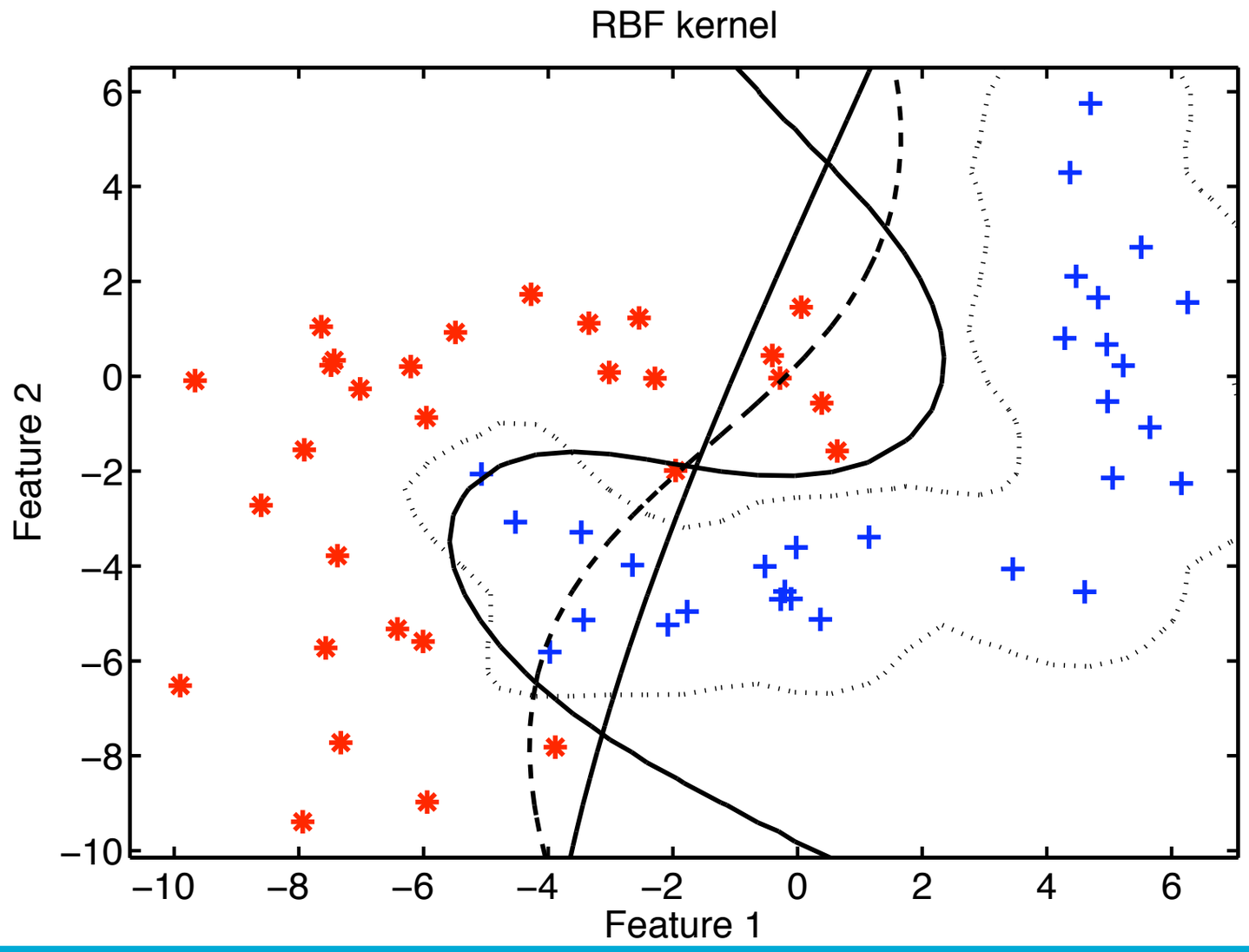
Complexity and Support Vector Classifiers



David M.J. Tax

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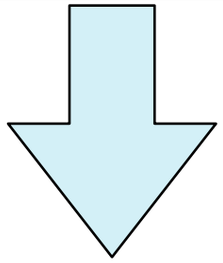
Contents

- How to characterise complexity?
- How to adapt the complexity?
- Measuring complexity: VC-dimension
- Support vector classifiers
  - Constrained optimisation
  - Advantages and disadvantages
- Examples
- Conclusions
- (Bonus?)



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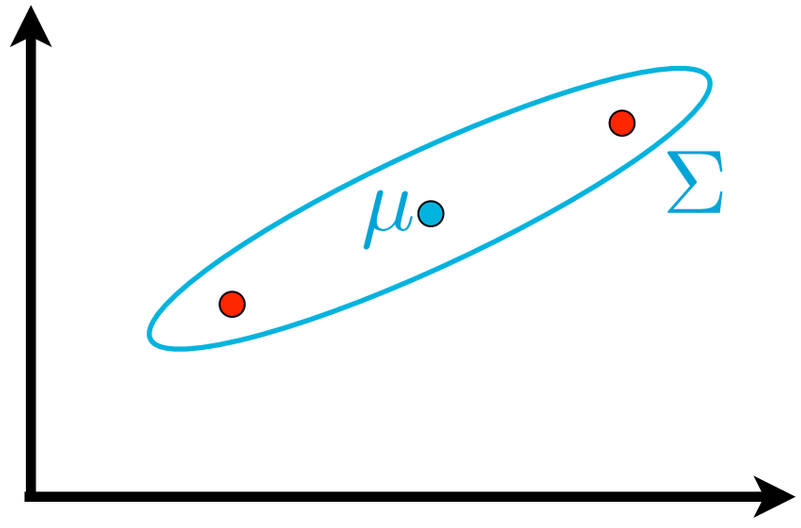
Quadratic classifier



- 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

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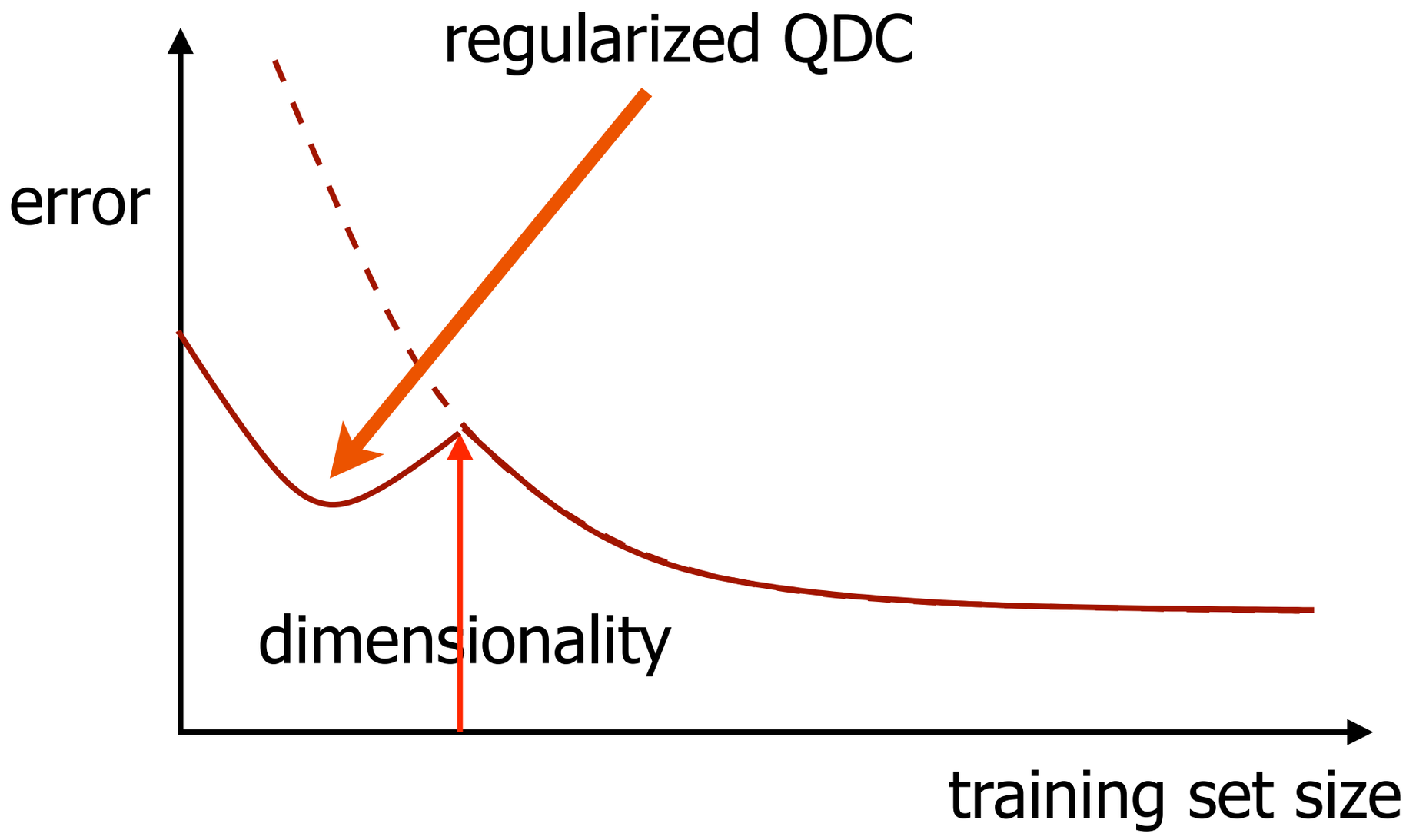
Quadratic classifier



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Bounding the true error

With probability at least $1-\eta$ the inequality holds:

$$\varepsilon \leq \varepsilon_A + \frac{\mathcal{E}(N)}{2}\left(1+\sqrt{1+\frac{\varepsilon_A}{\mathcal{E}(N)}}\right)$$

where

$$\mathcal{E}(N) = 4\frac{h(\ln(2N/h)+1)-\ln(\eta/4)}{N}$$

V.Vapnik, Statistical learning theory, 1998

- When h is small, the true error is close to the apparent error

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Is this bound practical?

