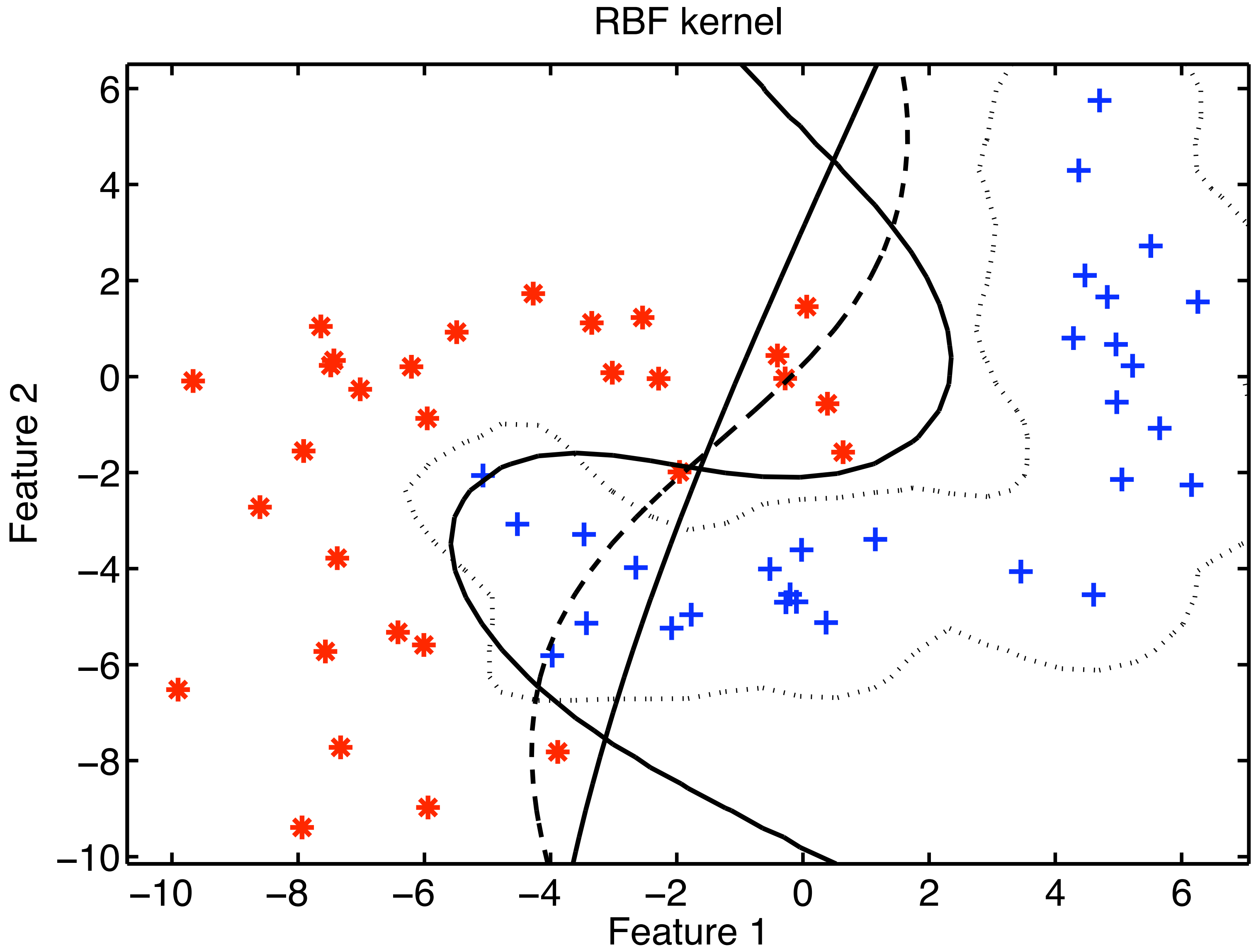
Complexity and Support Vector Classifiers



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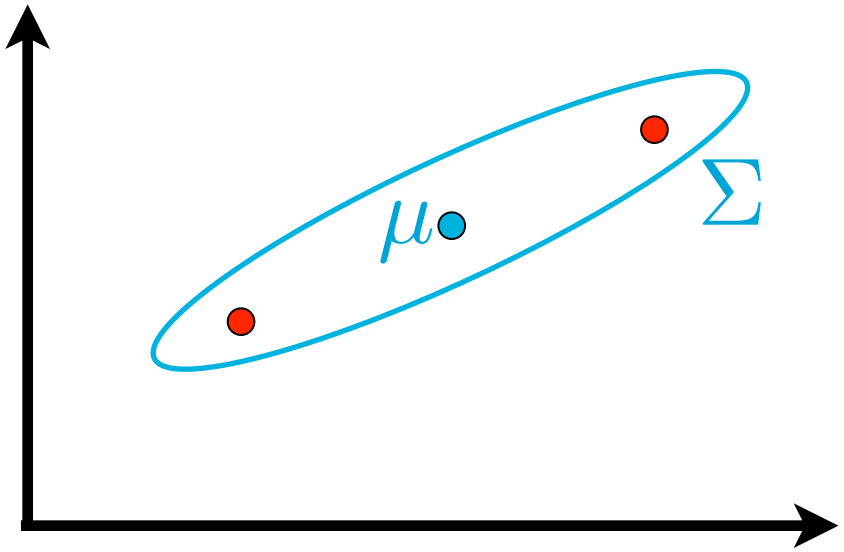
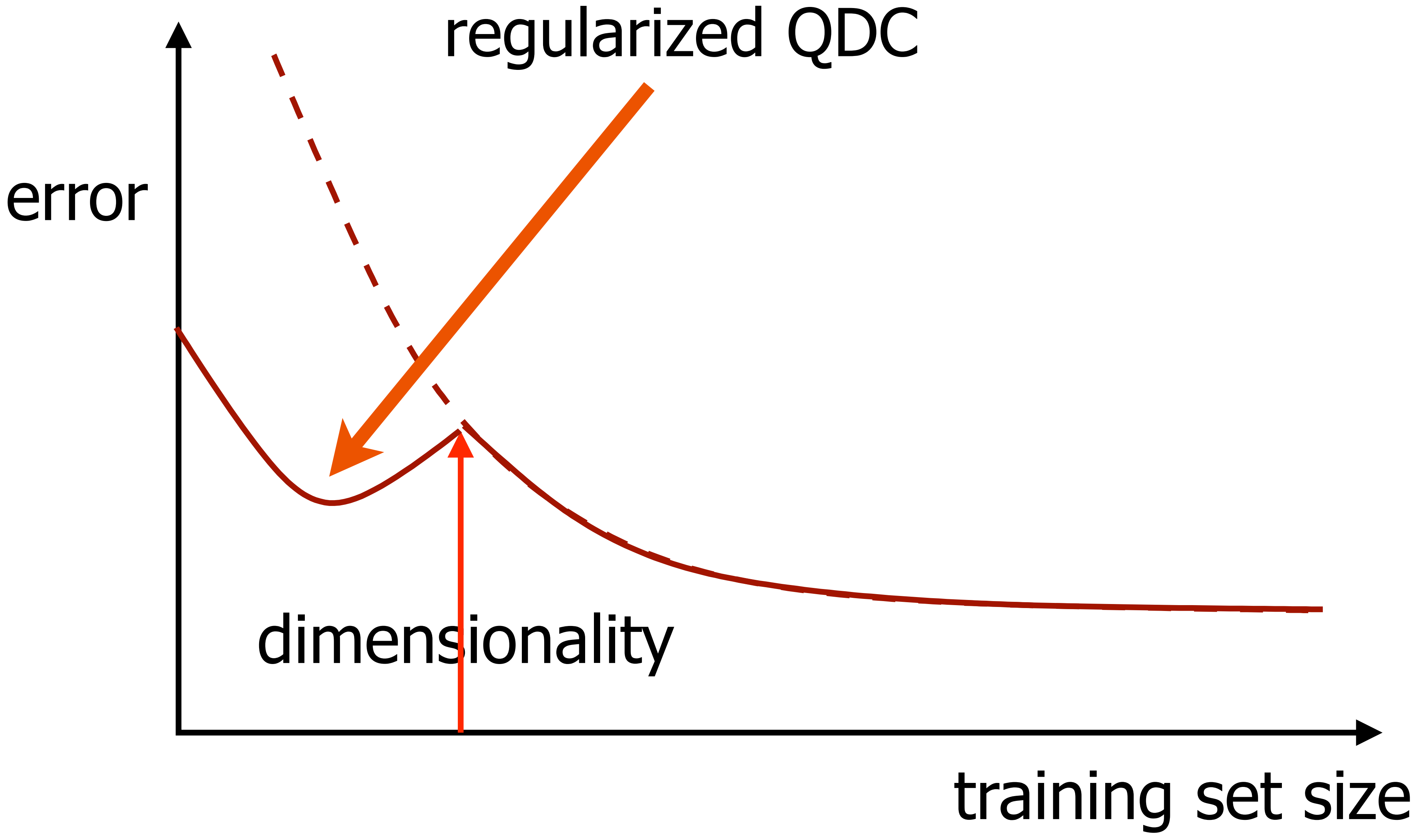


