Classification by Support Vector Machines

Florian Markowetz
Max-Planck-Institute for Molecular Genetics
– Computational Molecular Biology –
Berlin

Workshop on Practical Microarray Data Analysis
Heidelberg, 2002 Sep 26

Overview

I Large Margin Classifiers

II The Kernel Trick

III R package: e1071

Learning from examples

Gene expression is a complex process we can not describe explicitely.
$\Longrightarrow$ try to learn patterns from examples.

Given: $\mathcal{X} = \{x_i, y_i\}_{i=1}^{n}$ training set patients you've already seen

consisting of

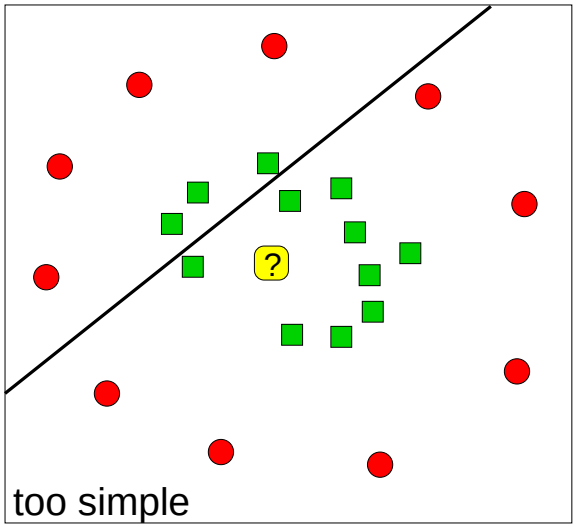
$x_i \in \mathbb{R}^g$	points	expression profiles
$y_i \in \{+1, -1\}$	labels	2 kinds of cancer

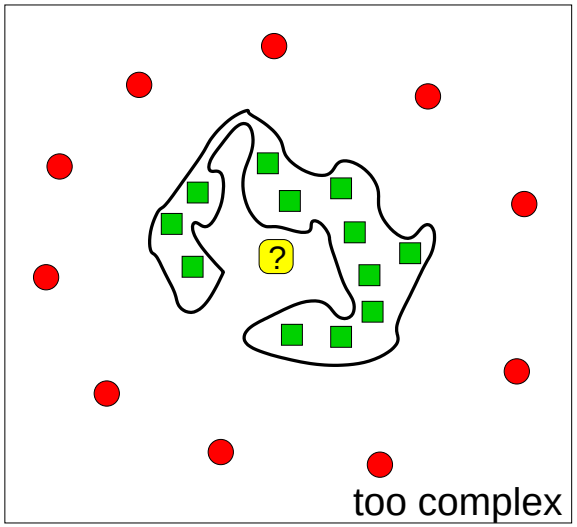
Goal: Learn a decision function that describes the data well.

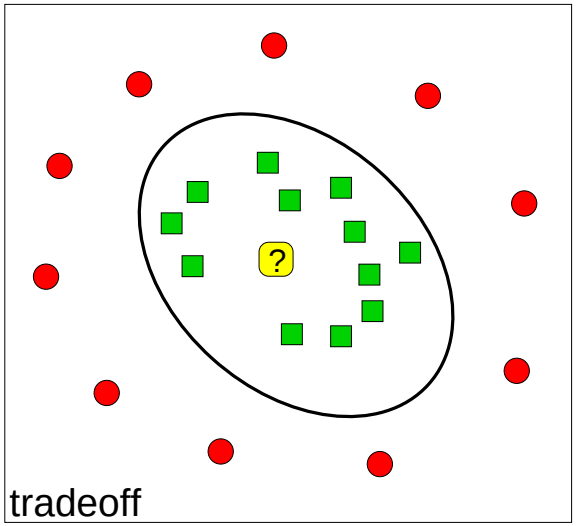
$$f_{\mathcal{X}}: \quad \mathbb{R}^g \mapsto \{+1, -1\}$$