- The given bound (and others) is very loose
- The worst case scenario is assumed: objects can be randomly labeled
- In practice, features are chosen such that objects from one class are nicely clustered and can be separated from other classes

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Compactness hypothesis

Representations of real world objects are close.
There is no ground for any generalization on representations that do not obey this demand.

A.G. Arkadev and E.M.Braverman,
Computers and Pattern Recognition, 1966

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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:

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

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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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Derivative of norm

- What is $\frac{1}{2}\frac{\partial \|\mathbf{w}\|^2}{\partial \mathbf{w}}$?
- Well, first $\frac{1}{2}\|\mathbf{w}\|^2 = \frac{1}{2}\sum_{i=1}^{p} w_i^2$
- Take derivative w.r.t. one parameter:

$$\frac{1}{2}\frac{\partial \|\mathbf{w}\|^2}{\partial w_1} = w_1 \qquad \frac{1}{2}\frac{\partial \|\mathbf{w}\|^2}{\partial w_2} = w_2$$

- In vector notation: $\frac{1}{2}\frac{\partial \|\mathbf{w}\|^2}{\partial \mathbf{w}} = \mathbf{w}$

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Derivative of inner product

- What is $\frac{\partial \mathbf{w}^T \mathbf{x}_i}{\partial \mathbf{w}}$?
- Write it out:

$$\frac{\partial}{\partial w_1}(\mathbf{w}^T \mathbf{x}_i) = \frac{\partial}{\partial w_1}\left(\sum_{j=1}^{N} w_j x_{ij}\right)$$

$$= \frac{\partial}{\partial w_1}(w_1 x_{i1}) = x_1$$

- Also for other w_j
- In vector notation:

$$\frac{\partial \mathbf{w}^T \mathbf{x}_i}{\partial \mathbf{w}} = \mathbf{x}_i$$

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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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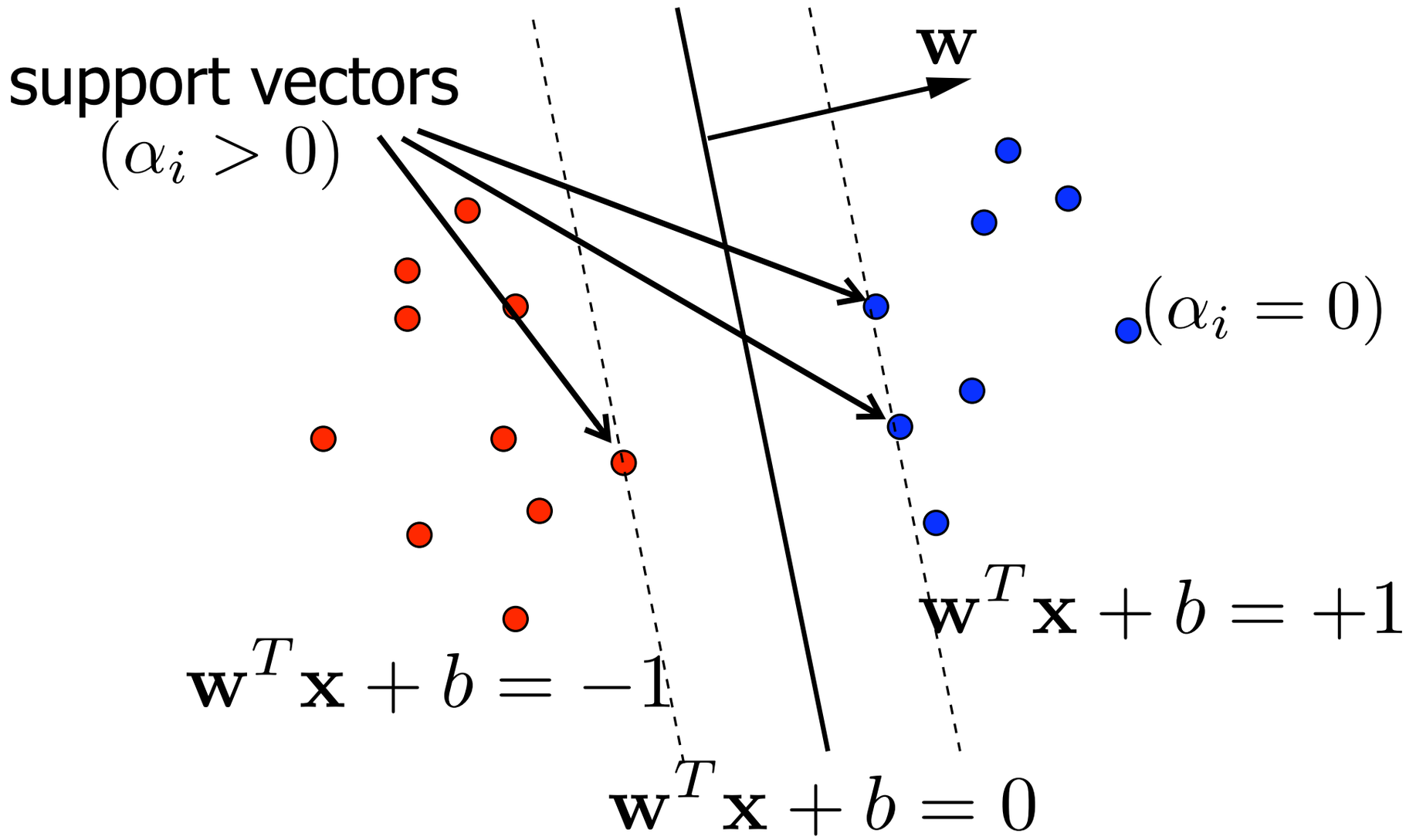
Support vector classifier



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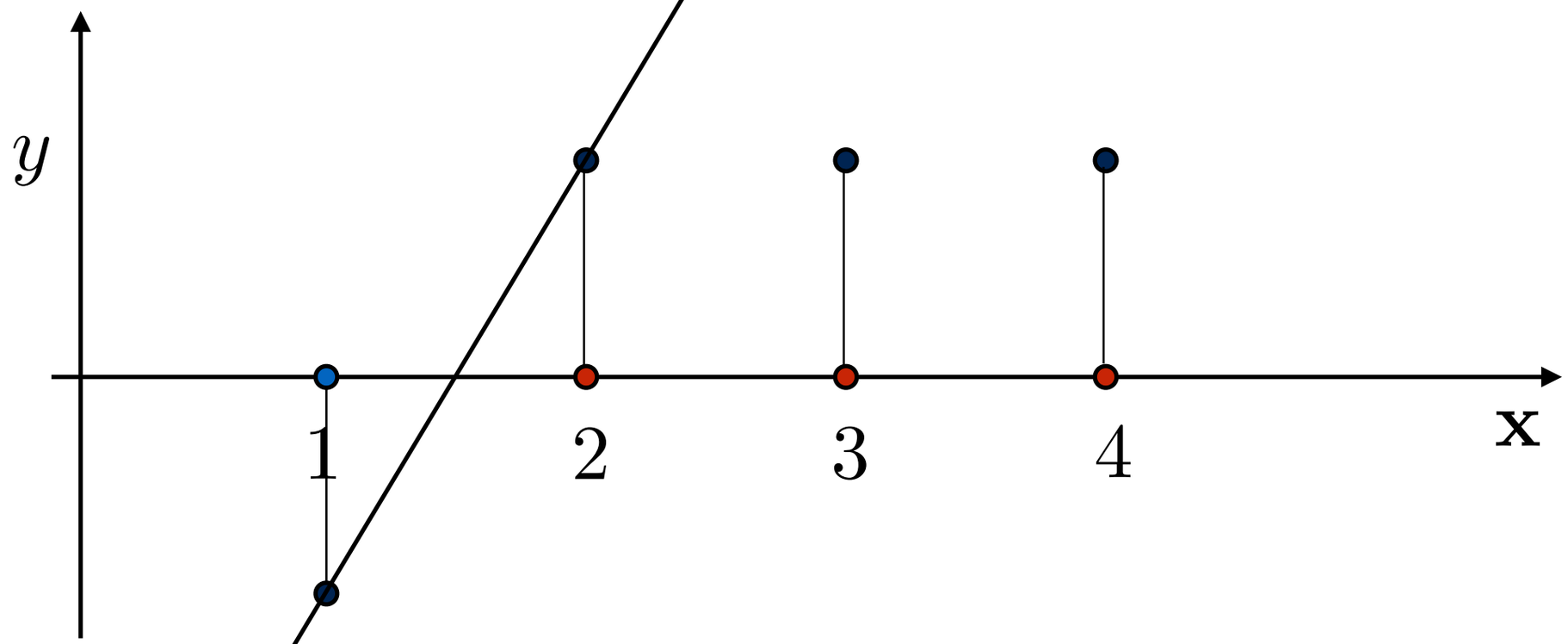
Use a linear classifier for:

$$y = \text{sign}(\mathbf{w}^T \mathbf{x} + w_0)$$

- What are the optimal **w** and w_0?



