Kernel Based Methods

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In the second lecture we will:

- show that the standard QP SVM is only one optimisation approach: we can use formulations which lead to linear programming, nonlinear programming semi-definite programming (SDP) for example.

- show that there are further tasks beyond classification/regression which can be handled by kernel machines and we shall show that there are different types of learning which can be performed using kernel mechines.

- we shall comment on different learning algorithms and strategies for model selection (finding kernel parameters).
- we will consider different kernels including how to combine kernels into composite kernels (data fusion).

2.1 Different types of optimisation: linear programming and non-linear programming.

2.2 Other types of kernel problems beyond classification/regression: novelty detection and its applications

2.3 Different types of learning: passive and active learning.

2.4 Training SVMs and other kernel machines.

2.5 Model Selection.

2.6 Different types of kernels and learning with composite kernels.

2.1. A Linear Programming Approach to Classification

The idea of kernel substitution isn't just restricted to the SVM framework, of course, and a very large range of methods can be kernelised, including:

- can kernelise simple neural network learning algorithms such as the perceptron, minover and the adatron (so we can handle non-linearly separable datasets). You can try the *kernel adatron* this afternoon.
- kernel principal component analysis (kernel PCA) or independent component analysis (kernel ICA).
- can devise new types of kernelised learning machines (e.g. the Bayes Point Machine).

For example, rather than using quadratic programming it is also possible to derive a kernel classifier using *linear programming (LP)* instead:

$$\min \left[\sum_{i=1}^{m} \alpha_i + C \sum_{i=1}^{m} \xi_i \right]$$

subject to:

$$y_i \left[\sum_{j=1}^{m} \alpha_i K(x_i, x_j) + b \right] \geq 1 - \xi_i$$

where $\alpha_i \geq 0$ and $\xi_i \geq 0$.

This classifier is, in my experience, slightly slower to train than normal QP SVM but it is robust.

2.2. Novelty Detection (one-class classifiers).

Other tasks can be handled beyond classification/regression ...

E.g. for many real-world problems the task is not to classify but to detect novel or abnormal instances.

Examples: condition monitoring or medical diagnosis.

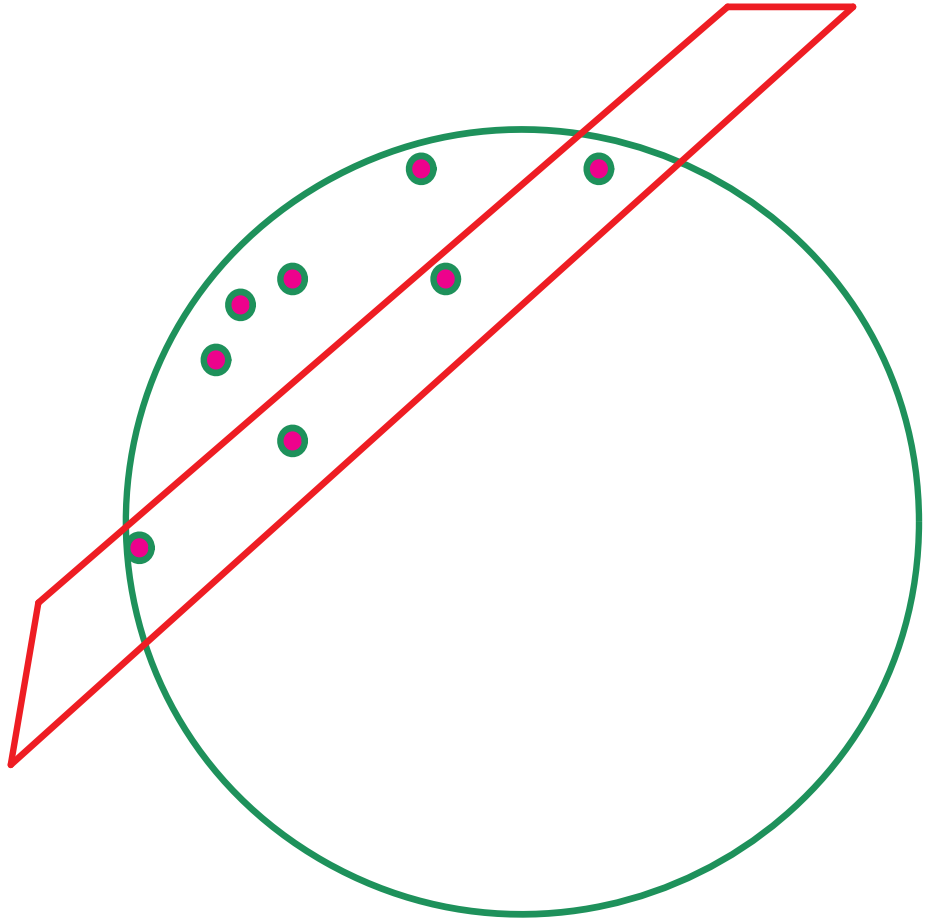
One approach: model the *support* of a data distribution.

Create a binary-valued function which is positive in those regions of input space where the normal data predominantly lies and negative elsewhere.

Various schemes possible: LP (here) or QP.

Objective: find a surface in input space which wraps around the data clusters: anything outside this surface is viewed as abnormal.

Feature space: corresponds to a hyperplane which is pulled onto the mapped datapoints.



This is achieved by minimising:

$$W(\alpha, b) = \sum_{i=1}^{m} \left(\sum_{j=1}^{m} \alpha_j K(\mathbf{x}_i, \mathbf{x}_j) + b \right)$$

subject to:

$$\sum_{j=1}^{m} \alpha_j K(\mathbf{x}_i, \mathbf{x}_j) + b \geq 0$$

$$\sum_{i=1}^{m} \alpha_i = 1, \quad \alpha_i \geq 0$$

Bias b is just treated as an additional unrestricted sign parameter.