- When insufficient data is available (nr of obj's is smaller than dimensionality), the inverse covariance matrices are not defined: the classifier is not defined
- **Regularization** solves it: $\tilde{\Sigma}_i = \Sigma_i + \lambda \mathbb{I}$
- With very large regularisation $\lambda \to \infty$ you get: nearest mean classifier

Quadratic classifier



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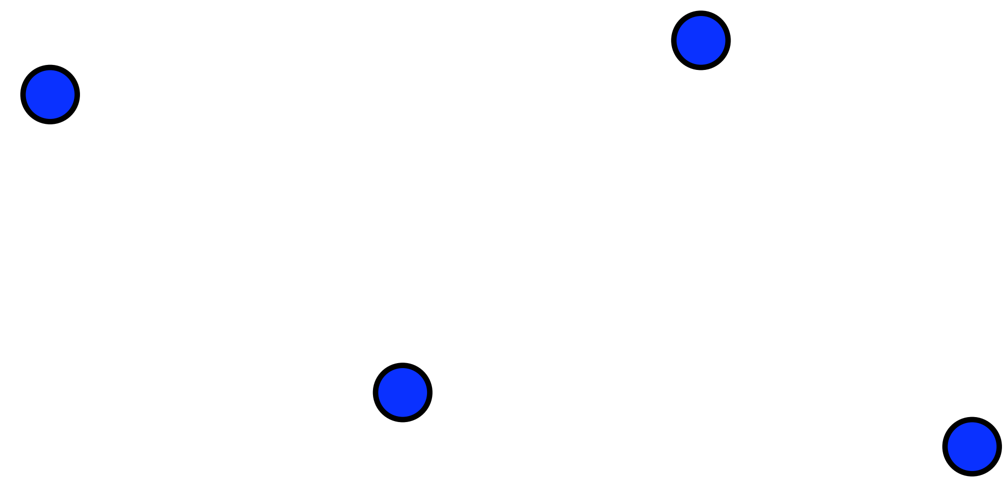
VC-dimension

- h: the VC-dimension of a classifier:



The largest number of vectors **h** that can be separated in all the 2^h possible ways.

Changing h for linear classifiers

- The linear classifier had $h = p + 1$

- By putting some constraints on this linear classifier, the VC dimension can be reduced
- Assume a linearly separable dataset, constrain the weights such that the output of the classifier is always larger than one:

$$\mathbf{w}^T \mathbf{x}_i + b \geq +1, \quad \text{for } y_i = +1$$
$$\mathbf{w}^T \mathbf{x}_i + b \leq -1, \quad \text{for } y_i = -1$$

Minimizing the Lagrangian

- Lagrangian:

$$\mathcal{L}(\mathbf{w},\alpha) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_i \alpha_i \left(y_i(\mathbf{w}^T\mathbf{x}_i + b) - 1 \right)$$

- Have to take the derivative with respect to **w**, b, and α_i and set the derivative to 0

$$\frac{\partial \mathcal{L}(\mathbf{w},\alpha)}{\partial \mathbf{w}} = \mathbf{w} - \sum_i \alpha_i y_i \mathbf{x}_i = 0$$

- Solve: $$\mathbf{w} = \sum_i \alpha_i y_i \mathbf{x}_i$$

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Optimizing the classifier

- Solving w.r.t. **w** and b is “simple”.
- Solving w.r.t. α_i gives:

$$\max_{\alpha} \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j}^{N} y_i y_j \alpha_i \alpha_j \mathbf{x}_i^T \mathbf{x}_j$$

$$\alpha_i \geq 0 \quad \forall i$$

$$\sum_{i=1}^{N} \alpha_i y_i = 0$$

$$\mathbf{w} = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i$$

- Quadratic Programming Problem

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Support vectors

- The classifier becomes:

$$\mathbf{w} = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i$$

- The solution is expressed in terms of objects, not features.
- Only a few weights become non-zero
- The objects with non-zero weight are called the support vectors

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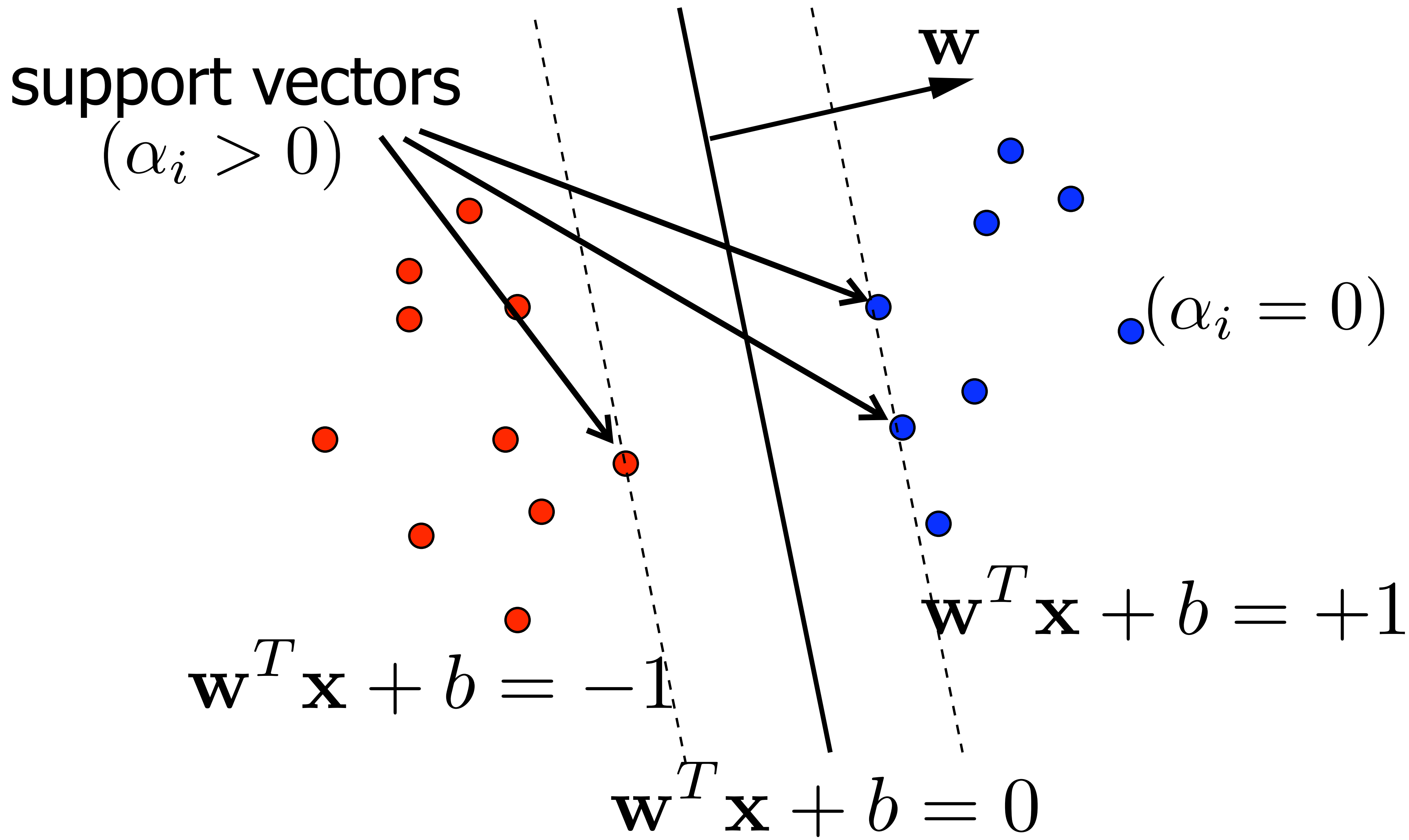
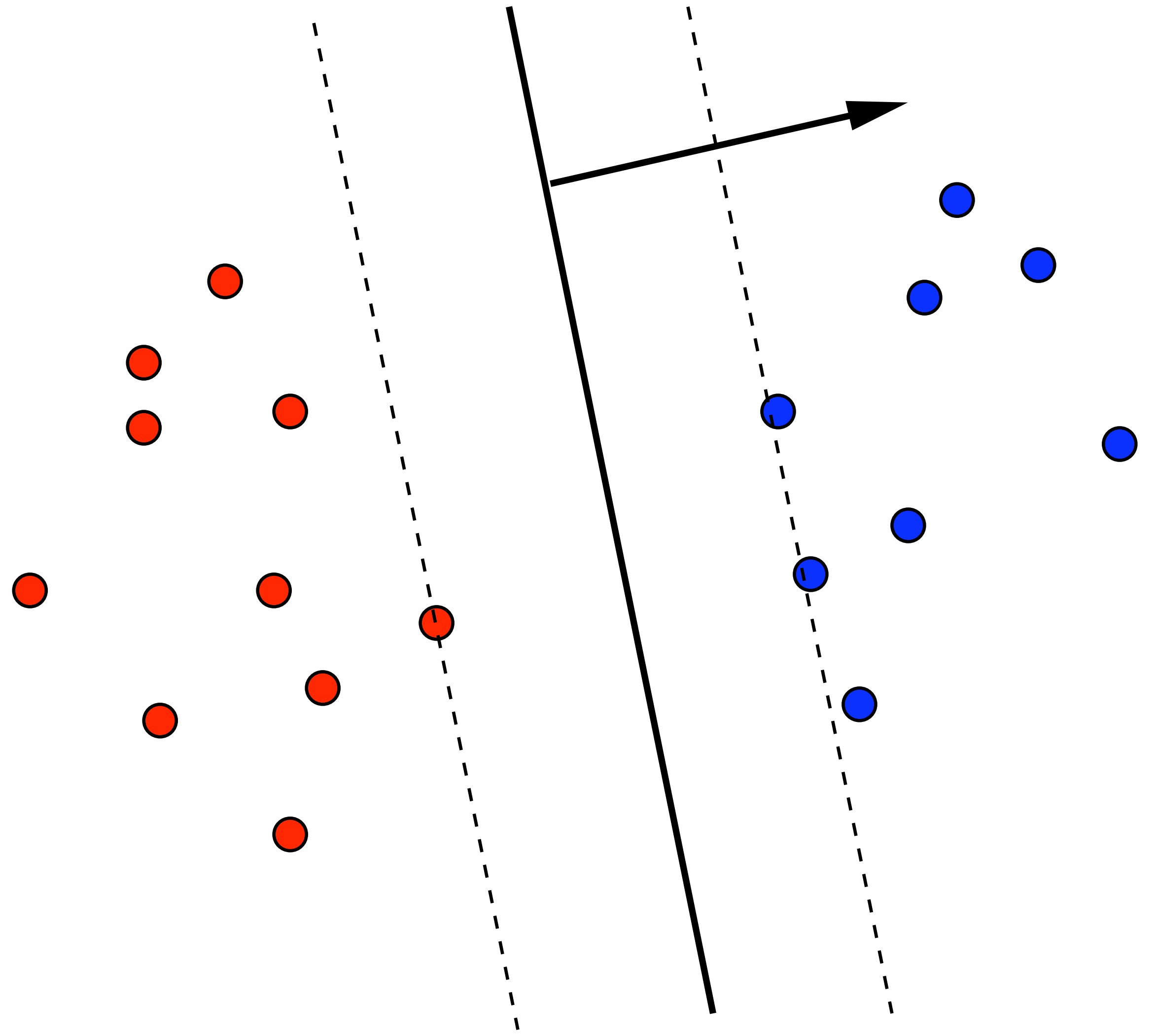
Support vector classifier