$$\text{Diagnosis} = f_{\mathcal{X}}(new\ patient)$$

Problems of learning







negative example
positive example
? new patient

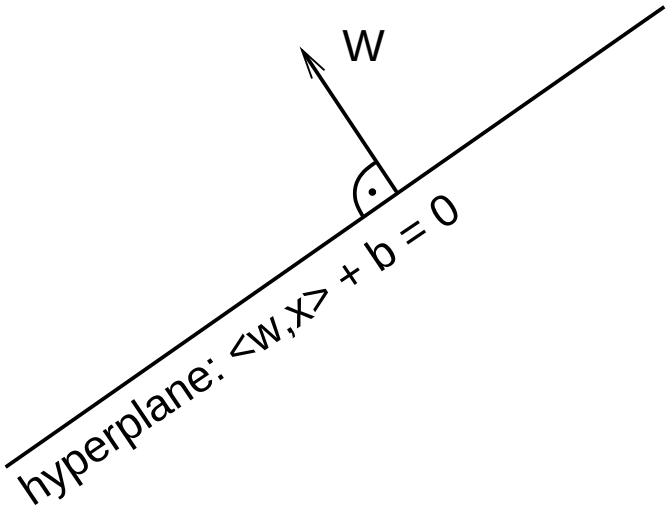
Linear separation

Most easy case: data set is linearly separable.

We need only a very simple classifier:

$$\mathcal{S} = \{\ x \mid \langle w, x \rangle + b = 0\}$$

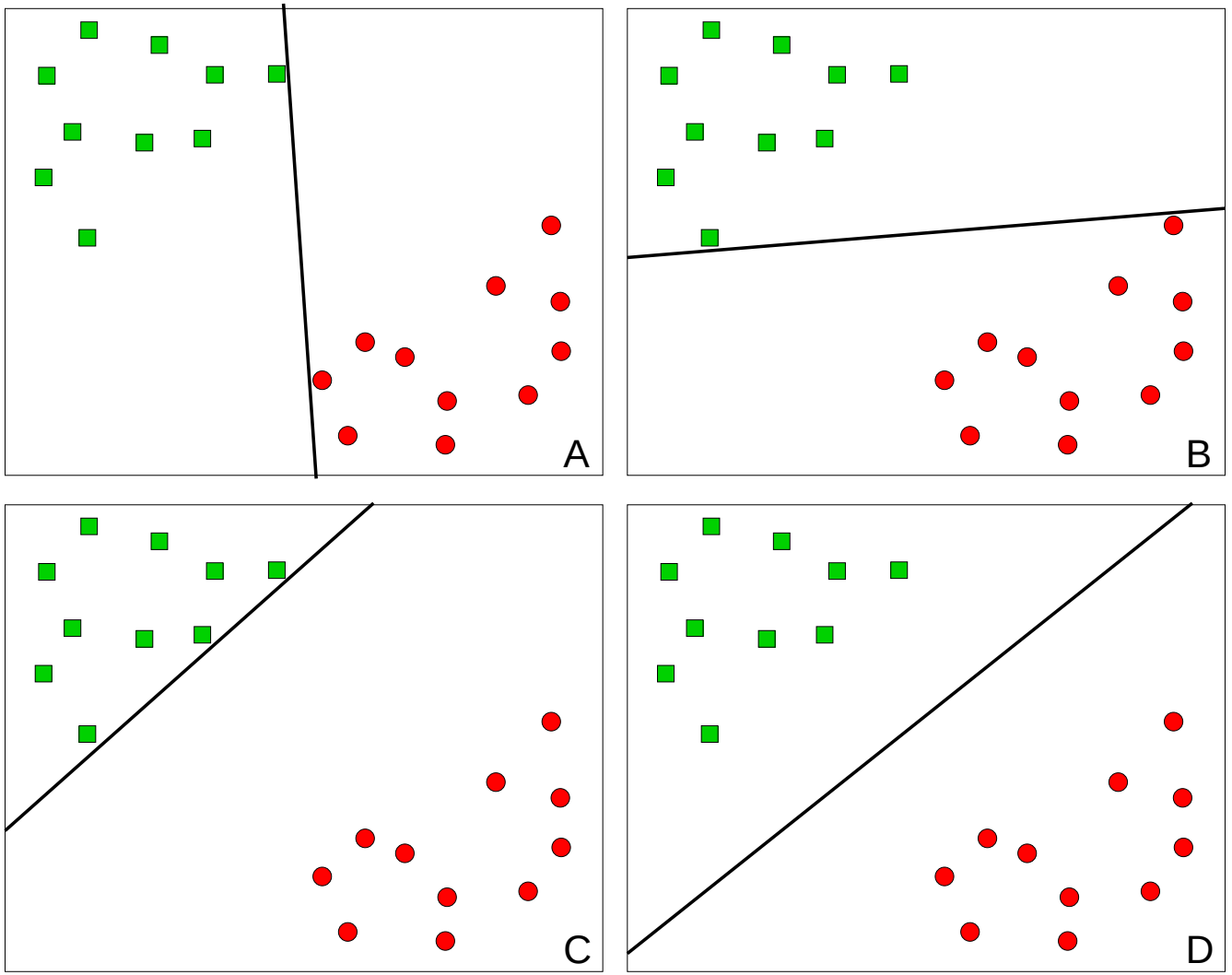
Choose w and b from the trainingset $\mathcal{X}$.