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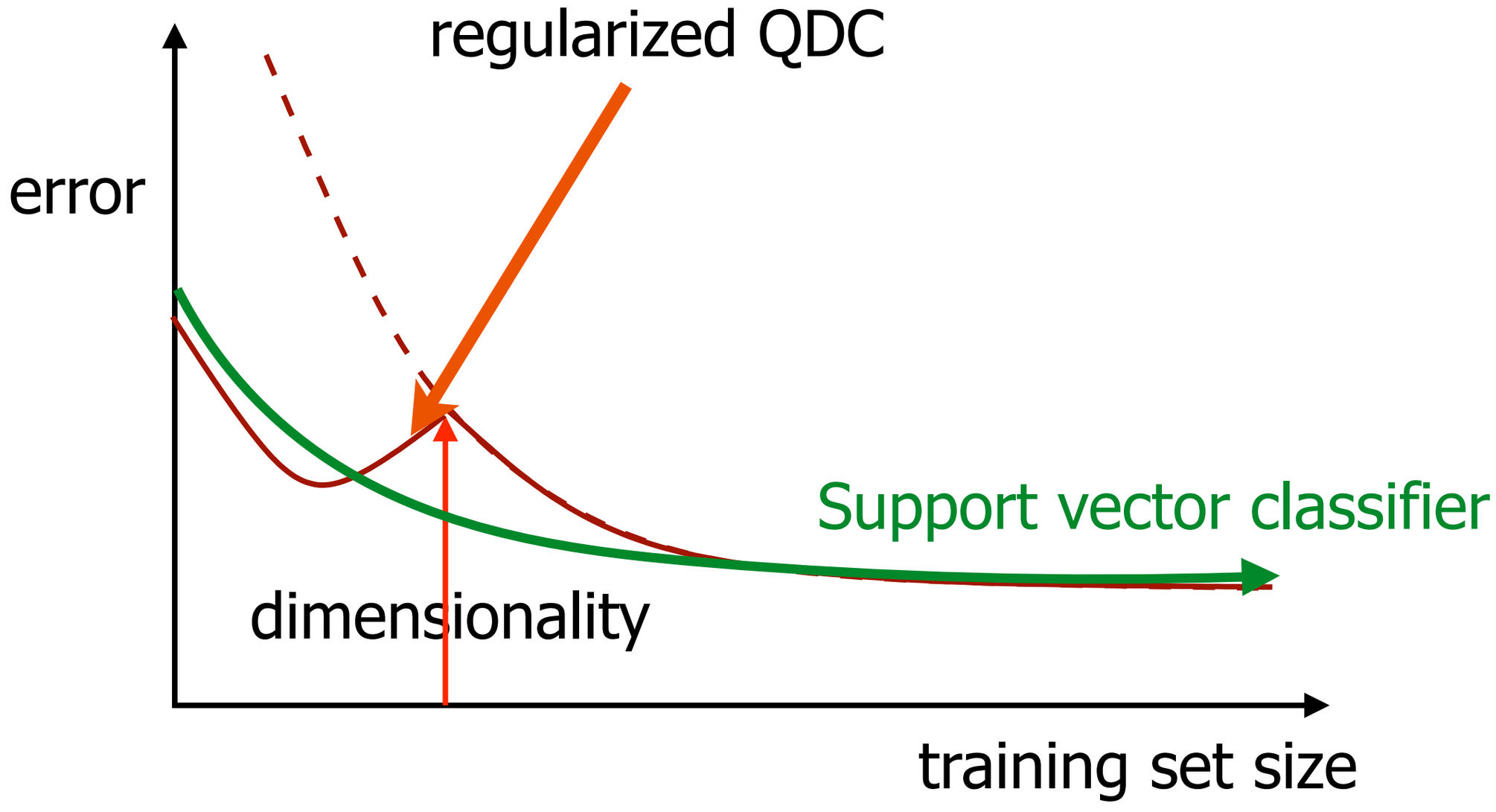
Quadratic classifier vs. SVC



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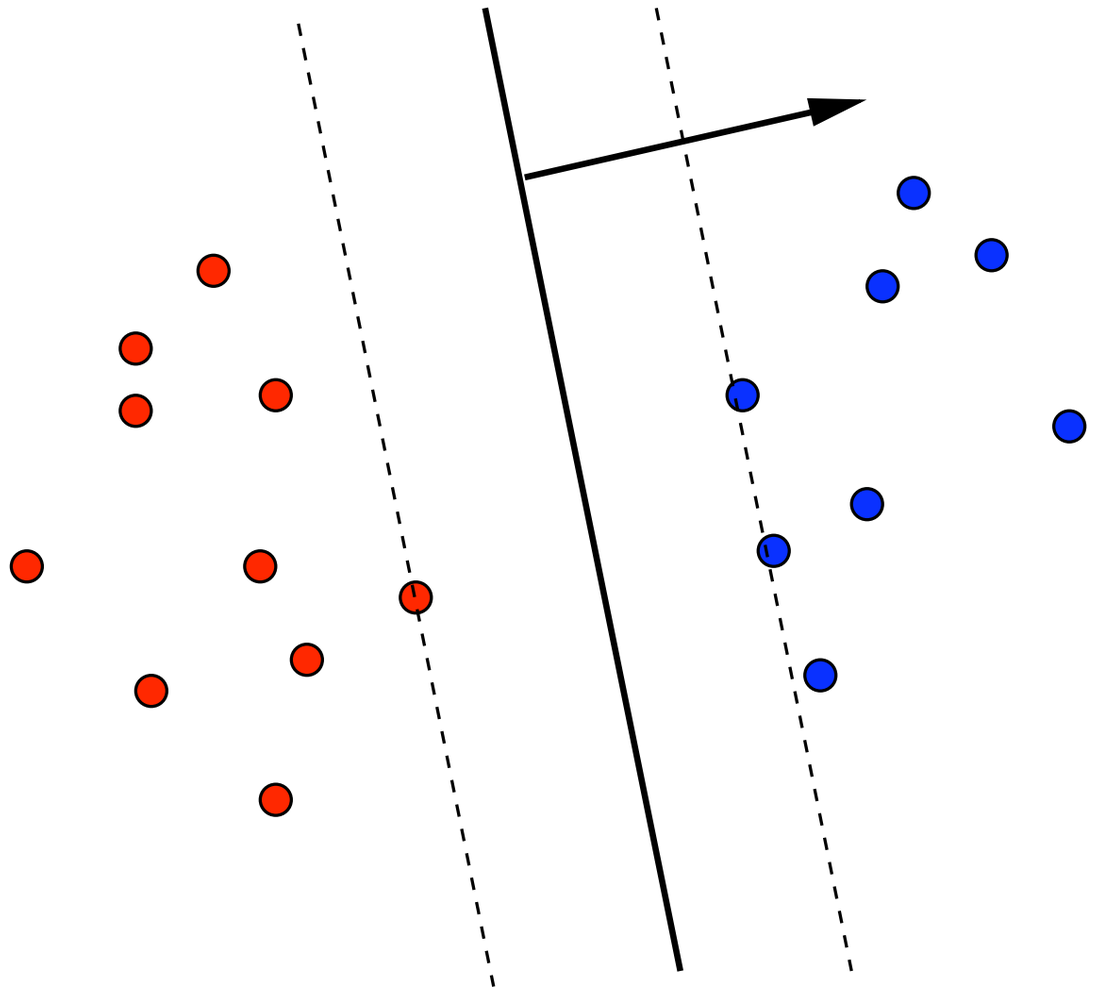
LOO Error estimation