Slack variables and a soft margin can also be introduced.

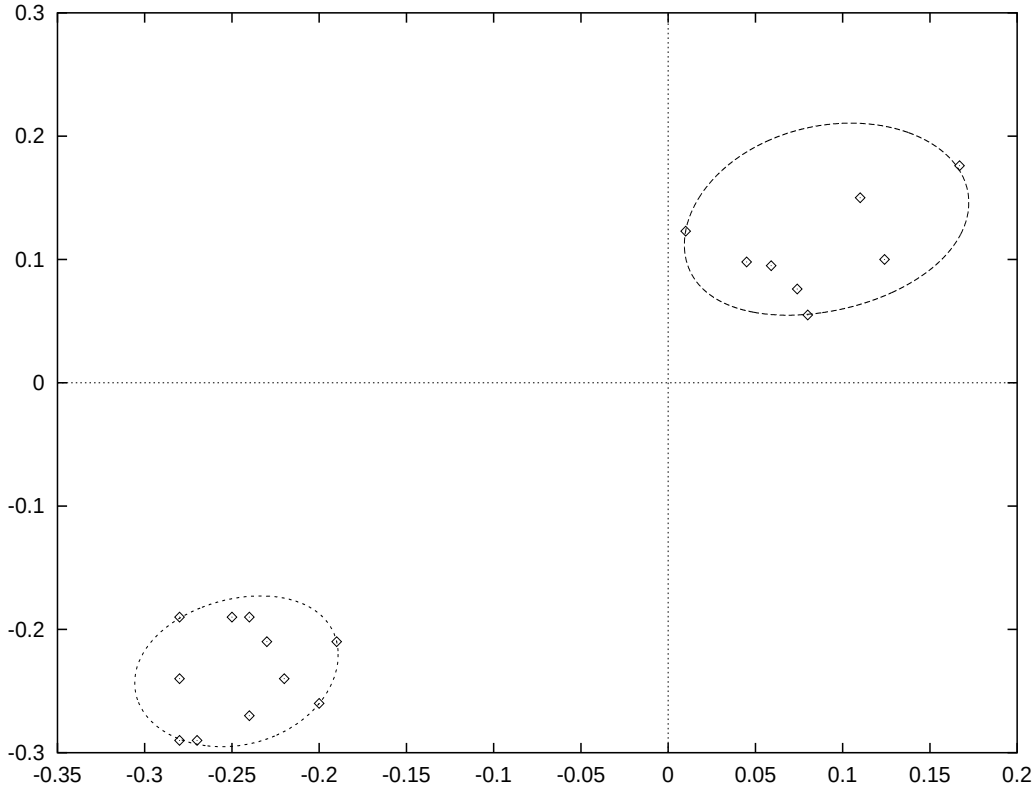


Figure 1: Hard margin and RBF kernel.

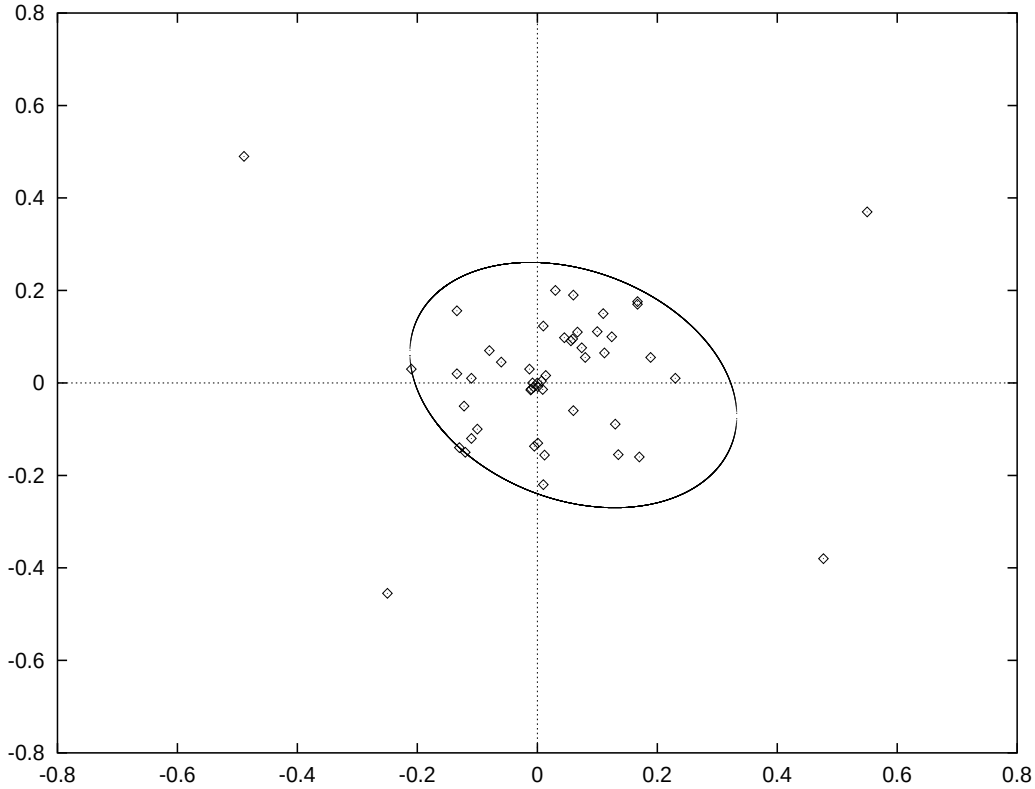


Figure 2: Using a soft margin (with $\lambda = 10.0$)