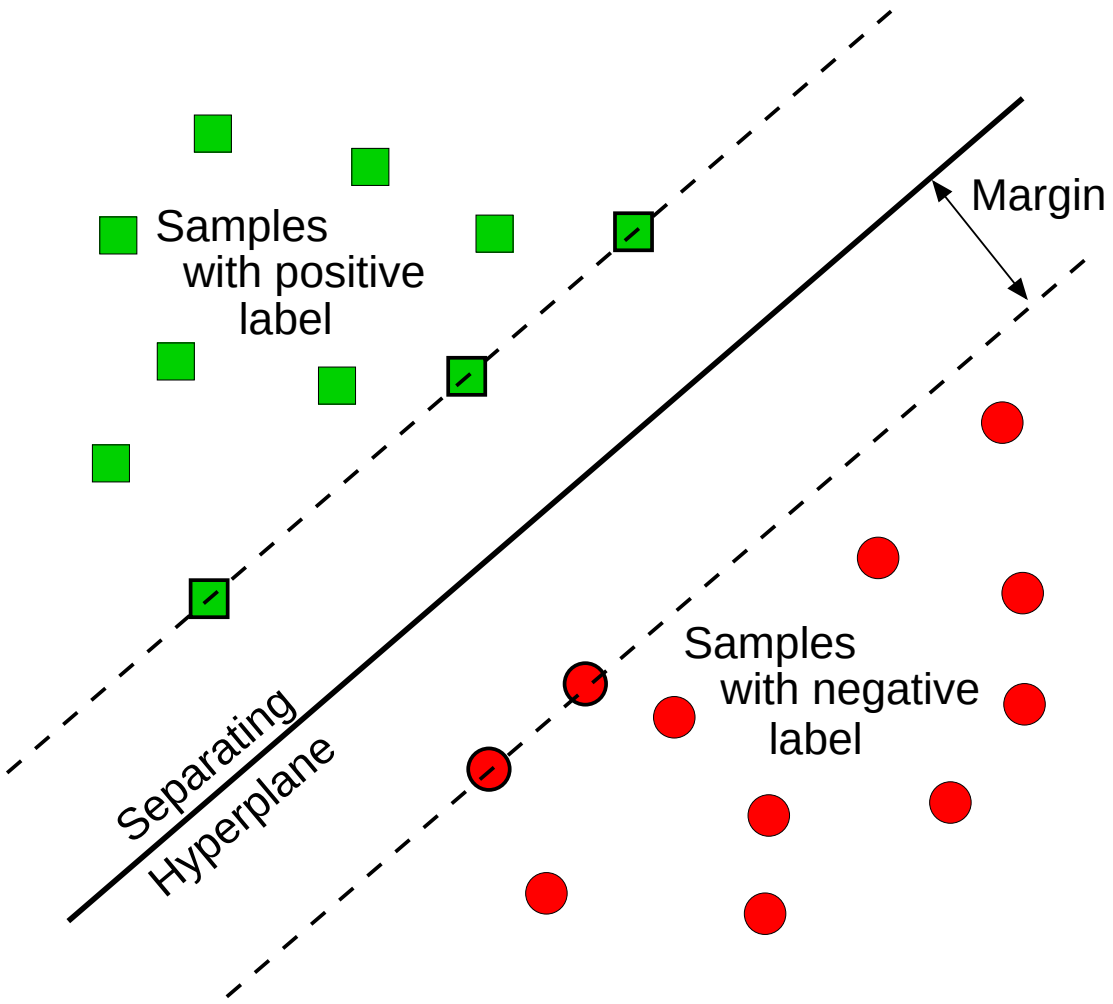
Prediction: On which side of the hyperplane does the new point lie?