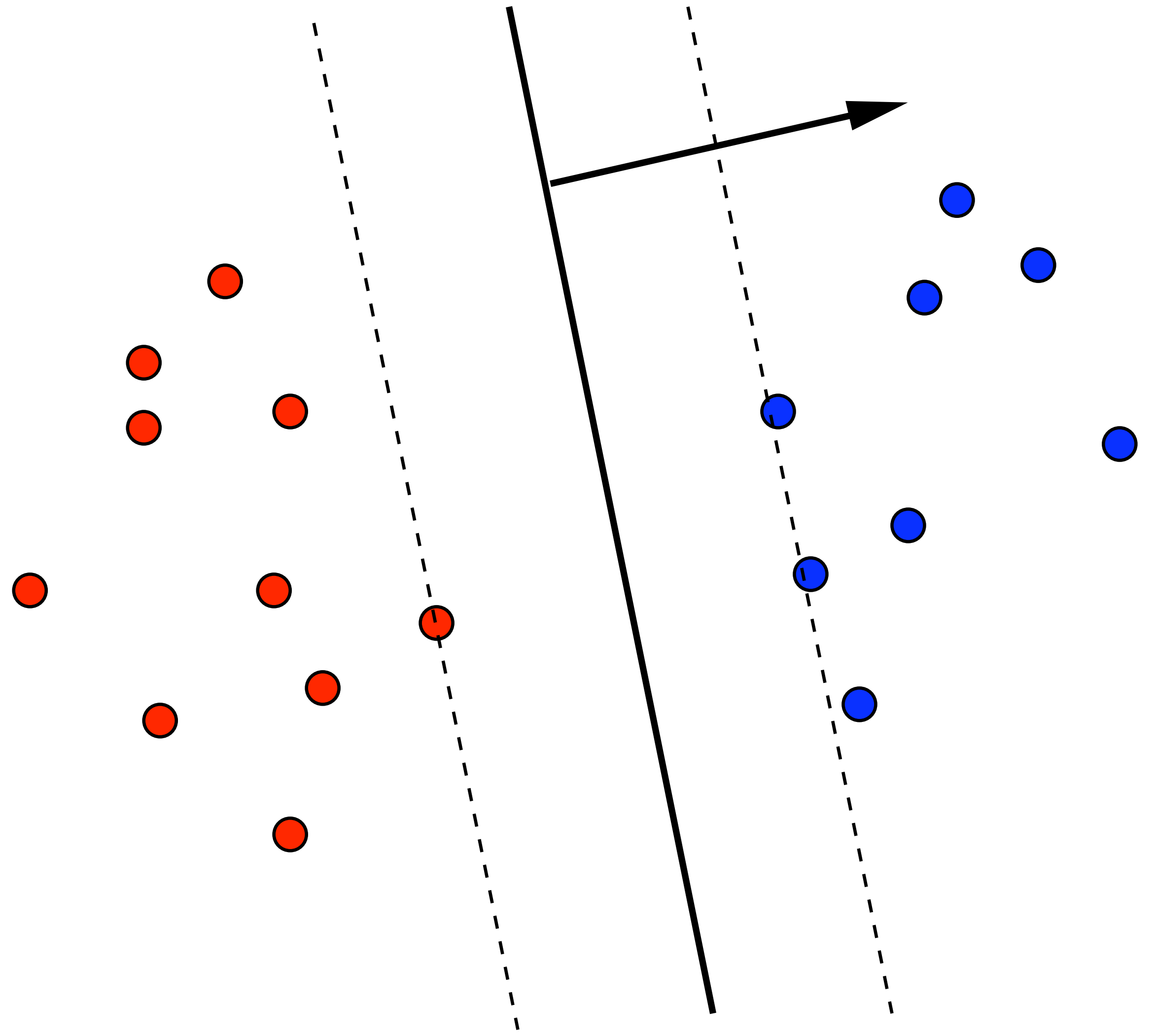


LOO Error estimation



Estimate the leave-one-out error on this data...

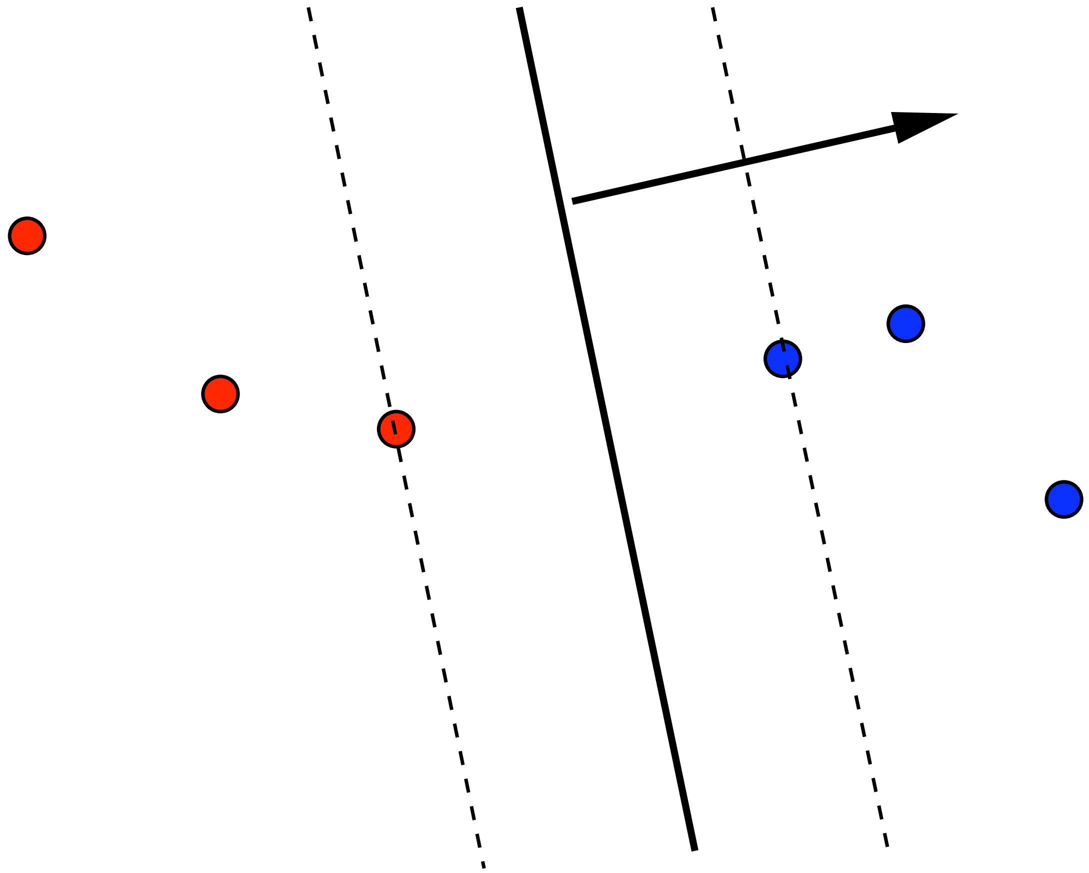
Error estimation



By leave-one-out you can obtain a bound on the error:

$$\varepsilon_{LOO} \leq \frac{\#\text{support vectors}}{N}$$

High dimensional feature spaces



The classifier is determined by objects, not features: the classifier tends to perform very well in high dimensional feature spaces.