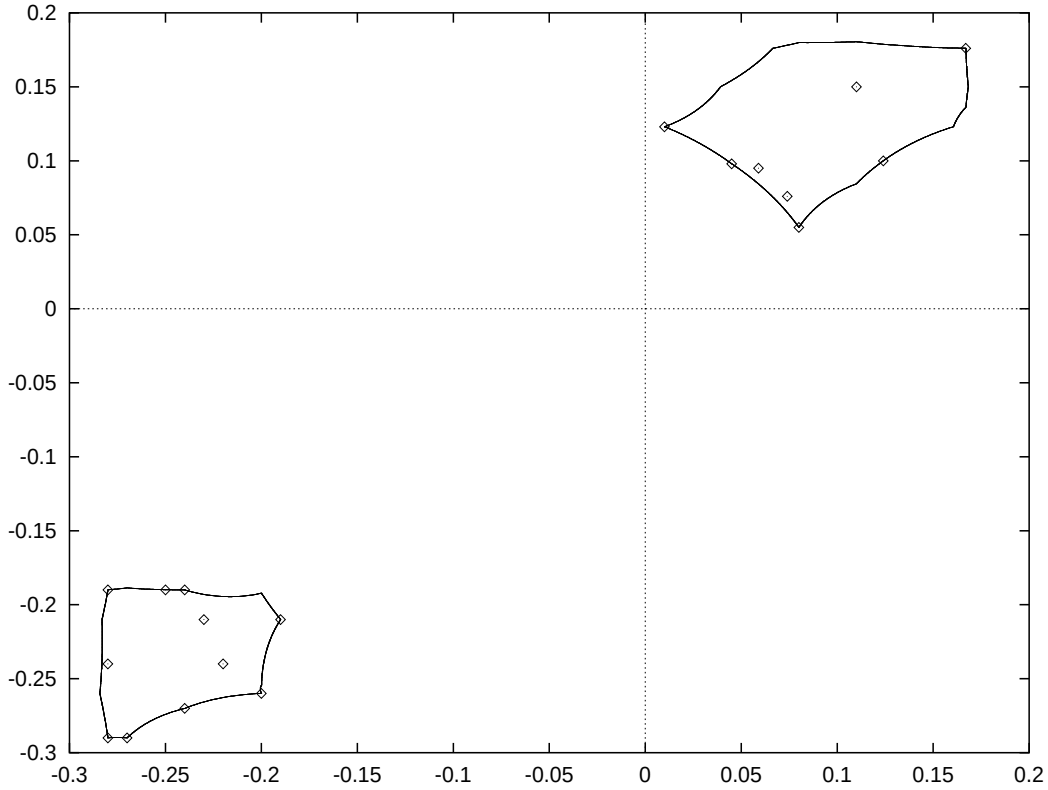


Figure 3: A modified RBF kernel

This basic model can be elaborated in various ways and the choice of kernel parameter (model selection) is important but it has worked well on real-life datasets e.g. detecting anomalies in blood samples.

2.3. Different types of learning: passive vs active learning.

Passive Learning: the learning machine receives examples, learns these and attempts to generalize to new instances.

Active Learning: the learning machine poses queries or questions to the oracle or source of information (the experimenatlist). With an efficient query learning strategy it can learn the problem efficiently.

Comments on active learning:

- Several strategies are possible:
- **Membership queries:** the algorithm selects unlabeled examples for the human expert to label (e.g. handwritten character).

- **Creating queries:** can create queries and ask for the label or answer. But sometimes the invented examples can be meaningless and impossible to label (e.g. I invent an unrecognisable handwritten character).

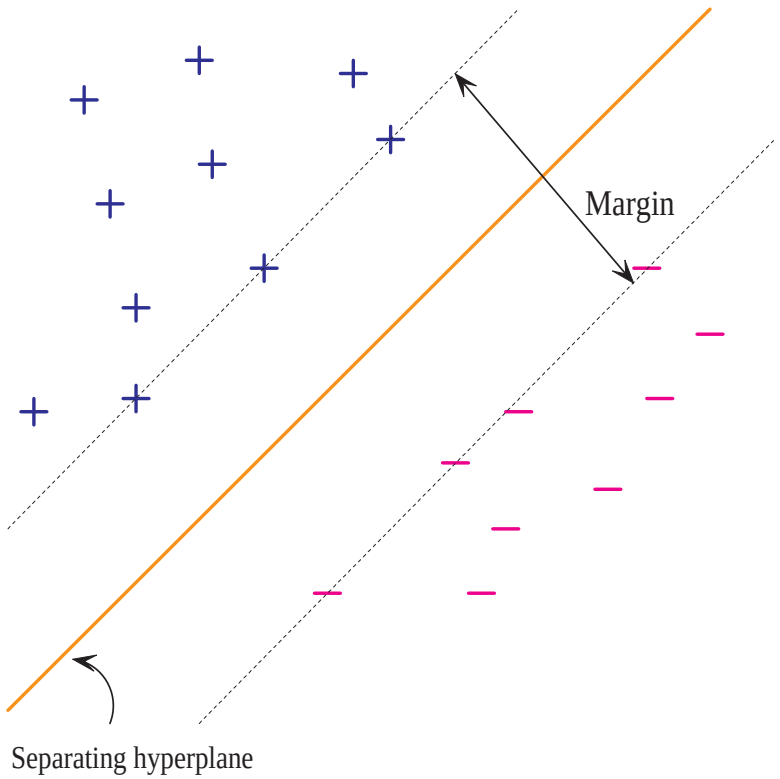
Worst case: possible to invent artificial examples for which number of queries equals sample size (hence no advantage to query learning)

but such adverse instances don't commonly occur in practice.