Decision function: $f_{\mathcal{X}}(x_{\text{new}}) = sign\left(\langle w, x_{\text{new}} \rangle + b\right)$

Which hyperplane is the best?

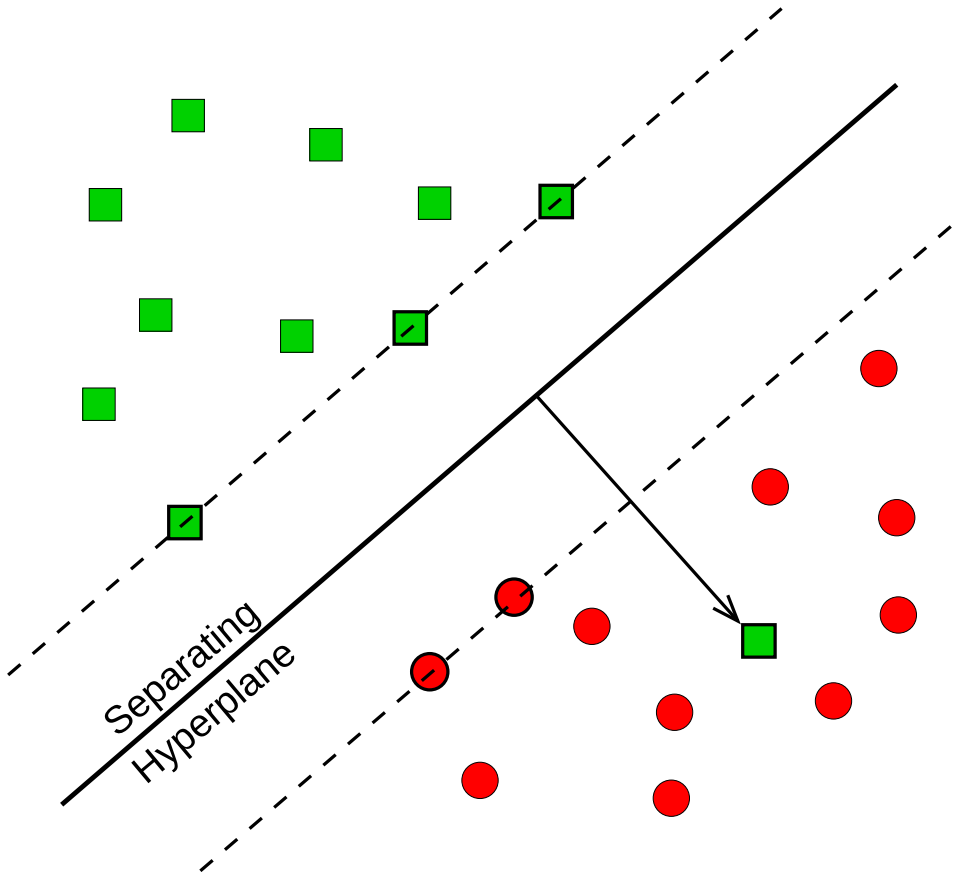


Separate the training set with maximal margin



Non-separable training sets

Use linear separation, but admit training errors.



Penalty of error: distance to hyperplane multiplied by *error cost* C.

Construction of the maximal margin hyperplane

Maximizing the margin is a problem of **constrained optimisation**, which can be solved by **Lagrange Method**.