Limitations of the SVM

1. The data should be separable
2. The decision boundary is linear

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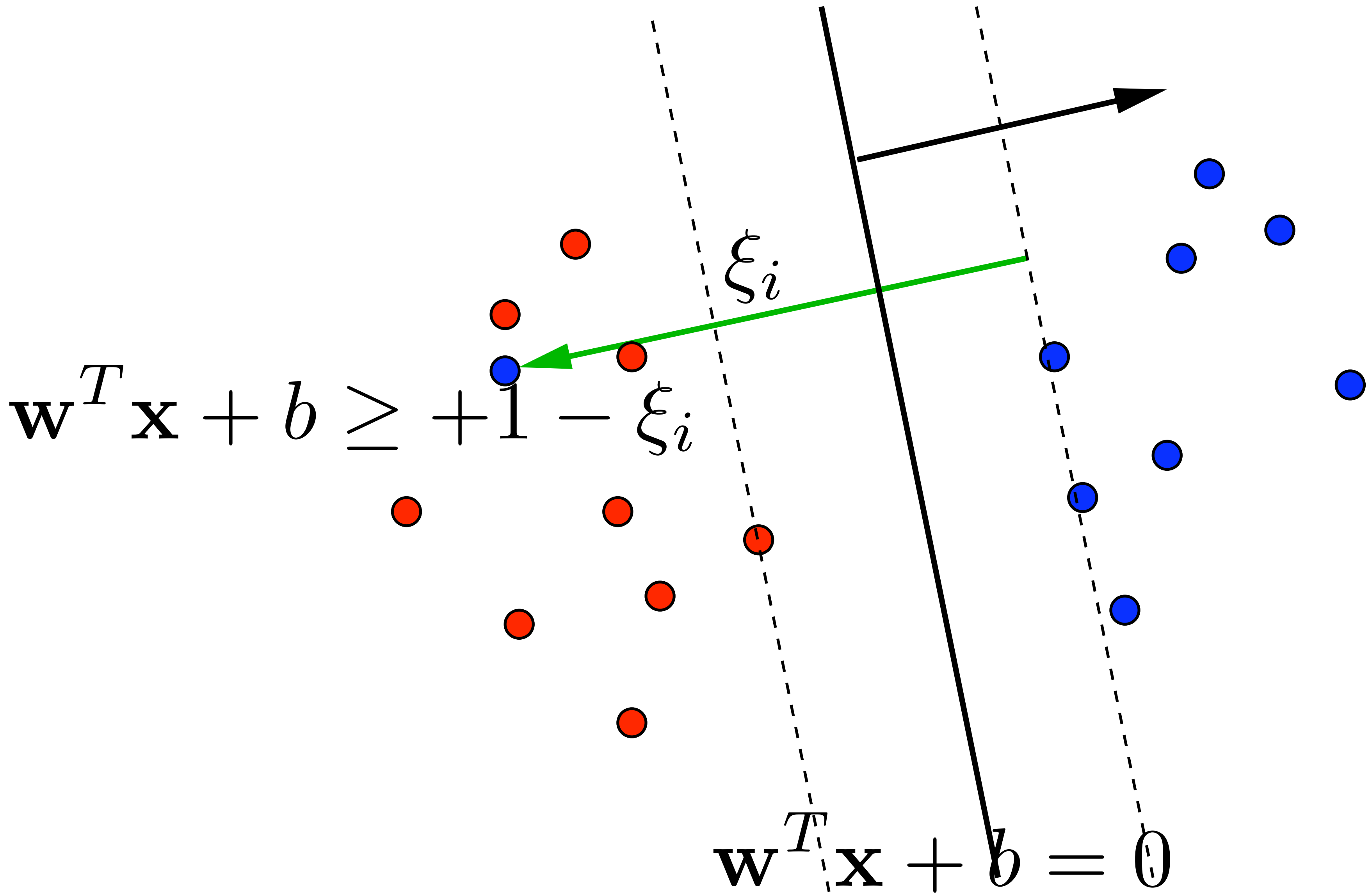
Problem 1

The classes should be separable...

Weakening the constraints



Introduce a 'slack' variable ξ_i for each object, to weaken the constraints

SVM with slacks

- The optimization changes into:

$$\min \|\mathbf{w}\|^2 + C\sum_{i=1}^{N} \xi_i$$

$$\mathbf{w}^T\mathbf{x}_i + b \geq +1 - \xi_i, \quad \text{for } y_i = +1$$

$$\mathbf{w}^T\mathbf{x}_i + b \leq -1 + \xi_i, \quad \text{for } y_i = -1$$

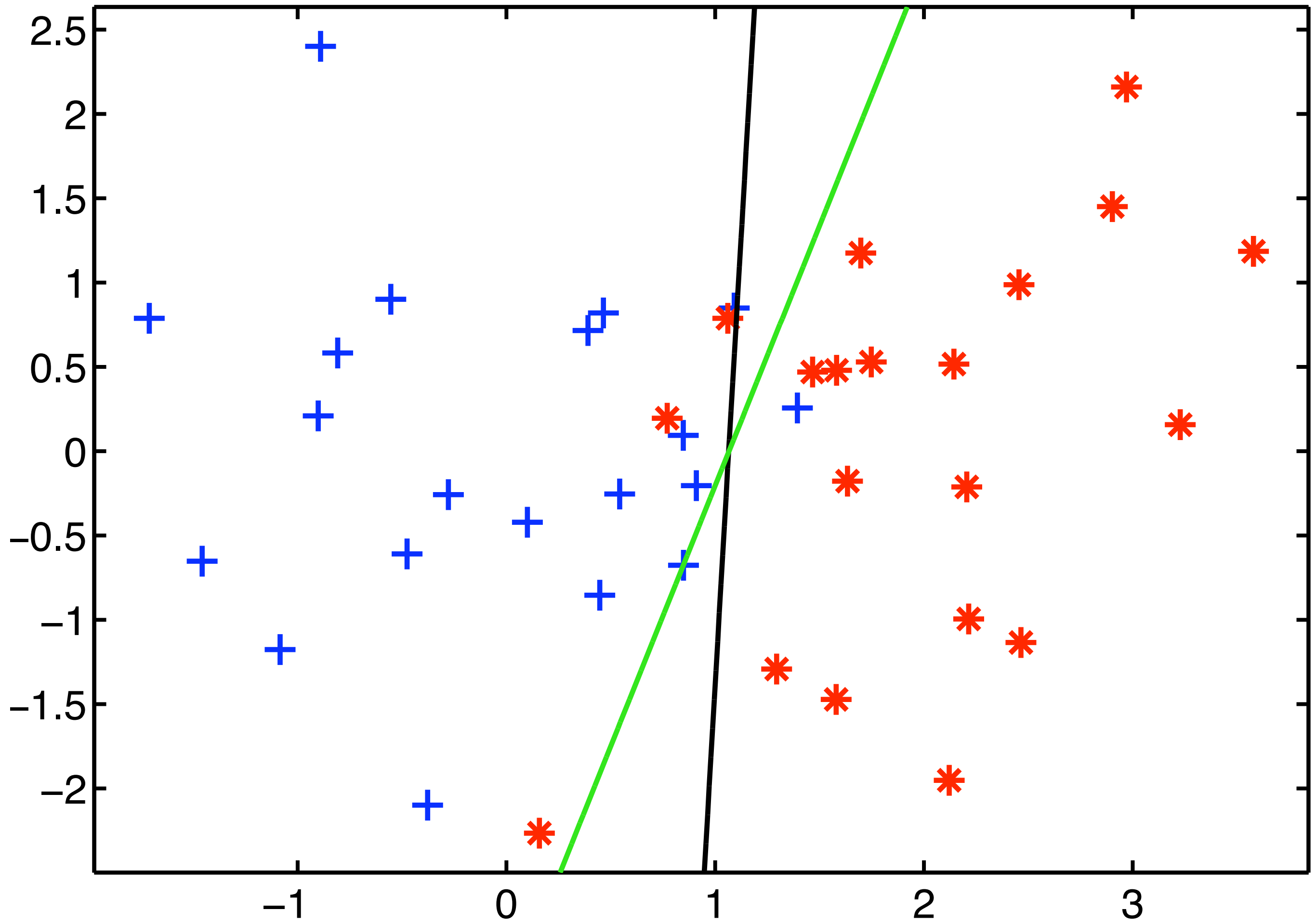
$$\xi_i \geq 0 \quad \forall i$$

Tradeoff parameter C

$$\min \|\mathbf{w}\|^2 + C \sum_{i=1}^{N} \xi_i$$

- Notice that the tradeoff parameter C has to be defined beforehand
- It weighs the contributions between the training error and the structural error
- Its values are often optimized using crossvalidation.

Influence of C



C=1

C=1000

Erroneous objects have still large influence when C is not optimized carefully

Problem 2

The decision boundary is only linear...

Trick: transform your data

$$\min_{\alpha} \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j}^{N} y_i y_j \alpha_i \alpha_j \mathbf{x}_i^T \mathbf{x}_j$$

$$\alpha_i \geq 0 \quad \forall i$$

$$\sum_{i=1}^{N} \alpha_i y_i = 0$$

$$f(\mathbf{z}) = \mathbf{w}^T \mathbf{z} + b = \sum_{i=1}^{N} \alpha_i y_i \mathbf{x}_i^T \mathbf{z} + b$$

- Magic: all operations are on inner products between objects
- Assume I have a magic transformation of my data that makes it linearly separable...