Average case analysis has been analysed using learning theory and we find:

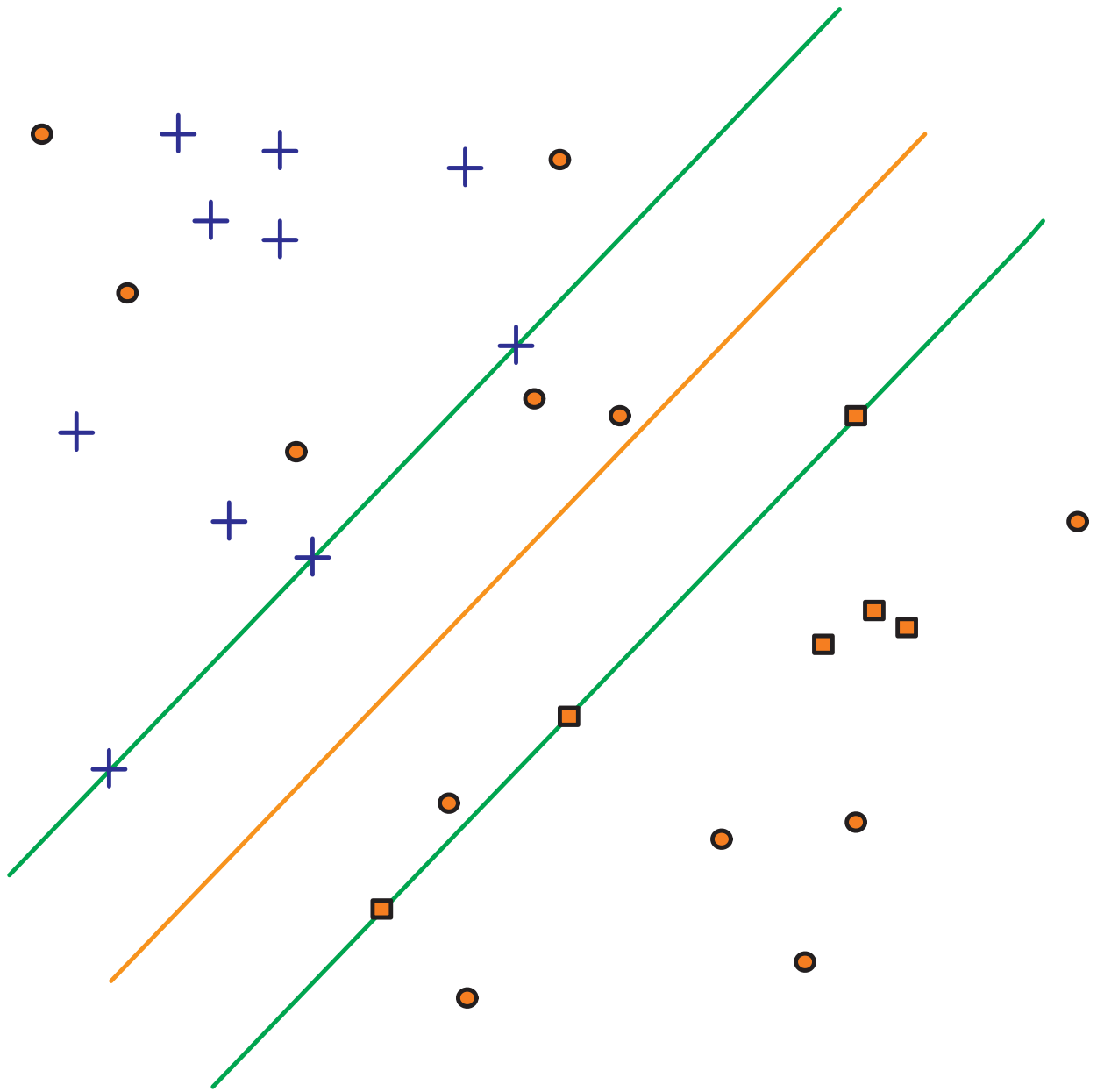
- Active learning is better than passive learning.
- For active learning the best choice for the next query is *a point lying within the current hyperplane* or as close as possible to the current hyperplane.

Support Vector Machines: construct hypothesis using the most informative patterns in the data (*the support vectors*) $\rightarrow$ good candidates for active learning.


Margin
Separating hyperplane

Suggests an algorithm:

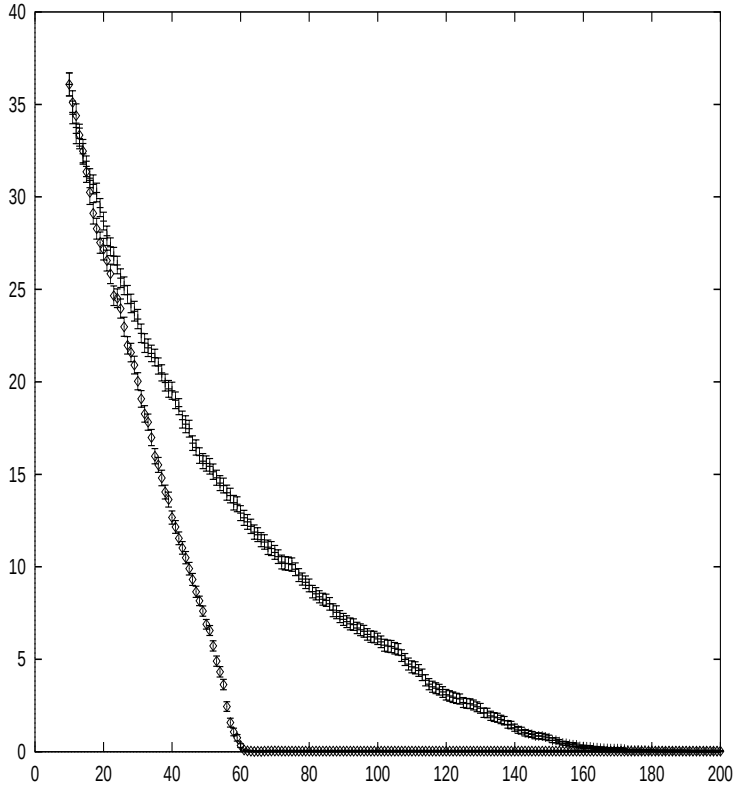
- Best points to query would be those points closest to the current hyperplane (maximally ambiguous).
- Querying a point within the margin band *always* guarantees a gain $\Delta W > 0$ whatever the label. Querying points outside the band only gives gain if current hypothesis predicts the label incorrectly.