Each training point x_i is described by a Lagrange multiplier α_i:

$\alpha_i = 0 \quad \Rightarrow \quad x_i$ has no influence on the hyperplane

$\alpha_i > 0 \quad \Rightarrow \quad x_i$ determines the sep. hyperplane
These points are called **Support Vectors**.
They lie nearest to the hyperplane.

Solution

Solution: $$w = \sum_{i=1}^{\#SV} \alpha_i y_i x_i^{sv}$$

Diagnosis: $$f(x_{\text{new}}) = sign\left(\sum_{i=1}^{\#SV} \alpha_i y_i \langle x_i^{sv}, x_{\text{new}} \rangle + b\right)$$

The decision function only depends on the Support Vectors.

They are the critical elements of the training set.

All other points could be removed without changing the solution.

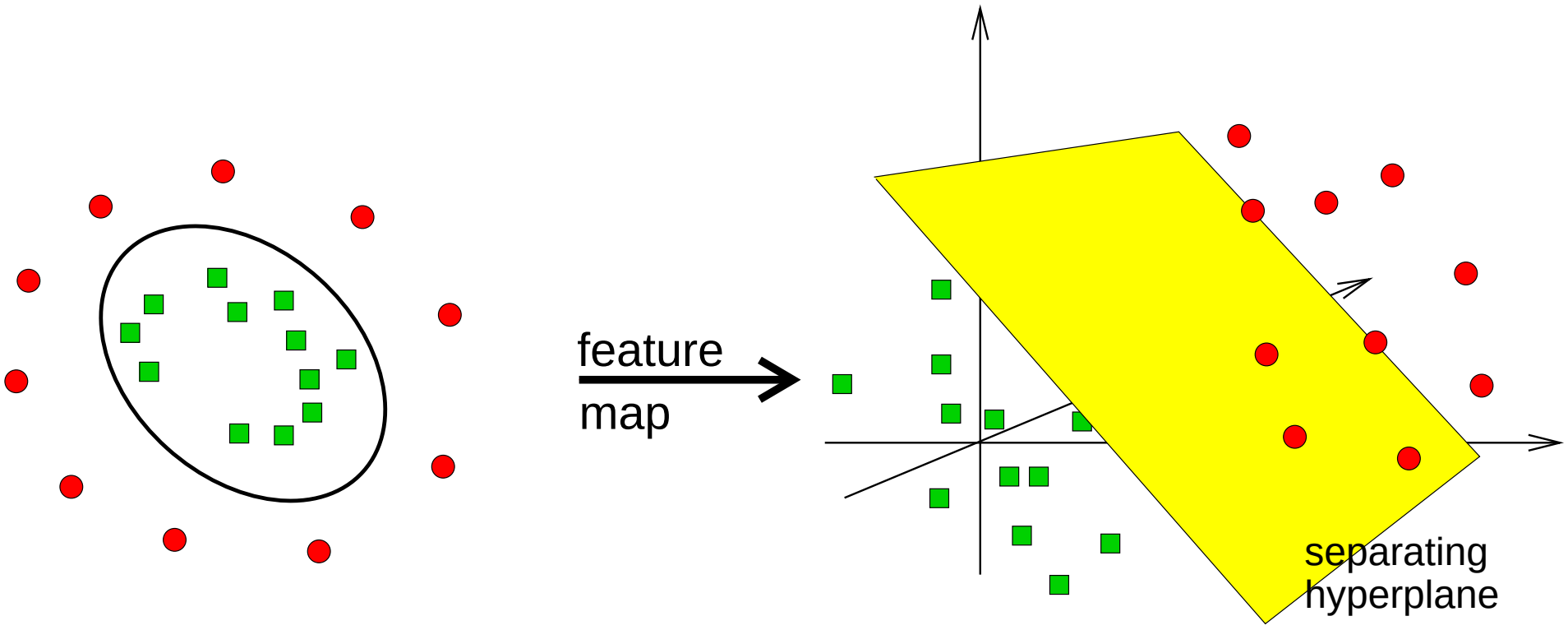
What's next?