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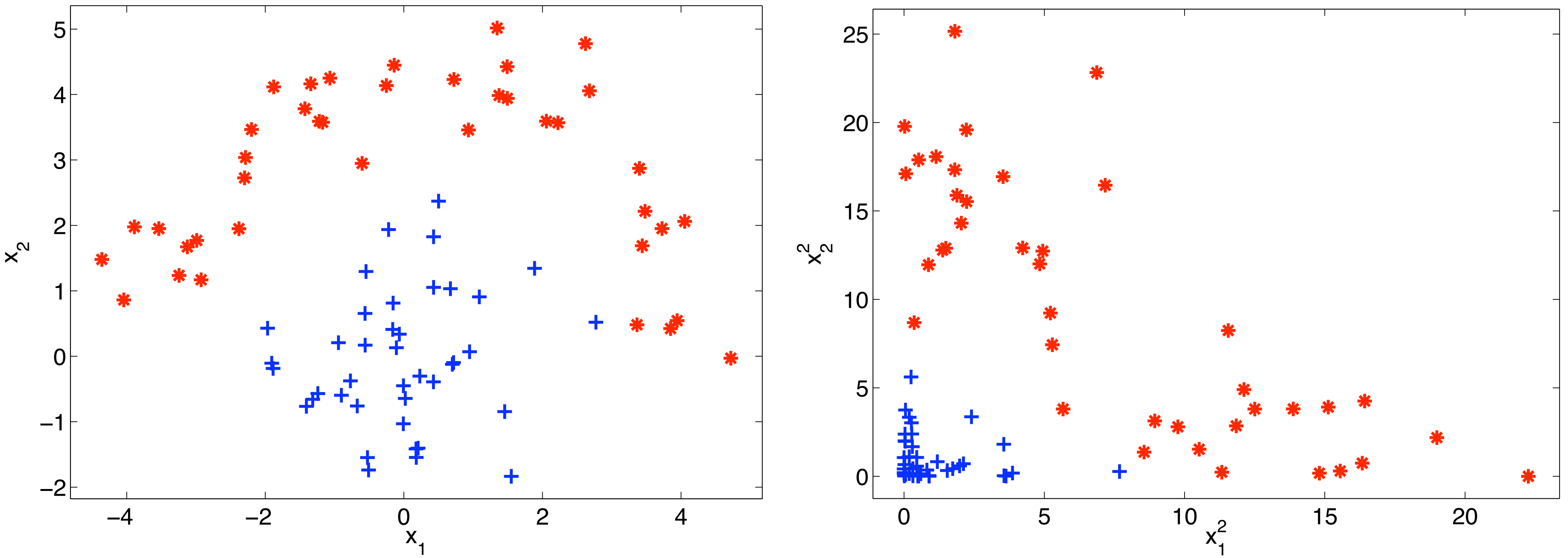
Example transformation



- Original data: $\mathbf{x} = (x_1, x_2)$
- Mapped data: $\mathbf{\Phi}(\mathbf{x}) = (x_1^2, x_2^2, \sqrt{2}x_1x_2)$

Polynomial kernel

- When we have two vectors

$$\mathbf{\Phi}(\mathbf{x}) = (x_1^2, x_2^2, \sqrt{2}x_1x_2)$$

$$\mathbf{\Phi}(\mathbf{y}) = (y_1^2, y_2^2, \sqrt{2}y_1y_2)$$

$$\begin{aligned} \mathbf{\Phi}(\mathbf{x})^T\mathbf{\Phi}(\mathbf{y}) &= x_1^2y_1^2 + x_2^2y_2^2 + 2x_1x_2y_1y_2 \\ &= \left((x_1, x_2)(y_1, y_2)^T\right)^2 \\ &= \left(\mathbf{x}^T\mathbf{y}\right)^2 \end{aligned}$$

it becomes very cheap to compute the inner product.

Transform your data

$$\min_{\alpha} \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j}^{N} y_i y_j \alpha_i \alpha_j \mathbf{\Phi}(\mathbf{x}_i)^T \mathbf{\Phi}(\mathbf{x}_j)$$

$$\sum_{i=1}^{N} \alpha_i y_i = 0 \quad \alpha_i \geq 0 \quad \forall i$$

$$f(\mathbf{z}) = \sum_{i=1}^{N} \alpha_i y_i \mathbf{\Phi}(\mathbf{x}_i)^T \mathbf{\Phi}(\mathbf{z}) + b$$

- If we have to introduce the magic $\mathbf{\Phi}(\mathbf{x})$
  we can as well introduce the magic kernel function:

$$K(\mathbf{x}, \mathbf{y}) = \mathbf{\Phi}(\mathbf{x})^T \mathbf{\Phi}(\mathbf{y})$$

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Transform your data

$$\max_{\alpha} \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j}^{N} y_i y_j \alpha_i \alpha_j K(\mathbf{x}_i, \mathbf{x}_j)$$

$$\sum_{i=1}^{N} \alpha_i y_i = 0 \quad \alpha_i \geq 0 \quad \forall i$$

$$f(\mathbf{z}) = \sum_{i=1}^{N} \alpha_i y_i K(\mathbf{x}_i, \mathbf{z}) + b$$

- We only define the kernel function, and forget about the mapping $\mathbf{\Phi}(\mathbf{x})$
- For instance:

$$K(\mathbf{x}_i, \mathbf{z}) = \exp\left(-\frac{\|\mathbf{x} - \mathbf{z}\|^2}{\sigma^2}\right)$$

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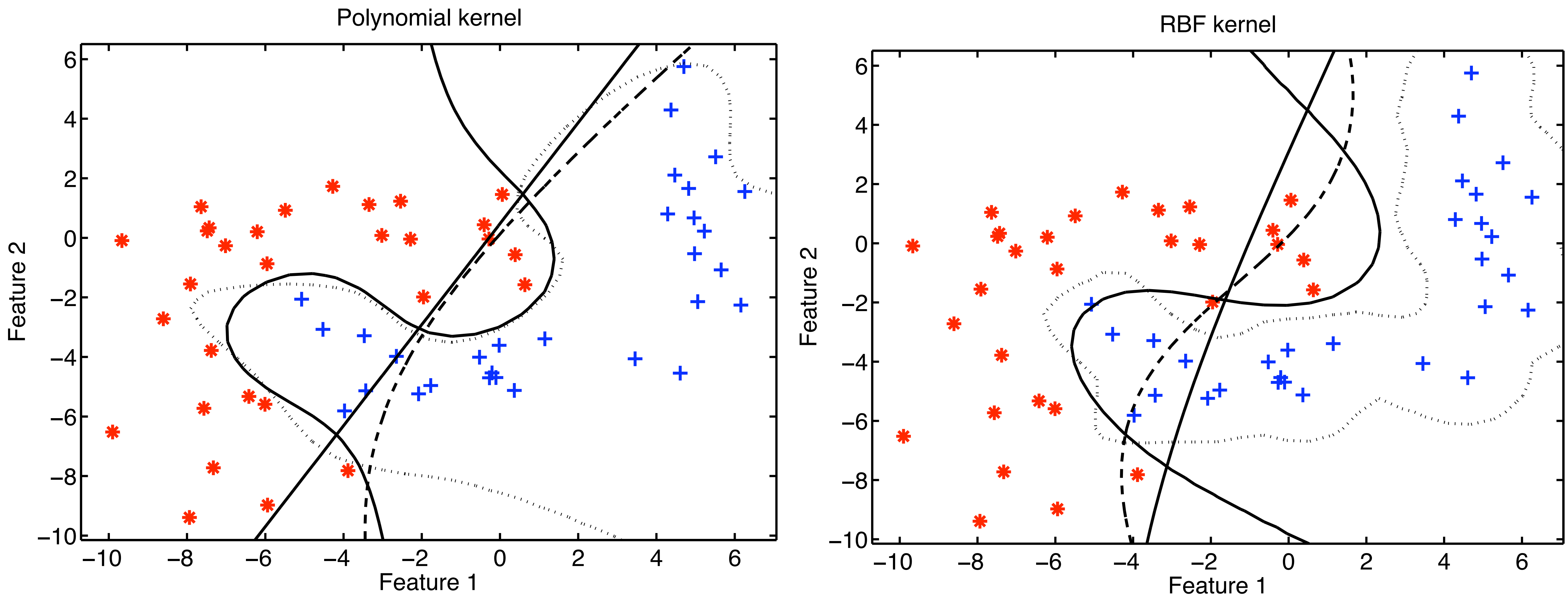
The ‘kernel-trick’