Example: first let us consider a toy problem.

Simple rule (majority rule) in which we create binary valued strings with components 0 or 1, e.g. if $(0, 1, 1, 0, 0, 0, 1, 0, 1, 0, 0, 0, 1, 0, 0, 1, 1, 0, 1, 0, 1, 1)$.

More 0's than 1's then target is 0, more 1's than 0's then target 1.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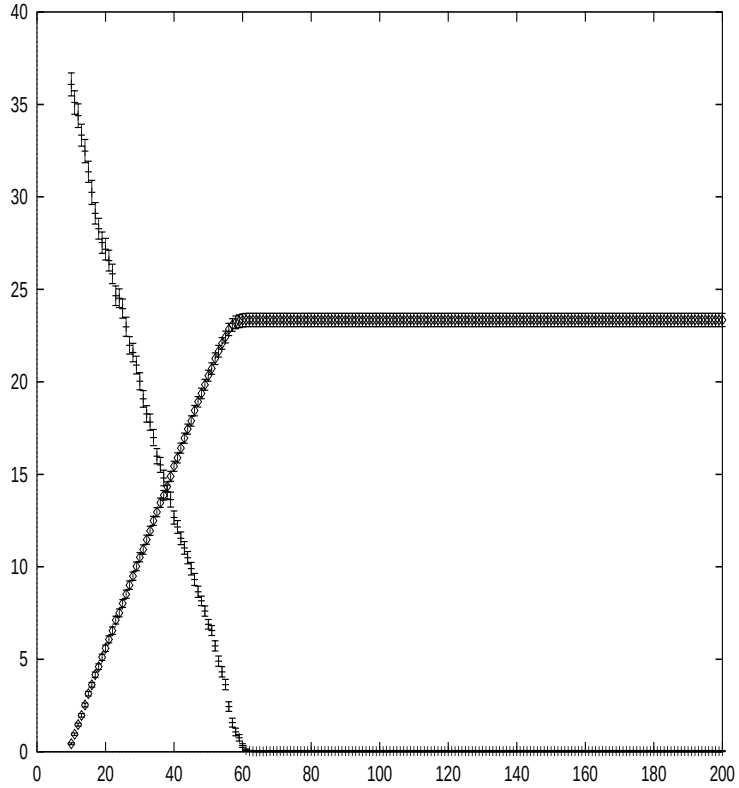
- How do we know when to stop asking queries?
- Several criteria are possible.
- One simple strategy (works for noiseless data) is to make a prediction and see if it agrees with what you find.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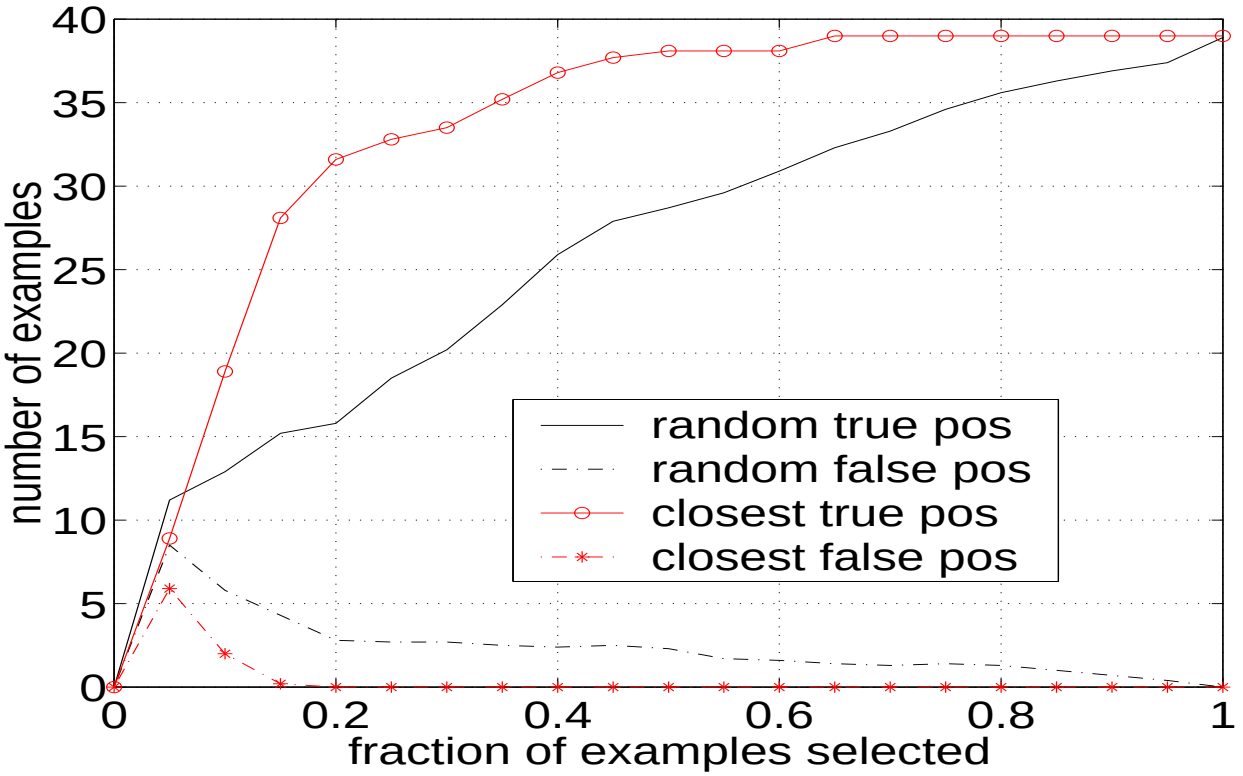
A real-life application: drug discovery

Each compound is described by a vector of 139,351 binary shape features and these vectors are typically sparse (on average 1378 features per *Round0* compound and 7613 per *Round1* compound)

Round0: dataset contained 1,316 chemically diverse examples, only 39 of which are positive.