Estimate the Leave-One-Out error on this data…

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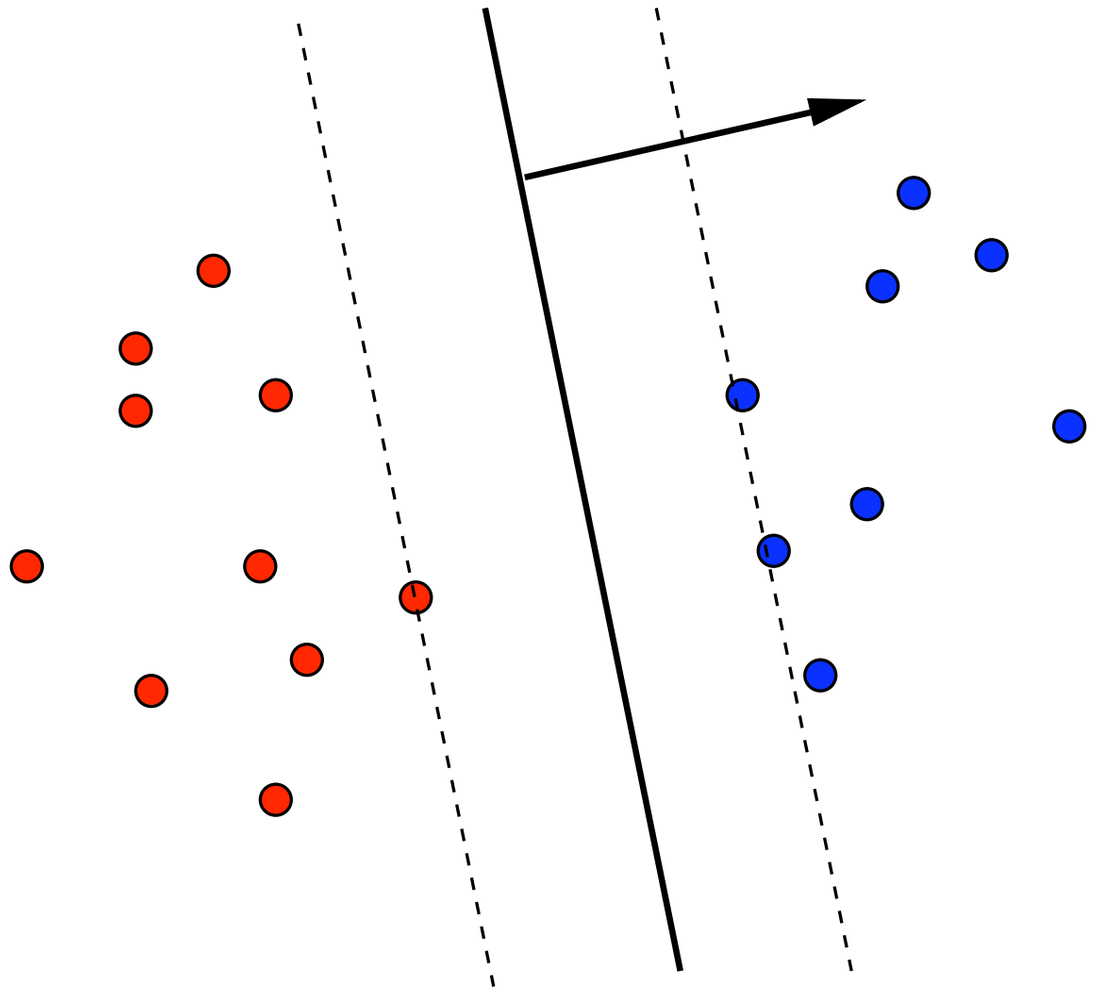
Error estimation



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

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

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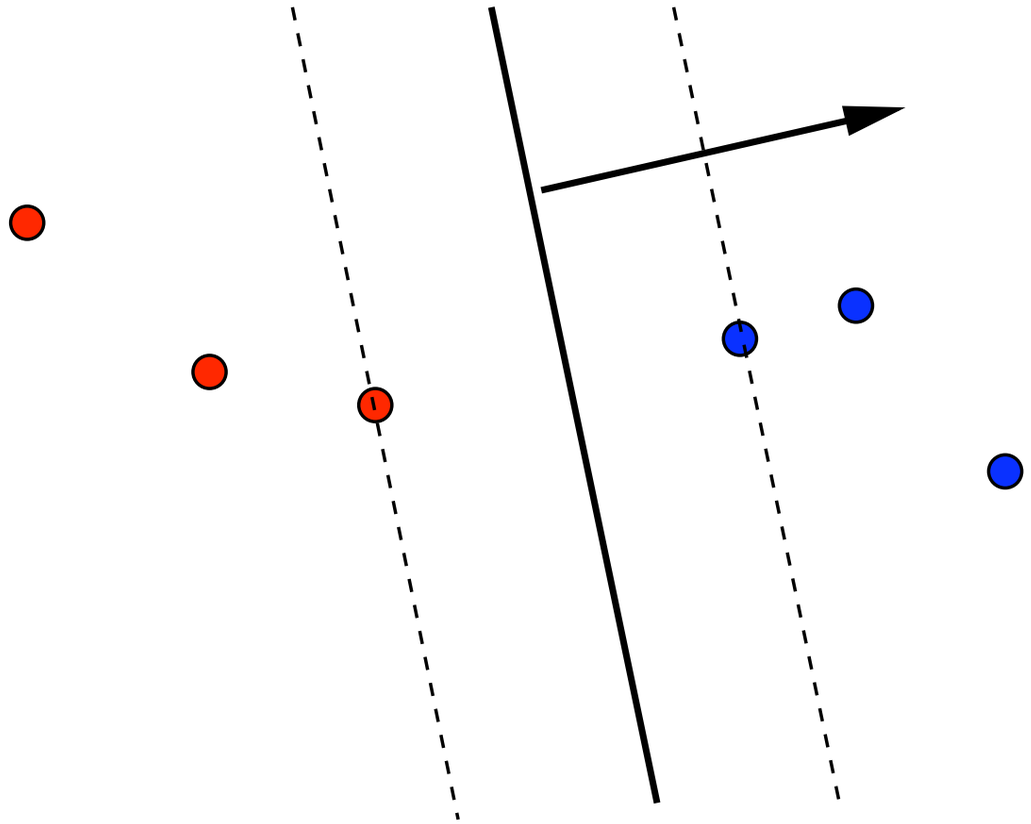
High dimensional feature spaces



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

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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...

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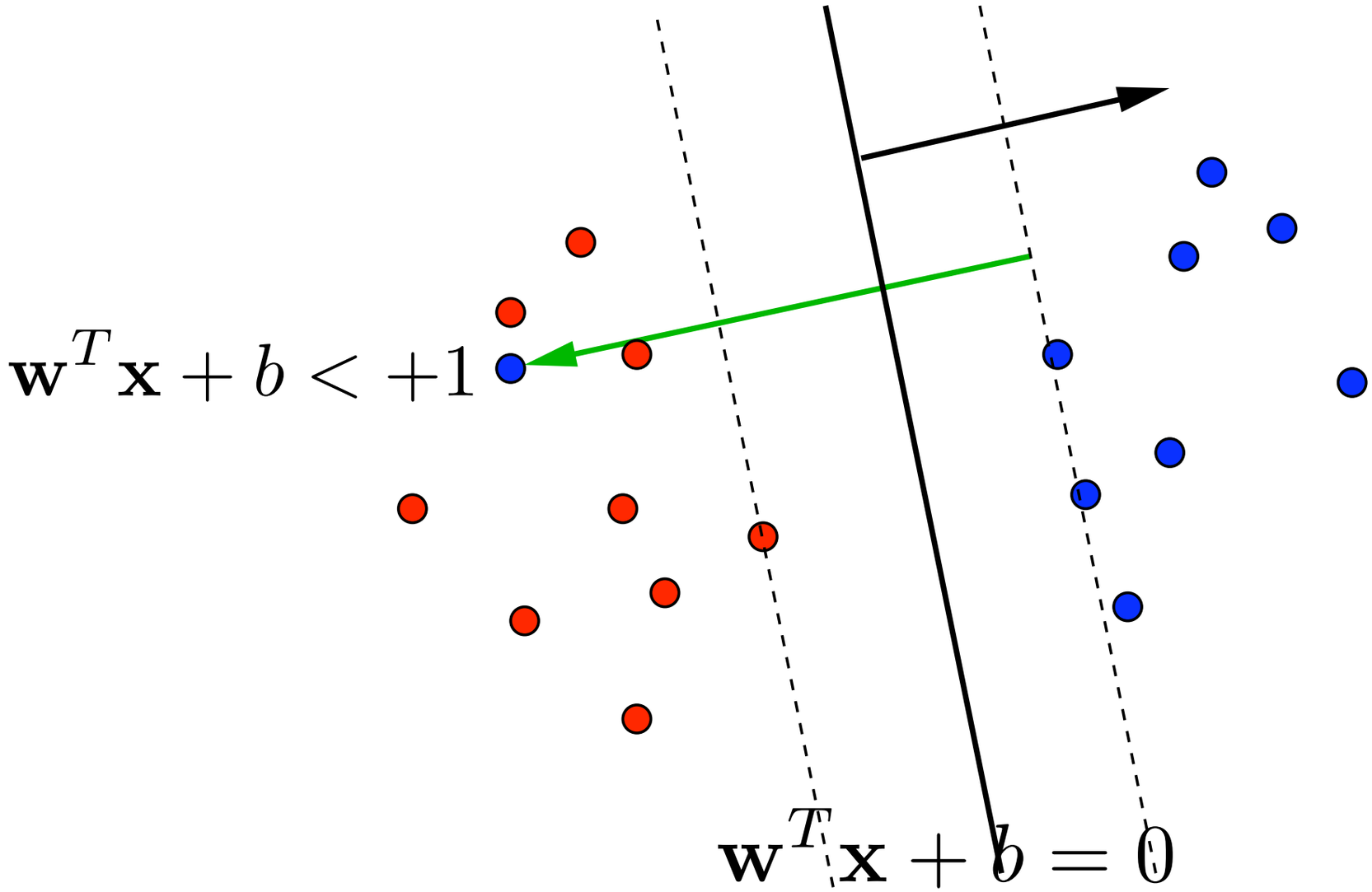
Problem 1