I Large Margin Classifiers

II **The Kernel Trick**

III R package: e1071

Separation may be easier in higher dimensions



complex in low dimensions

simple in higher dimensions

The kernel trick

Classification is easier in high dimensions.

In the construction of the maximal margin hyperplane, we have to evaluate high dimensional inner products of the form

$$\langle \Phi(x_1), \Phi(x_2) \rangle_{\mathcal{H}}$$

where $\Phi : \mathcal{L} \to \mathcal{H}$ is the feature map from a low to a high dimensional space.

Problem: Computationally expensive!

Idea: do the feature map **implicitely**!

Kernel Mapping

Mercer Theorem:
Under some conditions on $\mathcal{K}$ there exists an inner product $\langle \cdot\,, \cdot \rangle_{\mathcal{H}}$ and a mapping $\Phi : \mathcal{L} \longrightarrow \mathcal{H}$ such that

$$\langle \Phi(x_1), \Phi(x_2) \rangle_{\mathcal{H}} = \mathcal{K}(x_1, x_2)$$

Using this kernel the decision function becomes

$$f(x_{\text{new}}) = sign\left(\sum_{i=1}^{\#SV} \alpha_i y_i \mathcal{K}(x_i, x_{\text{new}}) + b \right)$$

Examples of Kernels

linear $\mathcal{K}(x_1, x_2) = \langle x_1, x_2 \rangle$

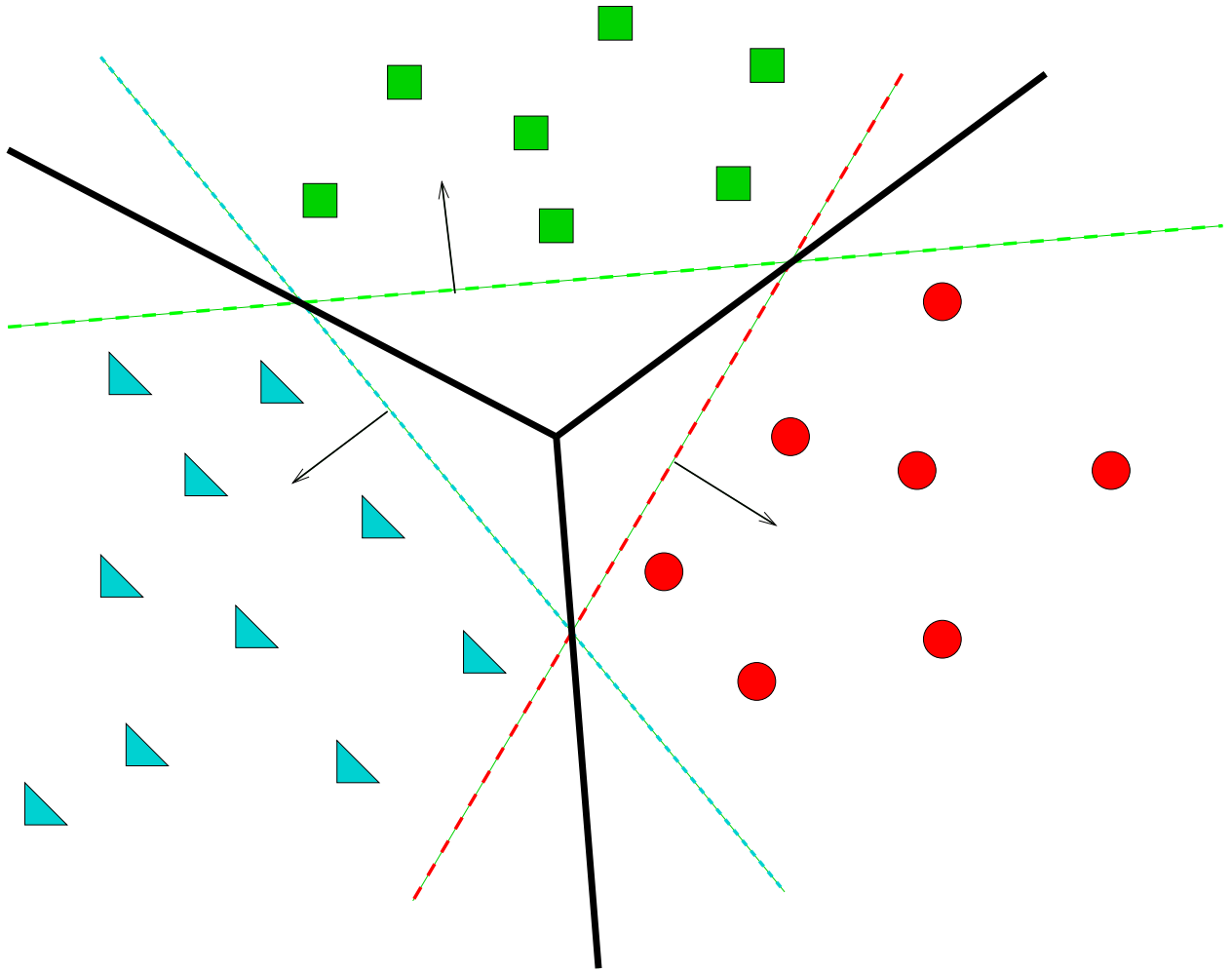
polynomial $\mathcal{K}(x_1, x_2) = (\gamma \langle x_1, x_2 \rangle + c_0)^d$