Evaluation is performed by virtual combinatorial chemistry.


number of examples
fraction of examples selected
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random false pos
closest true pos
closest false pos
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2.4. Training SVMs and other kernel machines.

So far the methods we have considered have involved linear or quadratic programming.

Linear programming can be implemented using column generation techniques (simplex or interior point methods).

For quadratic programming e.g. conjugate gradient.

QP packages: MINOS and LOQO.

Problem: kernel matrix is stored in memory.

Alternatives split into three categories:

- kernel components are evaluated and discarded during learning,
- *working set* methods in which an evolving subset of data is used
- algorithms that explicitly exploit the structure of the problem.

2.4.1. Chunking and Decomposition: update the α_i but using only a subset or *chunk* of data at each stage.

QP routine optimizes the lagrangian on an initial arbitrary subset of data.

The support vectors found are retained and all other datapoints (with $\alpha_i = 0$) discarded.

New working set derived from these support vectors and additional datapoints maximally violating storage constraints.

This *chunking* process iterated until margin maximized.

Of course, this procedure may still fail.

If so *decomposition* methods provide a better approach: these algorithms only use a fixed size subset of data with the α_i for the remainder kept fixed.

Decomposition and Sequential Minimal optimization (SMO).

Limiting case of decomposition in which only two α_i are optimized at each iteration.

The smallest set of parameters which can be optimized with each iteration is plainly two if the constraint $\sum_{i=1}^{m} \alpha_i y_i = 0$ is to hold.

Possible to derive an analytical solution which can be executed using few numerical operations.

Can handle classification, regression and other tasks such as novelty detection.

2.4.2. Further algorithms.

Directly approach training from an optimization perspective and create new algorithms.

Keerthi et al have proposed a very effective binary classification algorithm based on the dual geometry of finding the two closest points in the convex hulls.

The Lagrangian SVM (LSVM) method of Mangasarian and Musicant reformulates the classification problem as an unconstrained optimization task and then solves problem using an algorithm requiring the solution of systems of linear equalities.

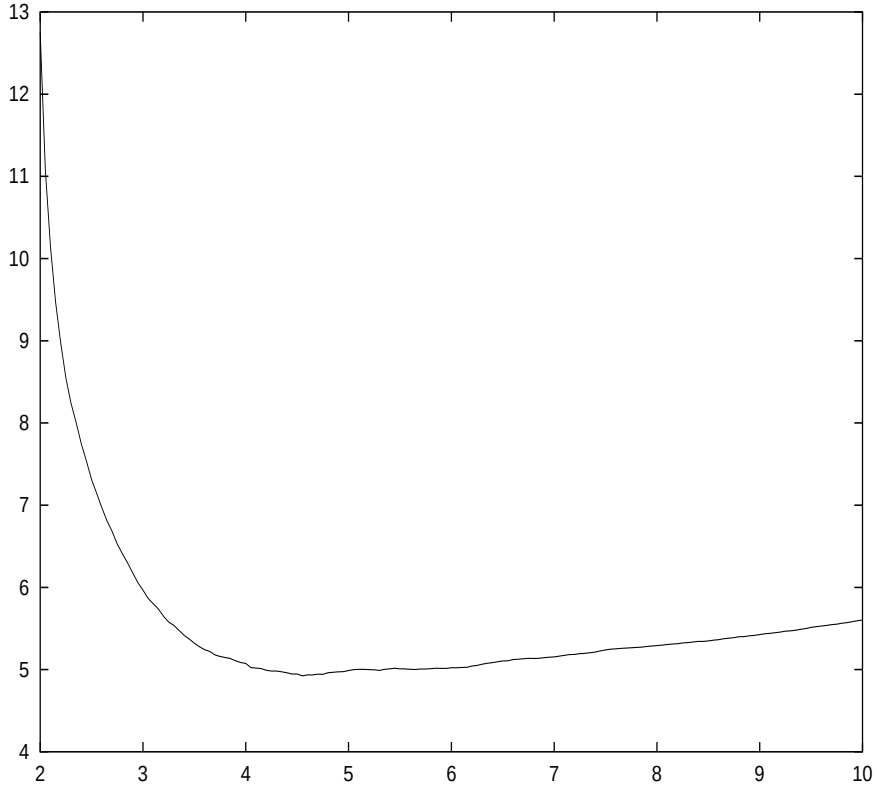
LSVM can solve linear classification problems for millions of points in minutes.

The interior-point and Semi-Smooth Support Vector Methods of Ferris and Munson can be used to solve linear classification problems with up to 60 million data points in 34 dimensions.

2.5. Model selection and Kernel Messaging

2.5.1. Model Selection. An important issue is the choice of kernel parameter (the σ in the Gaussian kernel, degree d of the polynomial kernel, etc).

If this parameter is poorly chosen the hypothesis modelling the data can be oversimple or too complex leading to poor generalisation.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The best value for this parameter can be found using cross-validation of course.

However, cross-validation is wasteful of data and it would be better to have a theoretical handle on the best choice for this parameter.

A number of schemes have been proposed to indicate a good choice for the kernel parameter without recourse to validation data.

We will only illustrate the idea with one of these.

Theorem: the number of leave-one-out errors of an L_1-norm soft margin SVM is bounded by:

$$\frac{|\{i : (2\alpha_i B^2 + \xi_i) \geq 1\}|}{m}$$

where α_i are the solutions of the SVM optimization task, B^2 an upper bound on $K(x_i, x_i)$ with $K(x_i, x_j) \geq 0$.