Classes should be separable

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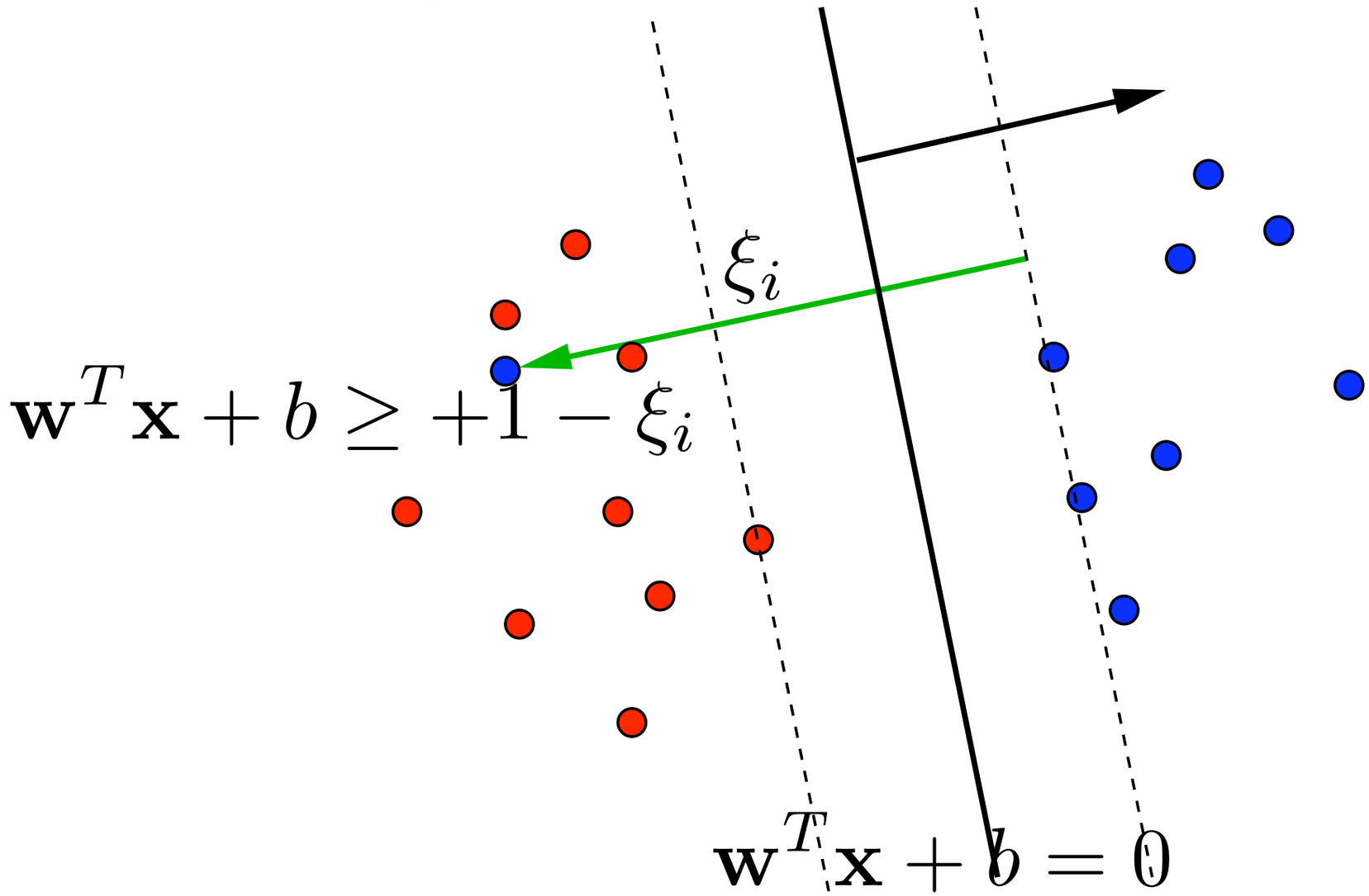
Weakening the constraints



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

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SVM with slacks

- The optimization changes into:

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

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

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

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

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Optimizing the classifier

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

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

$$0 \leq \alpha_i \leq C \quad \forall i$$

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

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

- Quadratic Programming Problem

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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.

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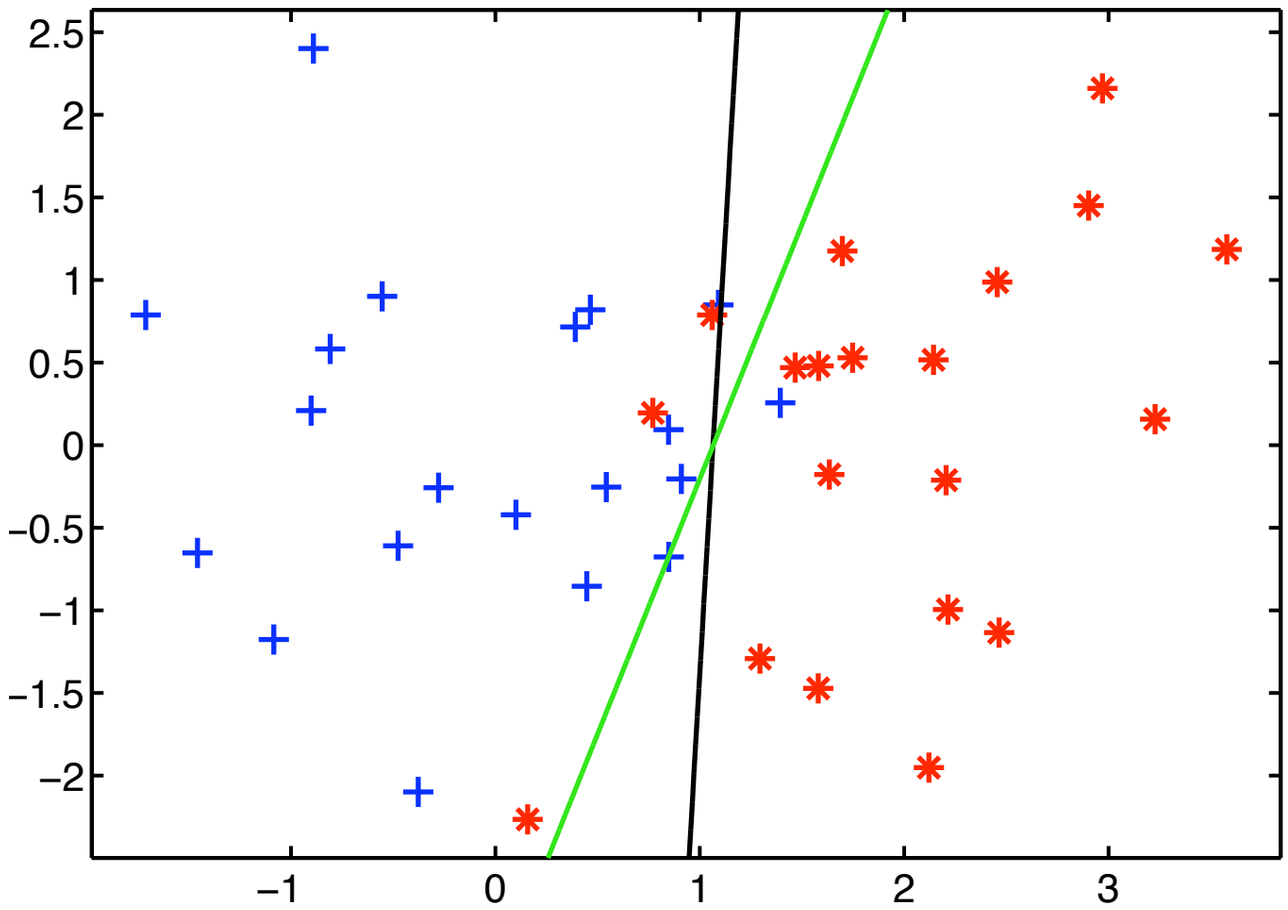
Influence of C



C=1

C=1000

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

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Problem 2

The decision boundary is only linear...