radial basis function $\mathcal{K}(x_1, x_2) = \exp\left(-\gamma \|x_1 - x_2\|^2\right)$

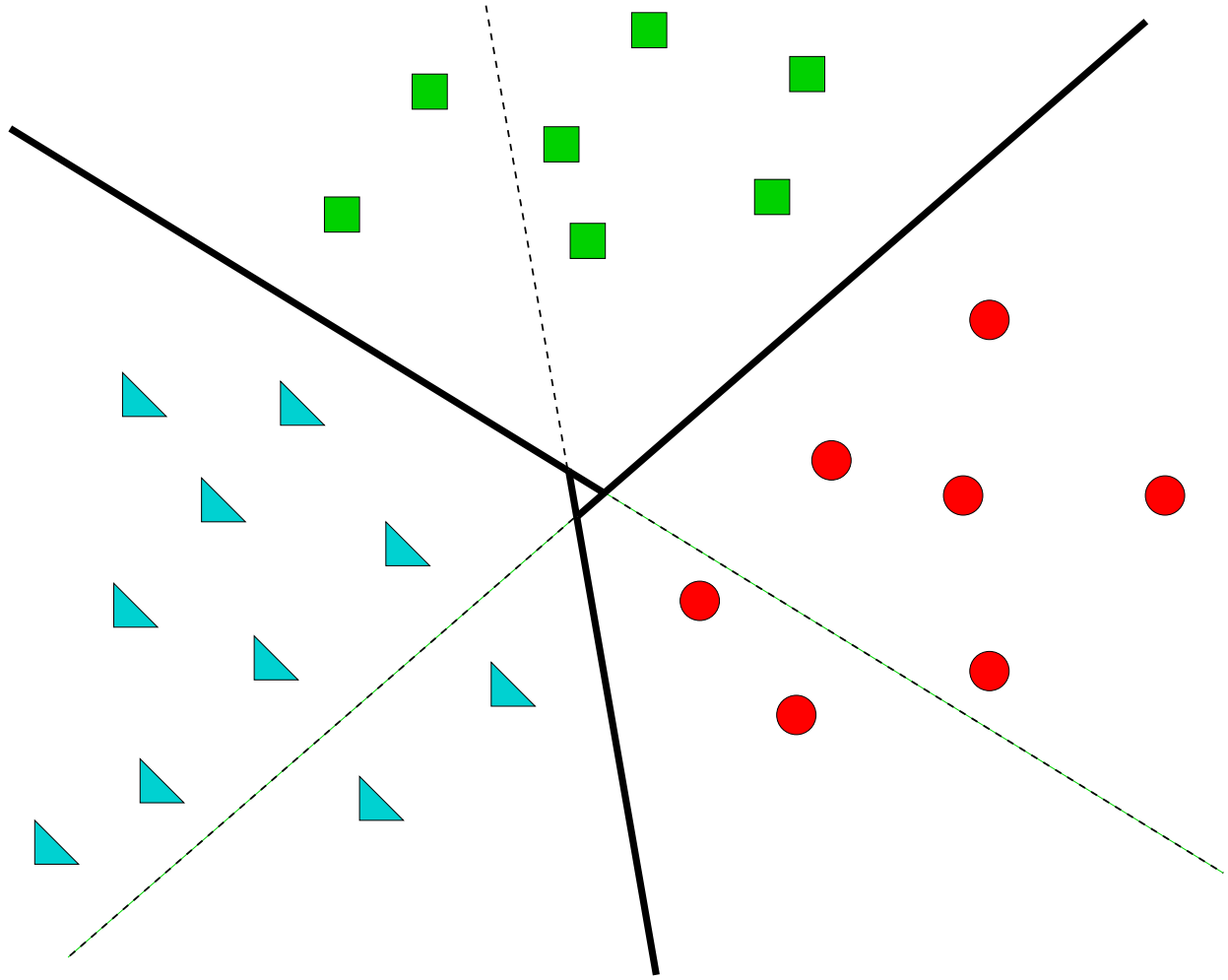
Parameters of SVM

Kernel Parameters	γ:	width of rbf coeff. in polynomial ($= 1$)
	d:	degree of polynomial
	c_0	additive constant in polynomial ($= 0$)
Error weight	C:	influence of training errors

More than 2 classes: *ONE-versus-ALL*



ONE-versus-ONE



Literature on SVM

- `http://www.kernel-machines.org`

- Vladimir Vapnik.
  Statistical Learning Theory. Wiley, NY, 1998.
  The comprehensive treatment of statistical learning theory, including a large amount of material on SVMs

  The Nature of Statistical Learning Theory. Springer, NY, 1995.
  An overview of statistical learning theory, containing no proofs, but most of the crucial theorems and milestones of learning theory. With a detailed chapter on SVMs for pattern recognition and regression

- Bernhard Schölkopf and Alex Smola.
  Learning with Kernels. MIT Press, Cambridge, MA, 2002.
  An introduction and overview over SVMs. A free sample of one third of the chapters (Introduction, Kernels, Loss Functions, Optimization, Learning Theory Part I, and Classification) is available on the book website.

What's next?

I Large Margin Classifiers

II The Kernel Trick

III **R package: e1071**

e1071

Misc Functions of the Department of Statistics (e1071), TU Wien

Functions for latent class analysis, short time Fourier transform, fuzzy clustering, support vector machines, shortest path computation, bagged clustering, ...