Thus, for a given value of the kernel parameter, the leave-one-out error is estimated from this quantity.

The kernel parameter is then incremented or decremented in the direction needed to lower the LOO bound.

2.5.2. Kernel Massaging and Semi-Definite Programming

Example: the existence of missing values is a common problem in many application domains.

We *complete* the kernel matrix (compensating for missing values) by solving the following semi-definite programming problem:

$$min_K \left| W \cdot (K - K^*) \right|^2$$

subject to:

$$AK = b \qquad A \geq 0$$

where K^* is the current kernel matrix, A the matrix of constraint coefficients, and b are slack variables to make inequalities up to equalities. W is a masking matrix of weights (0 or 1, with $W_{ii} > 0$)

2.6. Different types of kernels and learning with composite kernels

2.6.1. Different types of kernels

Keenels have been derived for a number of data objects and here we will only consider one: *string kernels*

Consider the following text strings **car**, **cat**, **cart**, **chart**. They have certain similarities despite being of unequal length. **dug** is of equal length to **car** and **cat** but differs in all letters.

A measure of the degree of alignment of two text strings or sequences can be found using algorithmic techniques e.g. edit codes (dynamic programming).

Frequent applications in

- bioinformatics e.g. Smith-Waterman, Waterman-Eggert algorithm (4-digit strings ... ACCGTATGTAAA ... from genomes),
- text processing (e.g. WWW), etc.

An appropriate kernel can be defined by a recurrence relation:

$$\begin{aligned} K(s,\epsilon) &= 1 \\ K(sa,t) &= K(s,t) + \sum_{k:t_k=a} K\left(s, t(1;k-1)\right) \end{aligned}$$

For a comparison of two strings with elements s, t, etc and ϵ the empty string.

Each element of the kernel quantifies the sequence similarity and the matrix as a whole is positive definite.

2.6.2. Data fusion using composite kernels

If we have kernels for different data objects we can combine then to create classifiers capable of handling disparate types of data using *composite kernels*:

$$K(\mathbf{x}_1, \mathbf{x}_2) = \sum_j \beta_j K_j(\mathbf{x}_1, \mathbf{x}_2)$$

First proposed Gunn and Kandola, 2002.

Example: Gert Lanckreit *et al*

Ref: JMLR **5** (2004) p. 27-72.

Task: predict functional classifications associated with yeast proteins (MIPS Yeast Genome Database).

Five different types of kernels used:

- amino acid sequences (inner product kernels, Smith-Waterman pairwise sequence comparison algorithm kernel),
- protein-protein interactions (graph kernel, diffusion kernel of Kondor-Lafferty),
- genetic interactions (graph kernel),
- protein complex data (weak interactions, graph kernel),
- expression data (Gaussian kernel)

Find that use of all 5 kernels better than using a single kernel.

Complex story but basically 13 functional classes: improvement 0.71 to 0.85 for fraction correctly classified on unseen hold-out data (0.71 is best comparator).

. . . but researchers are inclined to present appealing results in their papers . . .

If one type of data is dominant (e.g. microarray versus graph information and microarray much more plentiful) then learning algorithm can collapse onto one kernel ($K = \beta_1 K_1 + \beta_2 K_2$ and $\beta_2 \to 0$, say).

Despite this problem there are various successful applications (e.g. multimedia web page classification) and a number of proposed schemes:

- semi-definite programming (Lanckreit *et al*), leads to a quadratically constrained quadratic programme (QCQP).
- boosting schemes (Crammet *et al*, 2003, Bennett *et al*, 2002),
- a kernelised Fisher discriminant approach (Fung *et al* 2004),

- a kernel on kernels (*hyperkernels*, Ong *et al*, 2003),
- a Bayesian strategy to find the β_j coefficients for classification and regression (Mark Girolami and Simon Rogers, 2005, preprint, 2005), etc.

2.5. Applications of SVMs

Vast number number of applications: too many to summarise here ...

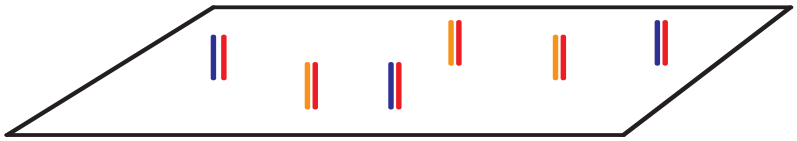
Just two applications to show how useful SVMs are ...

Example 1.

- Prediction of relapse/non relapse for Wilm's tumour using microarray technology.
- affects children/young adults
- with Richard Williams et al., ICR, London (*Genes, Chromosomes and Cancer*, 2004; 41: 65-79).