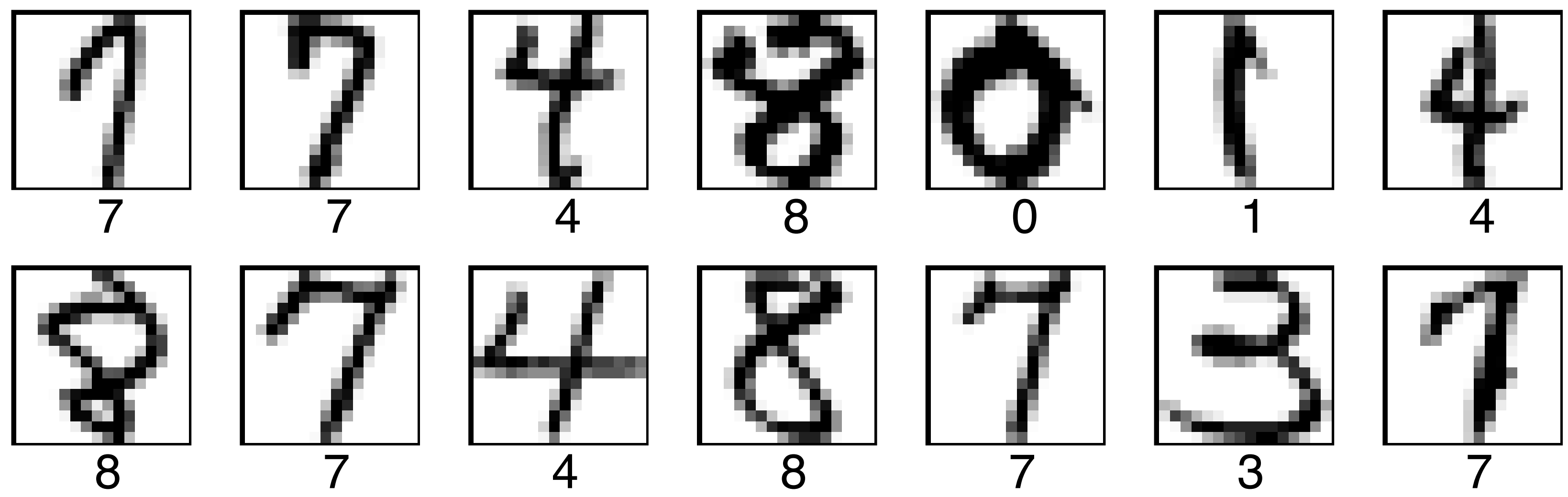
- The idea to replace all inner products by a single function, the kernel function K, is called the kernel trick
- It implicitly maps the data to a (most often) high dimensional feature space
- The practical computational complexity does not change (except for computing the kernel function)

Popular kernel functions



$$K(\mathbf{x}, \mathbf{y}) = (\mathbf{x}^T \mathbf{y} + 1)^d \qquad K(\mathbf{x}, \mathbf{y}) = \exp\left(-\frac{\|\mathbf{x} - \mathbf{y}\|^2}{\sigma^2}\right)$$

Results



USPS handwritten digits dataset

Cortes & Vapnik, Machine Learning 1995

Classifier	raw error, %
Human performance	2.5
Decision tree, CART	17
Decision tree, C4.5	16
Best 2 layer neural network	6.6
Special architecture 5 layer network	5.1

degree of polynomial	raw error, %	support vectors	dimensionality of feature space
1	12.0	200	256
2	4.7	127	~ 33000
3	4.4	148	$\sim 1 \times 10^6$
4	4.3	165	$\sim 1 \times 10^9$
5	4.3	175	$\sim 1 \times 10^{12}$
6	4.2	185	$\sim 1 \times 10^{14}$
7	4.3	190	$\sim 1 \times 10^{16}$

Advanced kernel functions

- People construct special kernel functions for applications:
  - Tangent distance kernels to incorporate rotation/ scaling insensitivity (handwritten digits recognition)
  - String matching kernels to classify DNA/protein sequences
  - Fisher kernels to incorporate knowledge on class densities
  - Hausdorff kernels to compare image blobs
  - …

High dimensional feature spaces

- SVM appears to work well in high dimensional feature spaces
  - The class overlap is often not large
  - Minimizing h minimizes the risk of overfitting
- The classifier is determined by the support objects and not directly by the features
- No density is estimated

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Advantages of SVM

- The SVM generalizes remarkably well, in particular in high-dimensional feature spaces with (relatively) low sample sizes
- Given a kernel and a C, there is one unique solution
- The kernel trick allows for a varying complexity of the classifier
- The kernel trick allows for especially engineered representations for problems

- No strict data model is assumed (when you can assume it, use it!)
- The foundation of the SVM is pretty solid (when no slack variables are used)
- An error estimate is available using just the training data (but it is a pretty loose estimate, and crossvalidation is still required to optimize K and C)

Disadvantages of SVM

- The quadratic optimization is computationally expensive (although more and more specialized optimizers appear)
- The kernel and C have to be optimized
- The SVM has problems with highly overlapping classes

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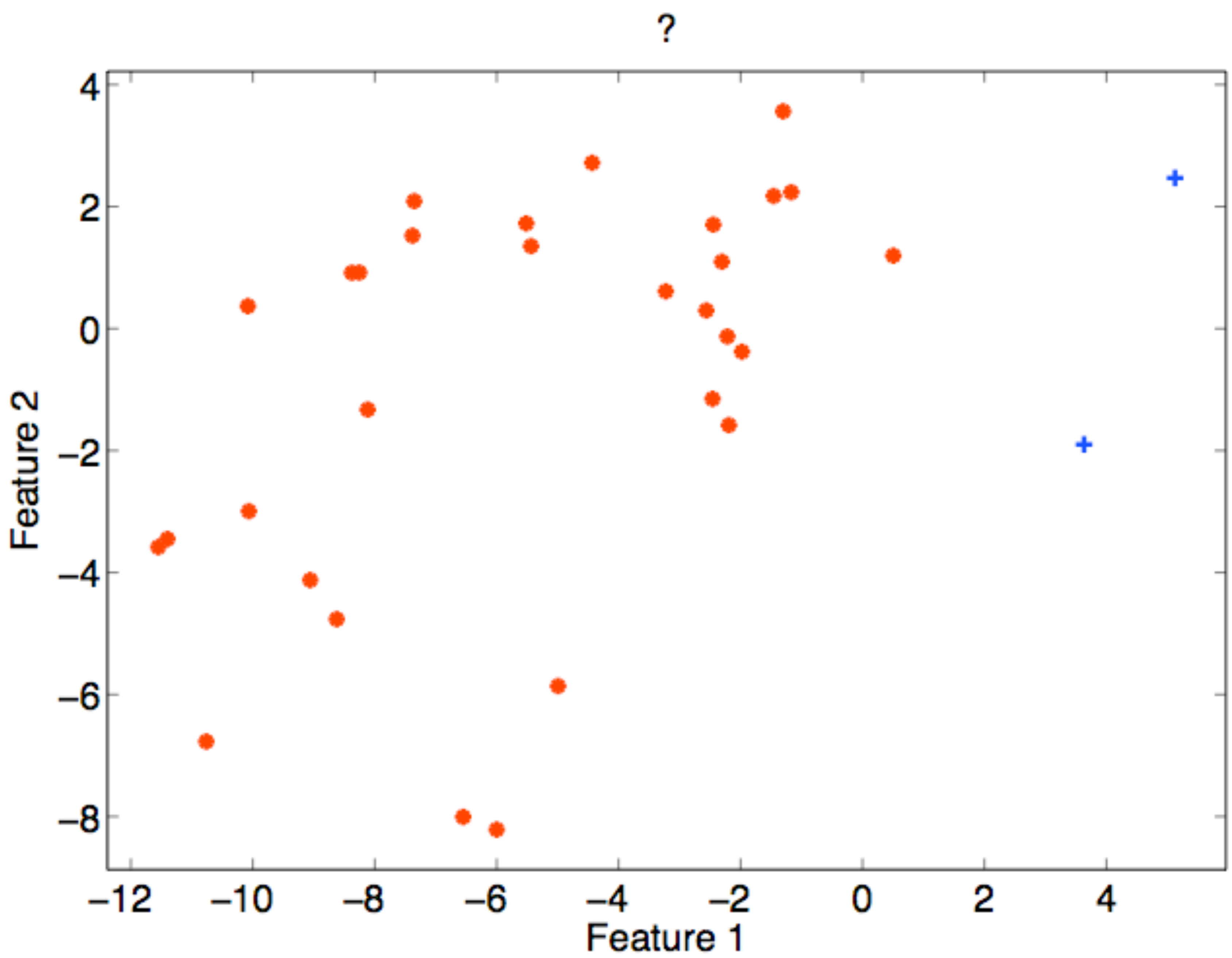
Conclusions

- Always tune the complexity of your classifier to your data (#training objects, dimensionality, class overlap, class shape...)
- A classifier does not need to estimate (class-) densities, like an SVM
- The SVM can be used in almost all applications (by adjusting K and C appropriately)

