
- Lets get an impression of the first one hundred pictures:



- # Taken from https://gist.github.com/brendano/39760
- # Copyright under the MIT licens:
- # I hereby license it as follows. This is the MIT license.
- # Copyright 2008, Brendan O'Connor
- # Permission is hereby granted, free of charge, to any person obtaining a copy of this softwar # and associated documentation files (the "Software"), to deal in the Software without restric
- # including without limitation the rights to use, copy, modify, merge, publish, distribute,
- # sublicense, and/or sell copies of the Software, and to permit persons to whom the Software i
- # furnished to do so, subject to the following conditions: The above copyright notice and this
- # Turnished to do so, subject to the following conditions: the above copyright notice and the
- # permission notice shall be included in all copies or substantial portions of the Software.

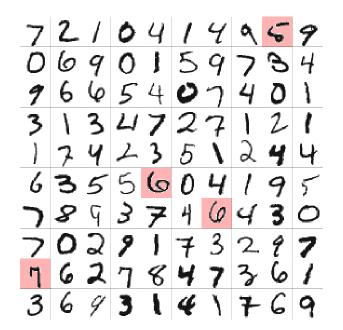
```
library(e1071)
load mnist <- function() {</pre>
  load image file <- function(filename) {</pre>
    ret = list()
    f = file(filename, 'rb')
    readBin(f,'integer',n=1,size=4,endian='big')
    ret$n = readBin(f,'integer',n=1,size=4,endian='big')
    nrow = readBin(f,'integer',n=1,size=4,endian='big')
    ncol = readBin(f,'integer',n=1,size=4,endian='big')
    x = readBin(f,'integer',n=ret$n*nrow*ncol,size=1,signed=F)
    ret$x = matrix(x, ncol=nrow*ncol, bvrow=T)
    close(f)
    ret
  load label file <- function(filename) {</pre>
    f = file(filename, 'rb')
    readBin(f,'integer',n=1,size=4,endian='big')
    n = readBin(f,'integer',n=1,size=4,endian='big')
    v = readBin(f,'integer',n=n,size=1,signed=F)
    close(f)
    У
  train <<- load image file('train-images-idx3-ubyte')
                                                             # Images
  test <<- load image file('t10k-images-idx3-ubyte')
  train$y <<- load label file('train-labels-idx1-ubyte')</pre>
                                                             # Labels
  test$v <<- load label file('t10k-labels-idx1-ubvte') }
show digit <- function(arr784, col=gray(12:1/12), ...) {
  image(matrix(arr784, nrow=28)[.28:1], col=col, ...)}
```

- This is the SVM-routine. Note that we chose linear and cost factor C = 10.
- Additionally, we only use 2000 samples for training (otherwise it takes quite long. 10.000 is feasiable...)

```
#prediction
testdat = data.frame(x=test$x[1:100,])
pred = predict(svmfit,testdat)
table(pred,test$y[1:100])
sprintf("Error rate: %f",1-sum(pred == test$y[1:100])/100)
# This gives the following result:
pred
    8 0 0 0 0 0 0
    0 0 0 0 14 0 0 0 0
   0 0 0 0 0 6 0 0 0
  6 0 0 0 0 0 0 8 0 0
  7 0 0 0 0 0 0 0 14 0 0
  8 0 0 0 0 0 0 0 0 2 0
    0 0 0 0 0 0 0 1 0 11
```

"Error rate: 0.040000"

Which is already remarkable. Which of the images are misclassified?



Regularization on RKHS

Classical regularization theory utilizes RKHS for the following minimization question:

$$\min_{f \in H} \frac{1}{n} \sum_{i=1}^{n} (y_i - f(x_i))^2 + \lambda \parallel f \parallel_H,$$