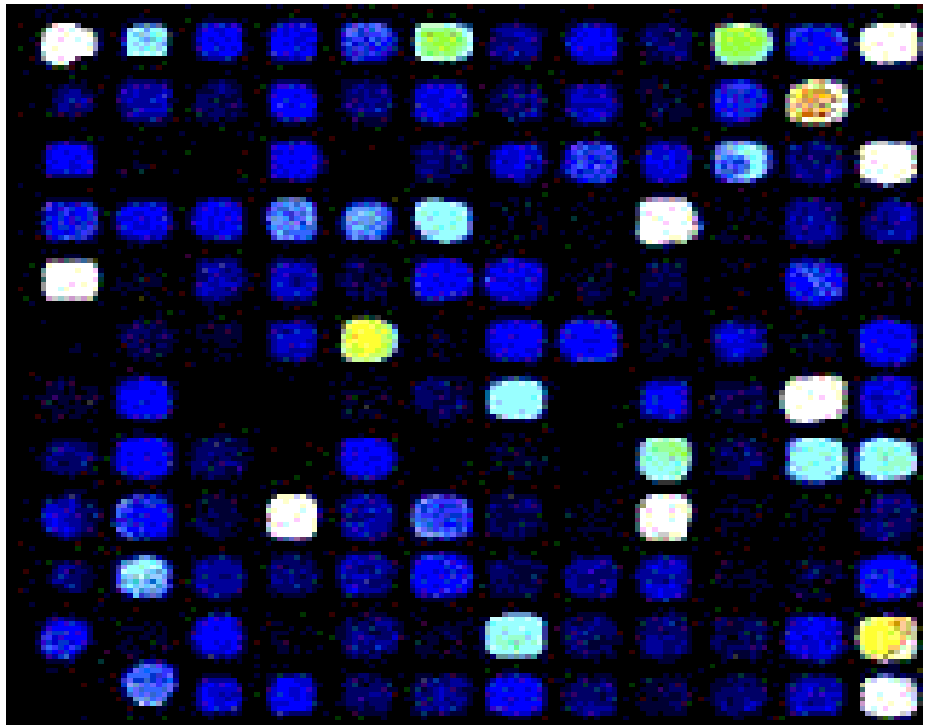
FRAGMENT AND LABEL ENDS WITH FLUORESCENT LABELS FOR EXAMPLE

FRAGMENTS HYBRIDIZE WITH DNA PROBES ON A SUBSTRATE



USE LASER EXCITATION TO FIND HOW MUCH mRNA DEPOSITED AT A PROBE SITE (INDICATES LEVEL OF EXPRESSION OF CORRESPONDING GENE)

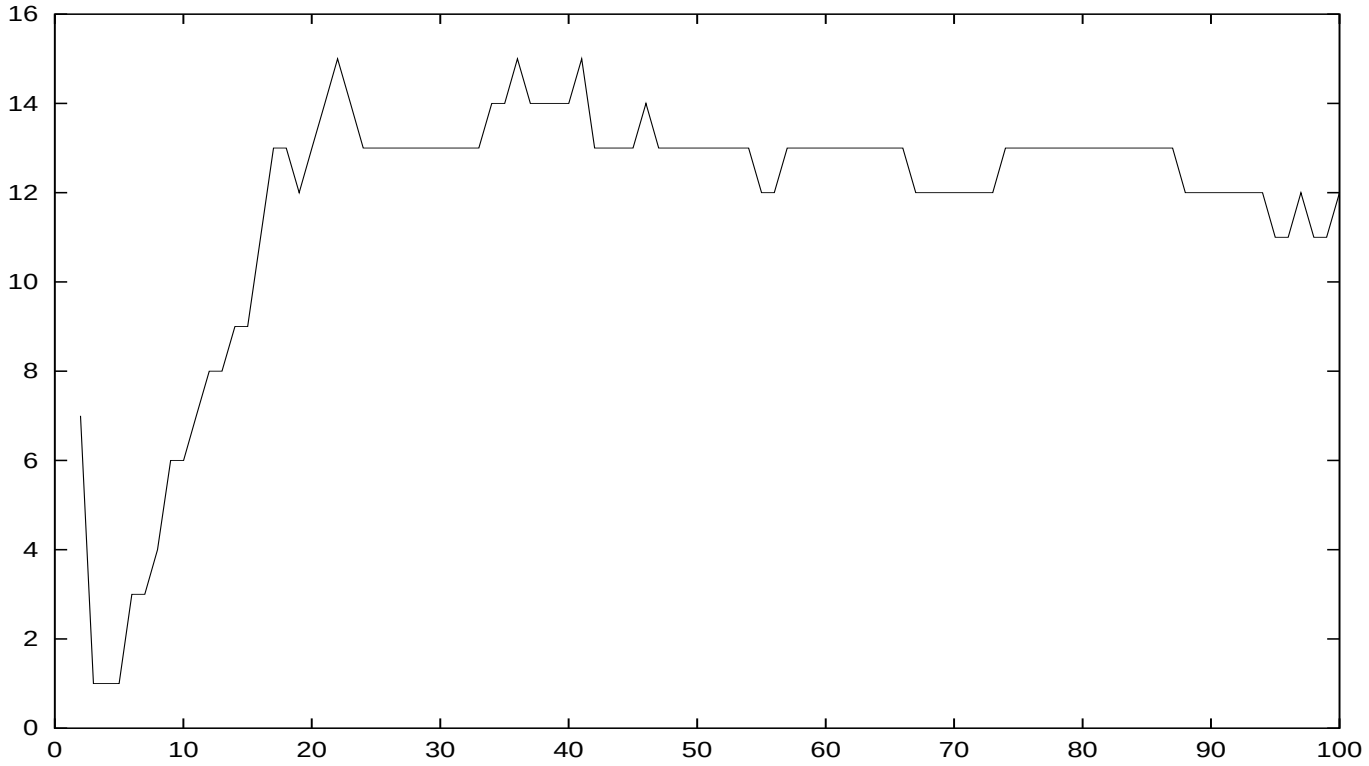
THE PROCESS IS USUALLY PERFORMED WITH A CONTROL TO IMPROVE ACCURACY



- 29 examples balanced dataset with 17836 features (probes)
- used a Support Vector Machine classifier with linear kernel and filter method for feature scoring.

- impute missing values,
- log data,
- use leave-one-out testing

Number of test errors (y-axis) versus number of remaining features (x-axis).



Example 2

Recognition of ZIP/postal codes: very important real-life application.

Standard benchmarking dataset is NIST (60,000 handwritten characters).

AT&T (Bell Labs): state-of-the-art was a layered neural networks (LeNet5, Yann Le Cun, et al).

Dennis de Coste/Bernhard Scholkopf (2002): used an SVM but with *virtual training vectors* as a means of ensuring invariant pattern recognition.

Improves on previous best by 0.15% test error reduction.

3. Conclusion.

Kernel methods: a powerful and systematic approach to classification, regression, novelty detection and many other machine learning problems.

Now widely used in many application domains including bioinformatics, machine vision, text analysis, finance, ...