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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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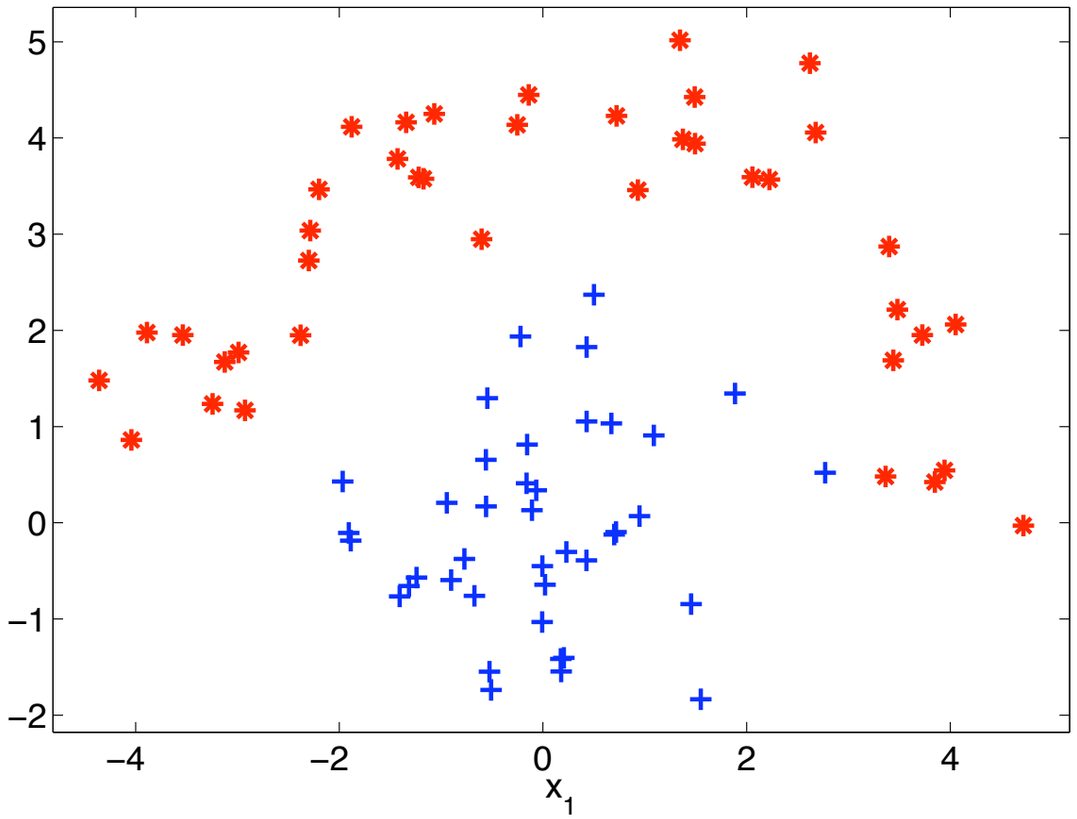
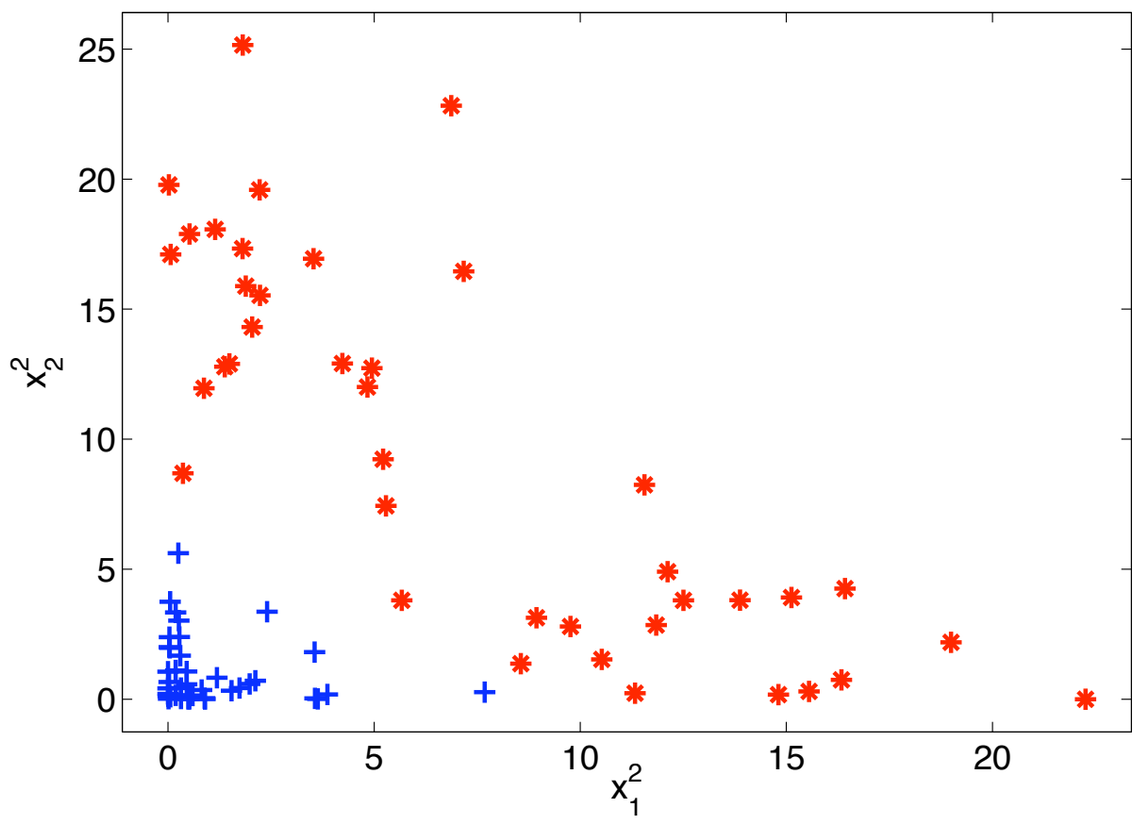
Example transformation





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

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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.

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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)

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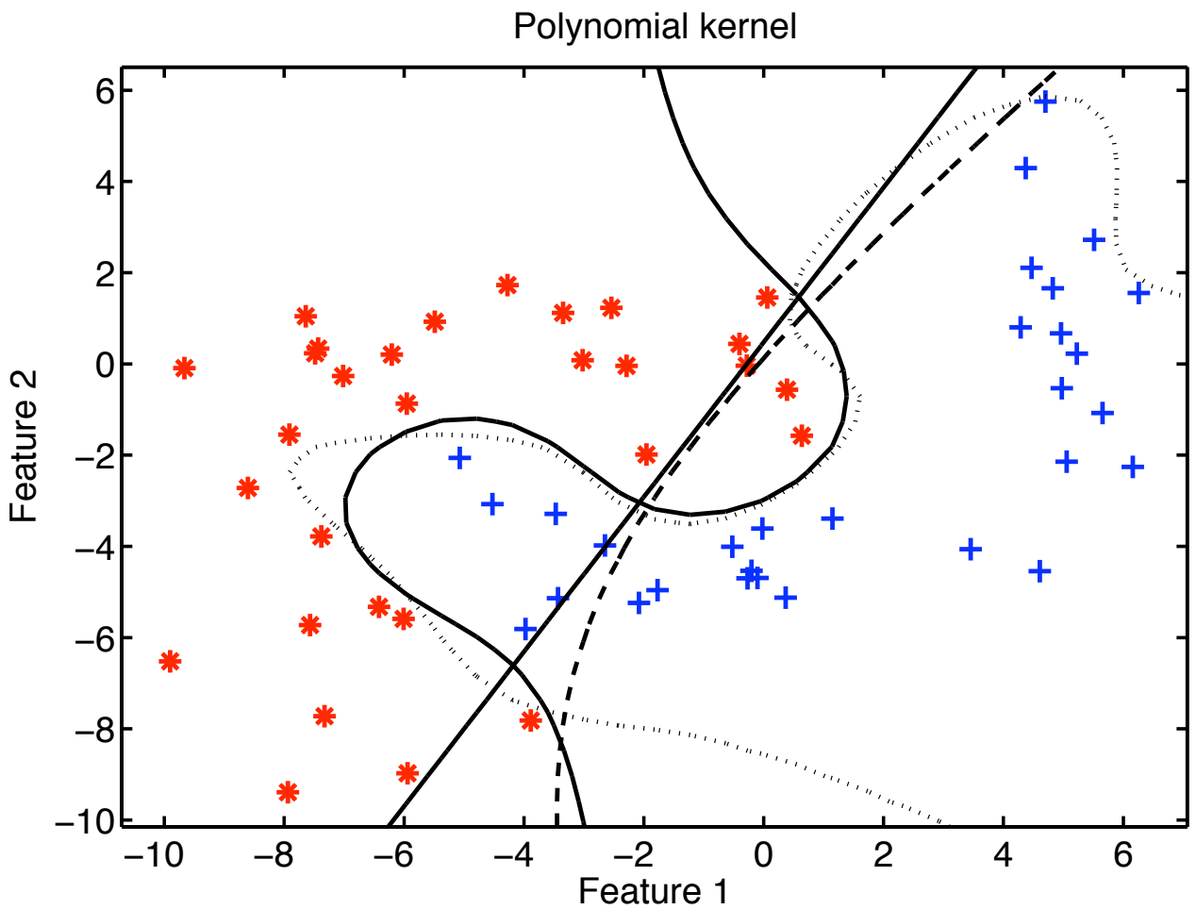
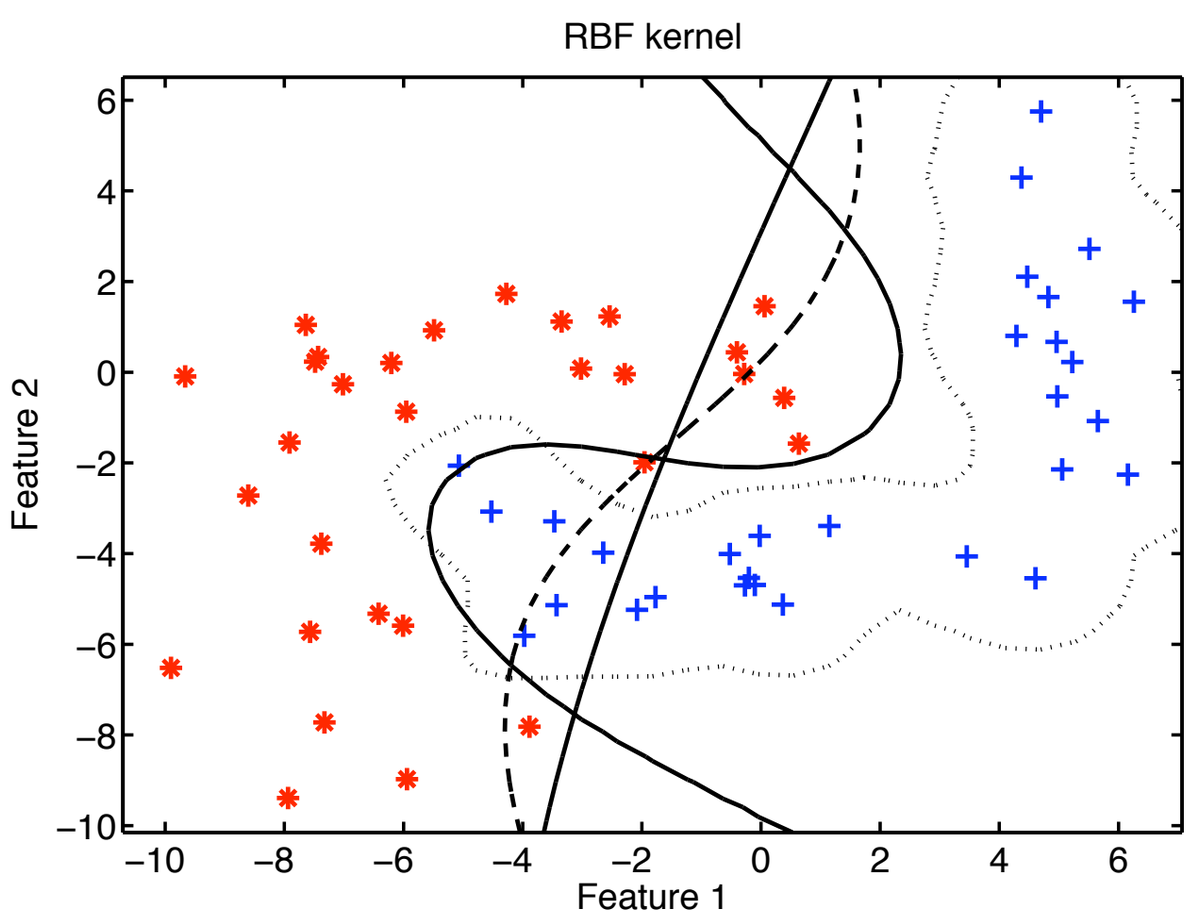
Popular kernel functions