Classification problem

BONUS



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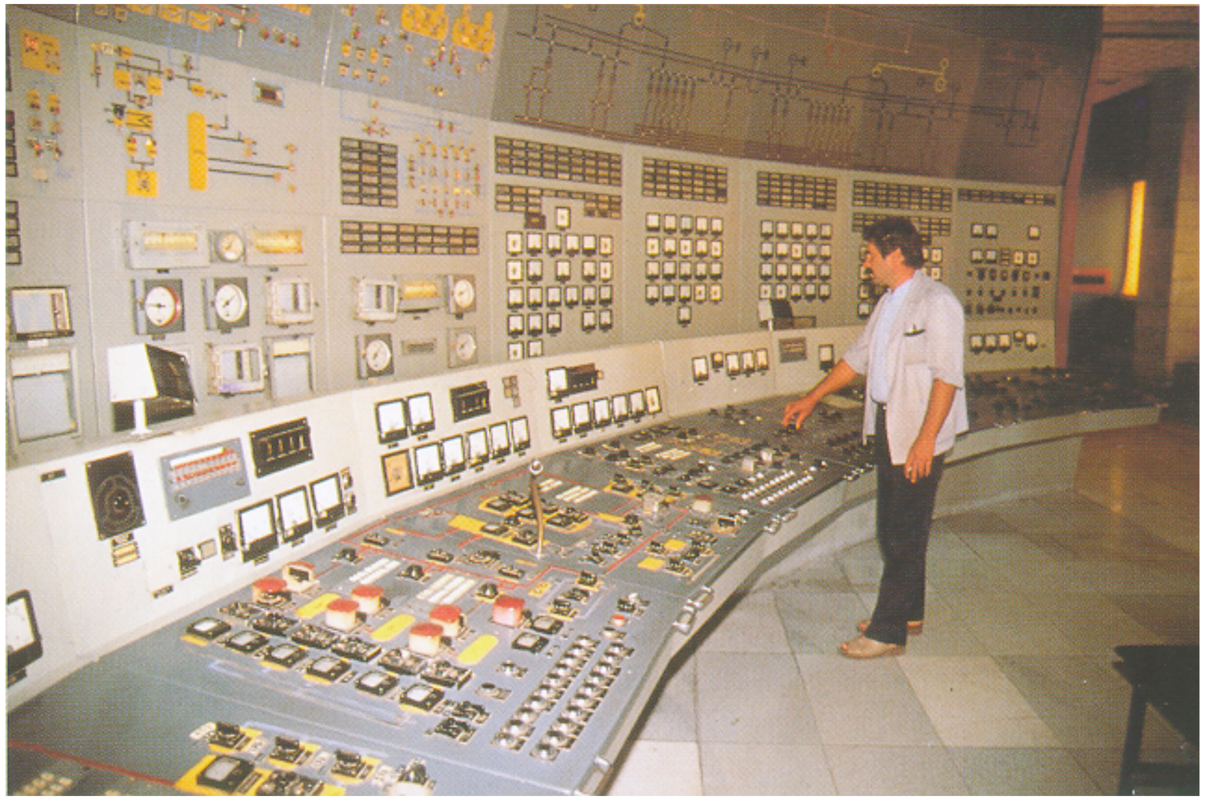
One-class classification



- Normal operating condition (target class) can be sampled well
- Abnormal conditions (outlier class) are rare, or are hard to sample reliably

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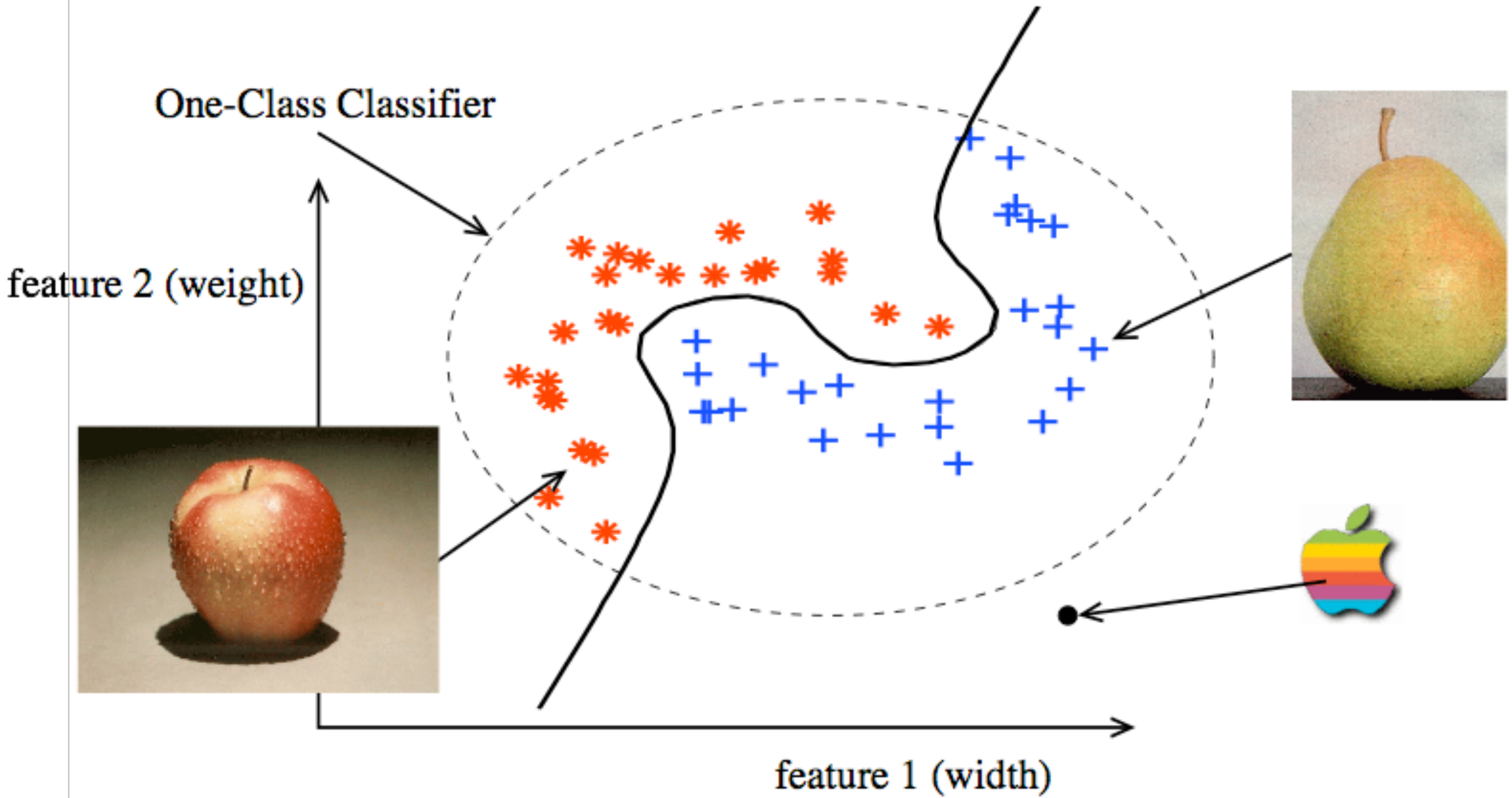
One-class classification



- Many example target objects are present
- Few (reliable) outlier objects are available

From classifiers to outlier detection

$$p(y|\mathbf{x})$$

generative classifiers:

$$\hat{p}(y|\mathbf{x}) = \frac{\hat{p}(\mathbf{x}|y)\hat{p}(y)}{\hat{p}(\mathbf{x})}$$

discriminative classifiers:

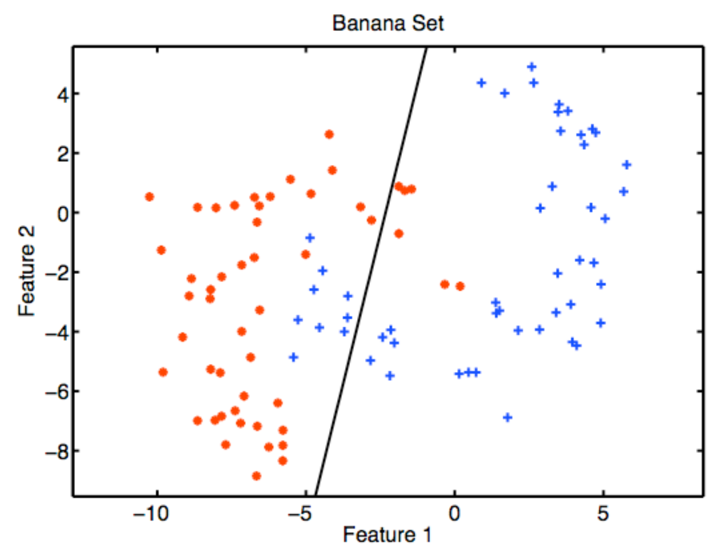
$$\hat{p}(y|\mathbf{x}) = f(\mathbf{x};\mathbf{w})$$