Source + Reference Manual:
The Comprehensive R Archive Network:

`http://cran.r-project.org/`

e1071: training

```
svm.model <- svm(x=data, y=labels, type="C-classification",
                 kernel="linear")

svm.model <- svm(x=data, y=labels, type="C-classification",
                 kernel="linear", cost="42")

svm.model <- svm(x=data, y=labels, type="C-classification",
                 kernel="polynomial", degree="2")

svm.model <- svm(x=data, y=labels, type="C-classification",
                 kernel="radial", gamma="0.002")
```

e1071: cross validation

```
> svm.model <- svm(data, labels, type="C-classification",
                   kernel="linear", cross=10)
> svm.model

Call:
 svm.default(x = data, y = labels, type = "C-classification",
             kernel = "linear", cross = 10)

Parameters:
   SVM-Type:  C-classification
 SVM-Kernel:  linear
       cost:  1
      gamma:  0.0001402721

Number of Support Vectors:  42 ( 22 20 )
```

e1071: cross validation *cont'd*

```
Number of Classes:  2

Levels: (as integer)
 1 -1

Rho:
 -0.2118043

10-fold cross-validation on training data:

Total Accuracy: 87.7551
Single Accuracies:
 75 80 100 80 100 100 80 80 100 80
```

e1071: testing

```
predicted <- predict(svm.model, data)  # test on training set

sum(predicted != labels)               # count differences

table(true=labels, pred=predicted)     # confusion matrix
```

```
      pred
      -1  1
true
  -1  24  0
   1   0 25
```

Thank you!