$$K(\mathbf{x}, \mathbf{y}) = (\mathbf{x}^T \mathbf{y} + 1)^d$$

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

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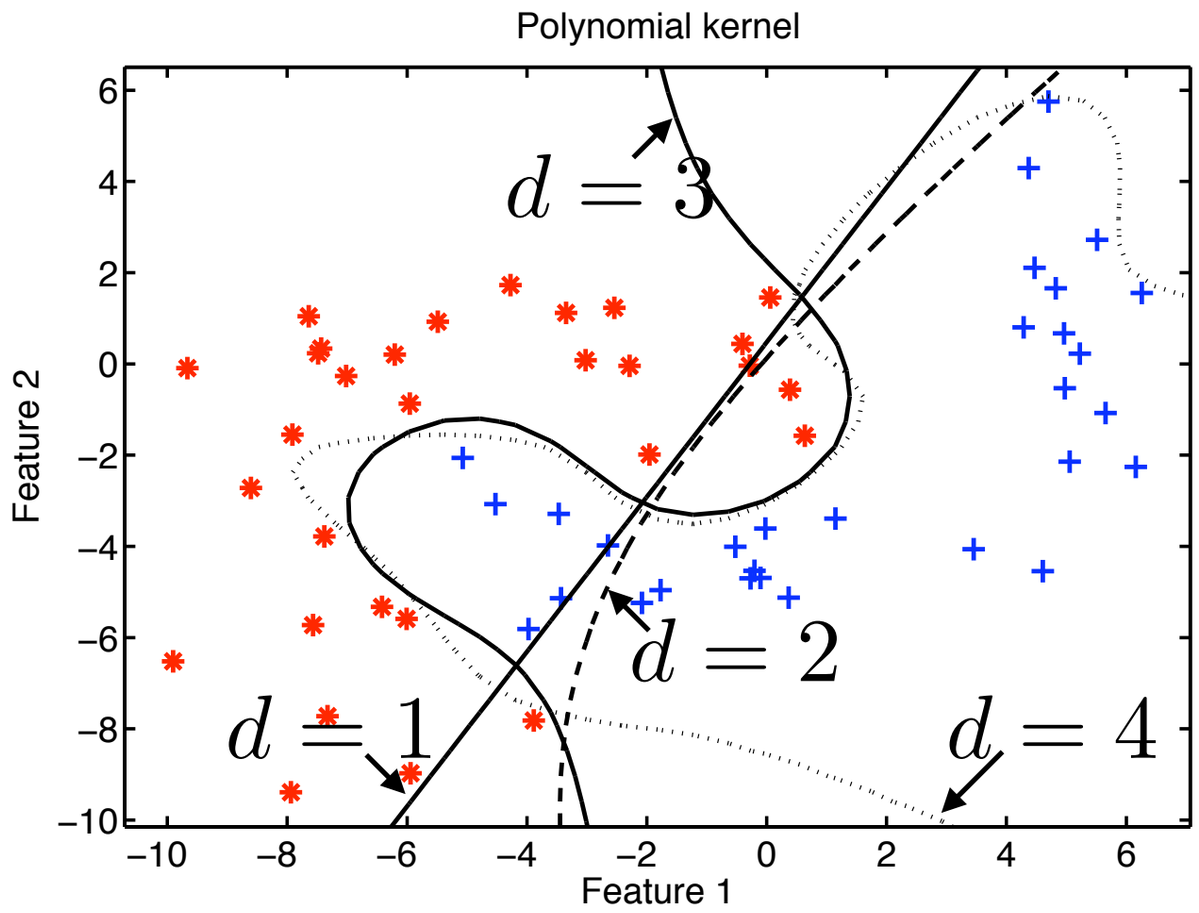
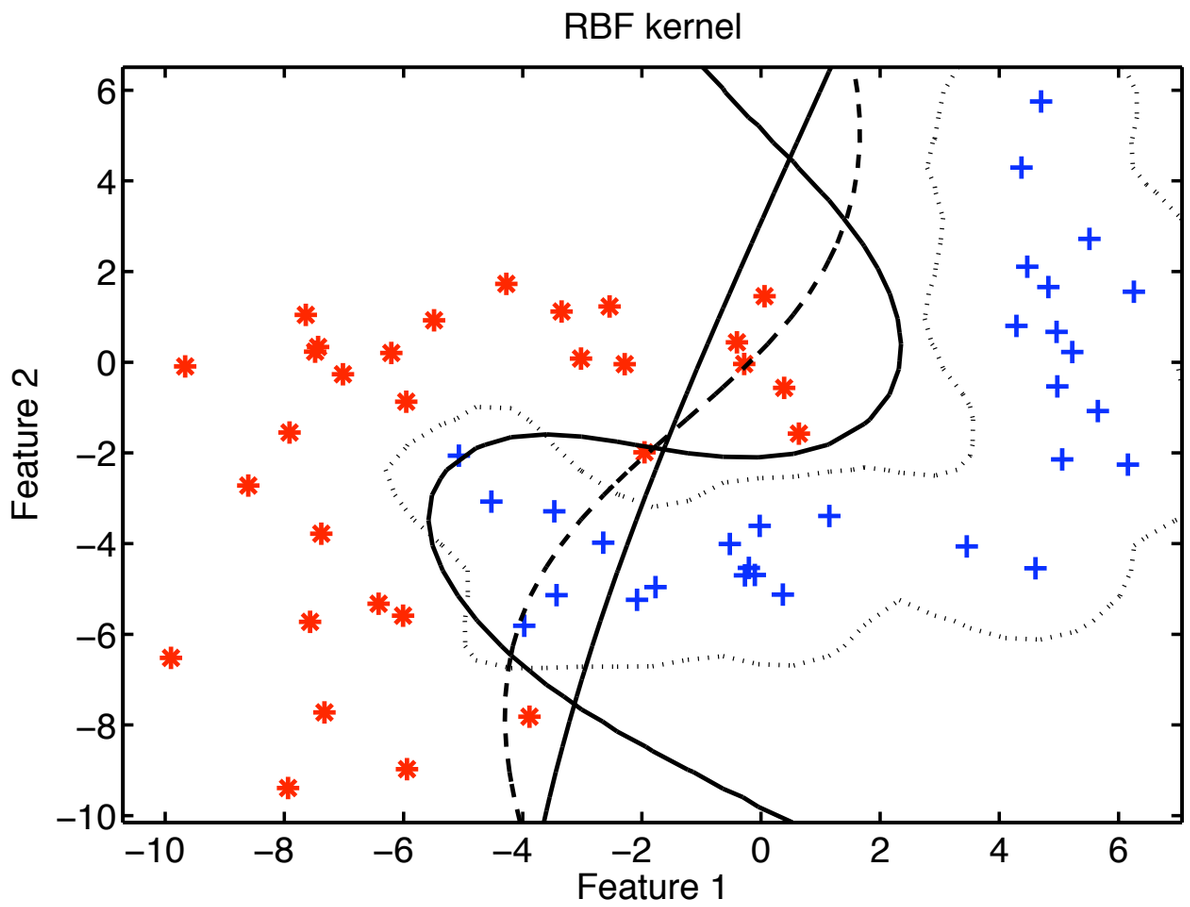
Popular kernel functions