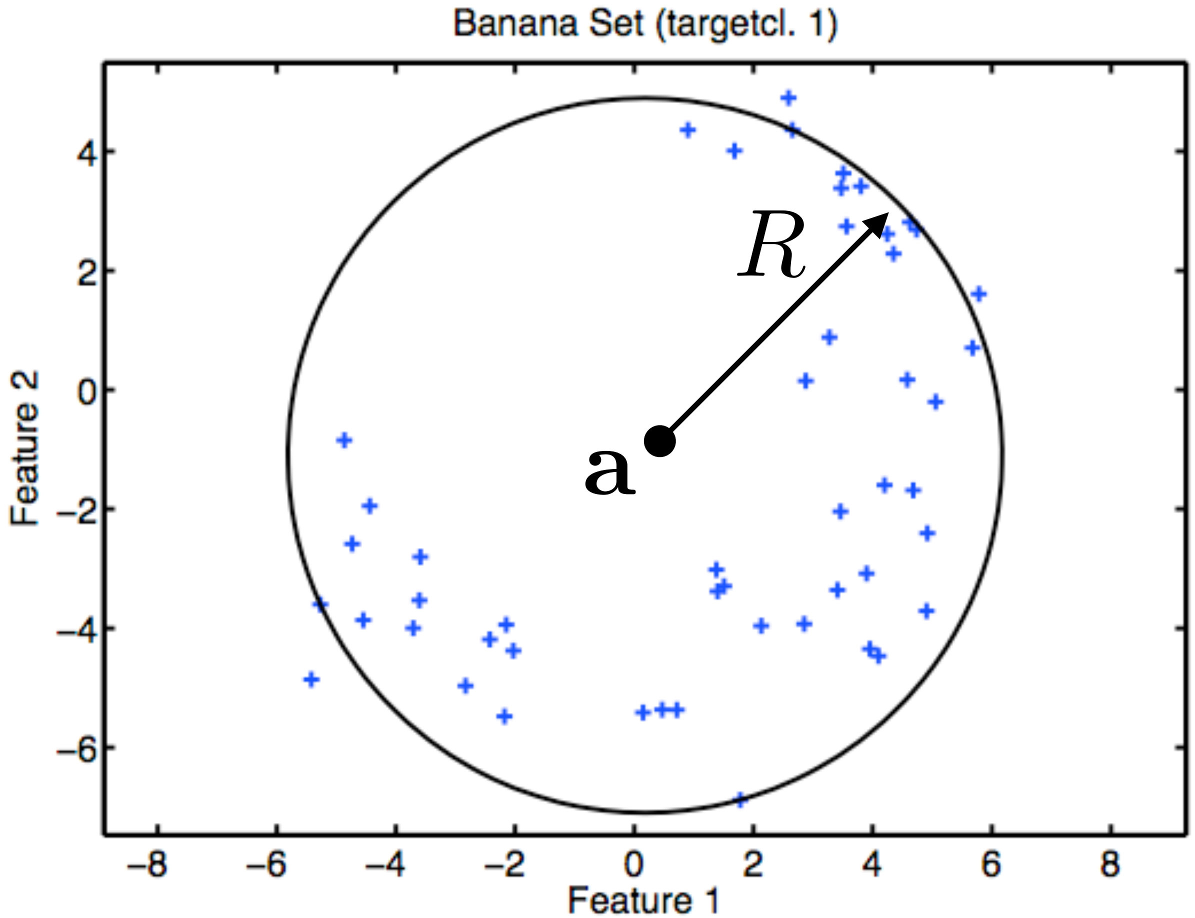
$$\hat{p}(\mathbf{x}) = \sum_i \hat{p}(\mathbf{x}|y_i)\hat{p}(y_i)$$

?

- Outlier detection without density estimation?

Decision boundary OCC





- Fit only a boundary (inspired by the support vector classifier)
- Instead of a linear decision boundary, a hypersphere around the target class

Support Vector Data Description

	Support Vector cl.	**Support vector DD**
model	hyperplane $\mathbf{w}, b$	hypersphere $\mathbf{a}, R$
complexity	$\lVert\mathbf{w}\rVert^2$	R^2
error	$\lVert\mathbf{w}\rVert^2 + C\sum_i \xi_i$	$R^2 + C\sum_i \xi_i$
SVs	objects on the plane	objects on the sphere
slacks	objects on the wrong side of the plane	objects outside the sphere

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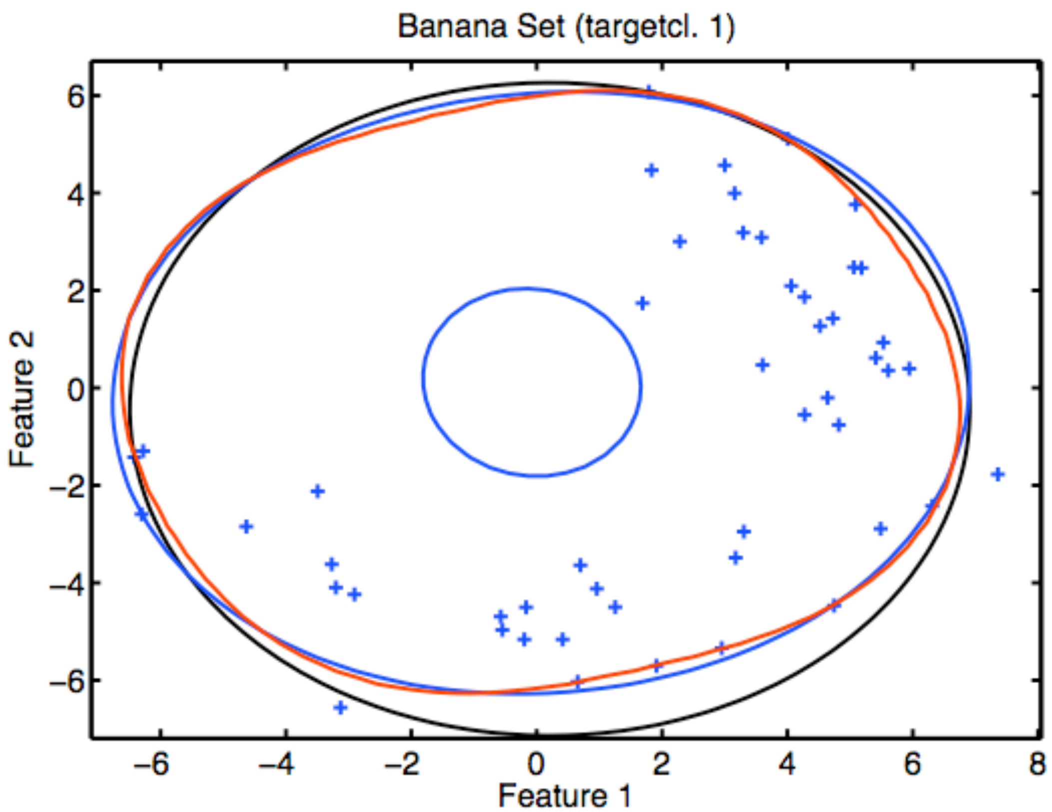
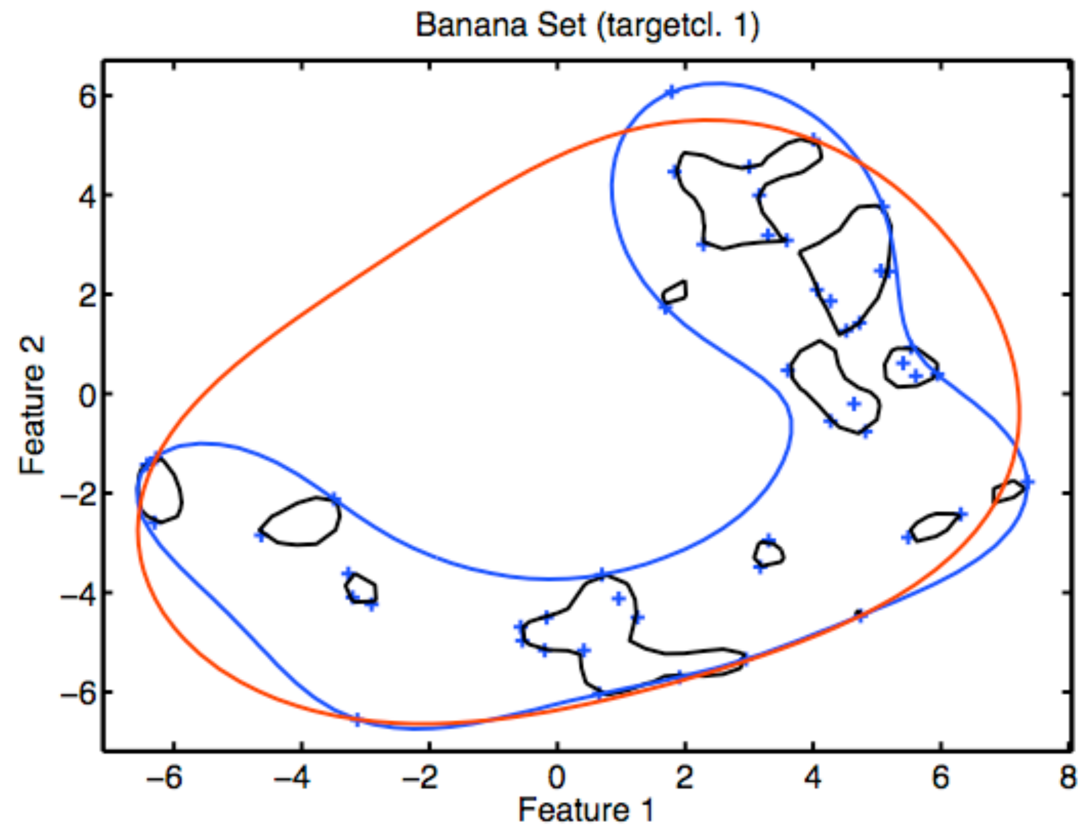
Different kernels





Polynomial

Radial basis (Gaussian)

$$K(\mathbf{z}, \mathbf{x}) = (\mathbf{x}^T \mathbf{z} + 1)^d \qquad K(\mathbf{z}, \mathbf{x}) = \exp\left(-\frac{\|\mathbf{x} - \mathbf{z}\|^2}{\sigma^2}\right)$$