$$K(\mathbf{x}, \mathbf{y}) = (\mathbf{x}^T \mathbf{y} + 1)^d$$

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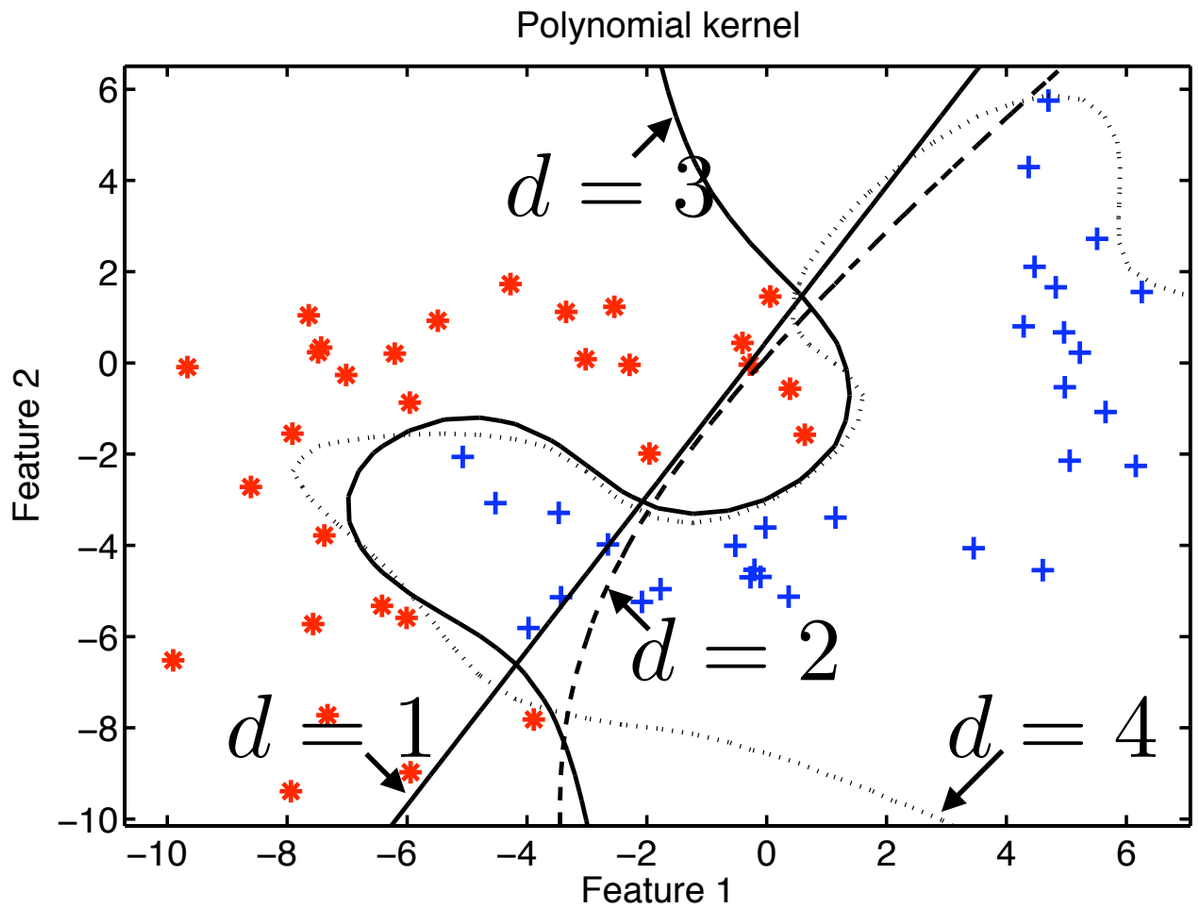
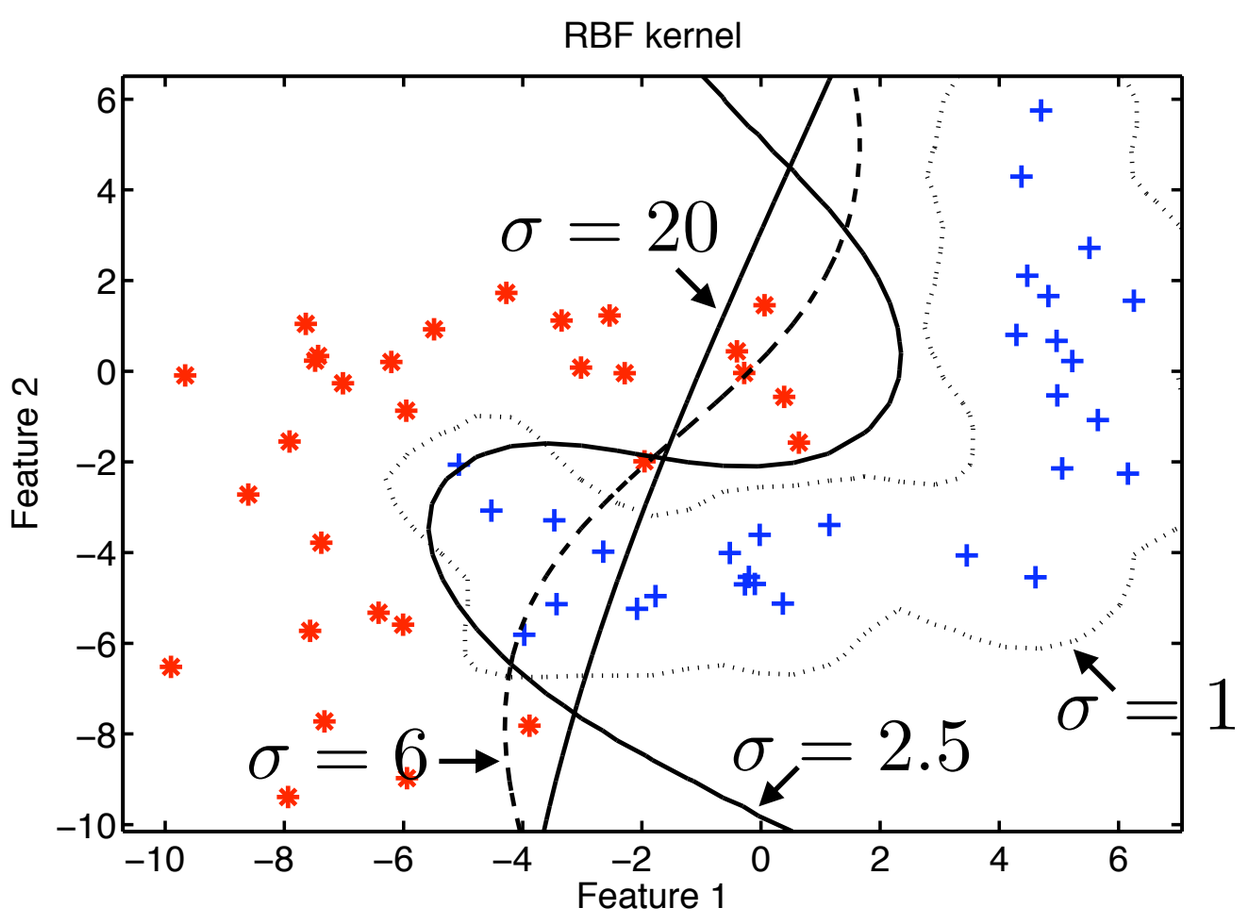
Popular kernel functions





$$K(\mathbf{x}, \mathbf{y}) = (\mathbf{x}^T \mathbf{y} + 1)^d$$

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

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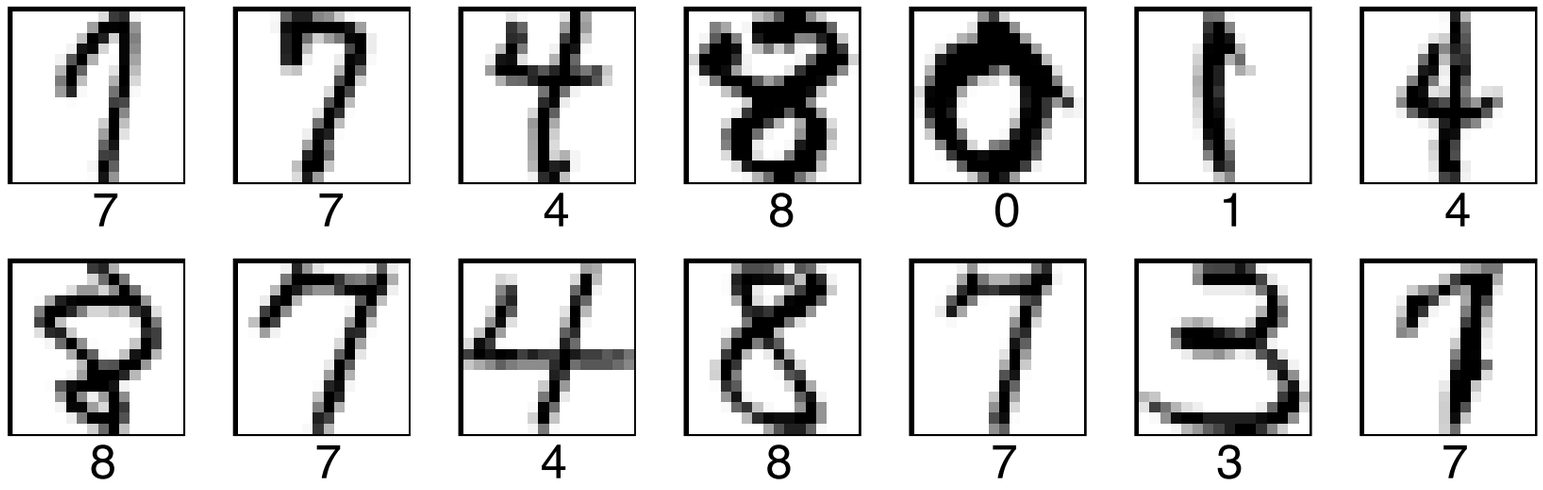
Results



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	$\sim 1 \times 10^{16}$

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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
  - …

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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)

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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...)

- 'Avoid solving a more general intermediate problem, when you have limited data' can be implemented by the SVM: no need to estimate (class-) densities

- The SVM can be used in almost all applications (by adjusting K and C appropriately)

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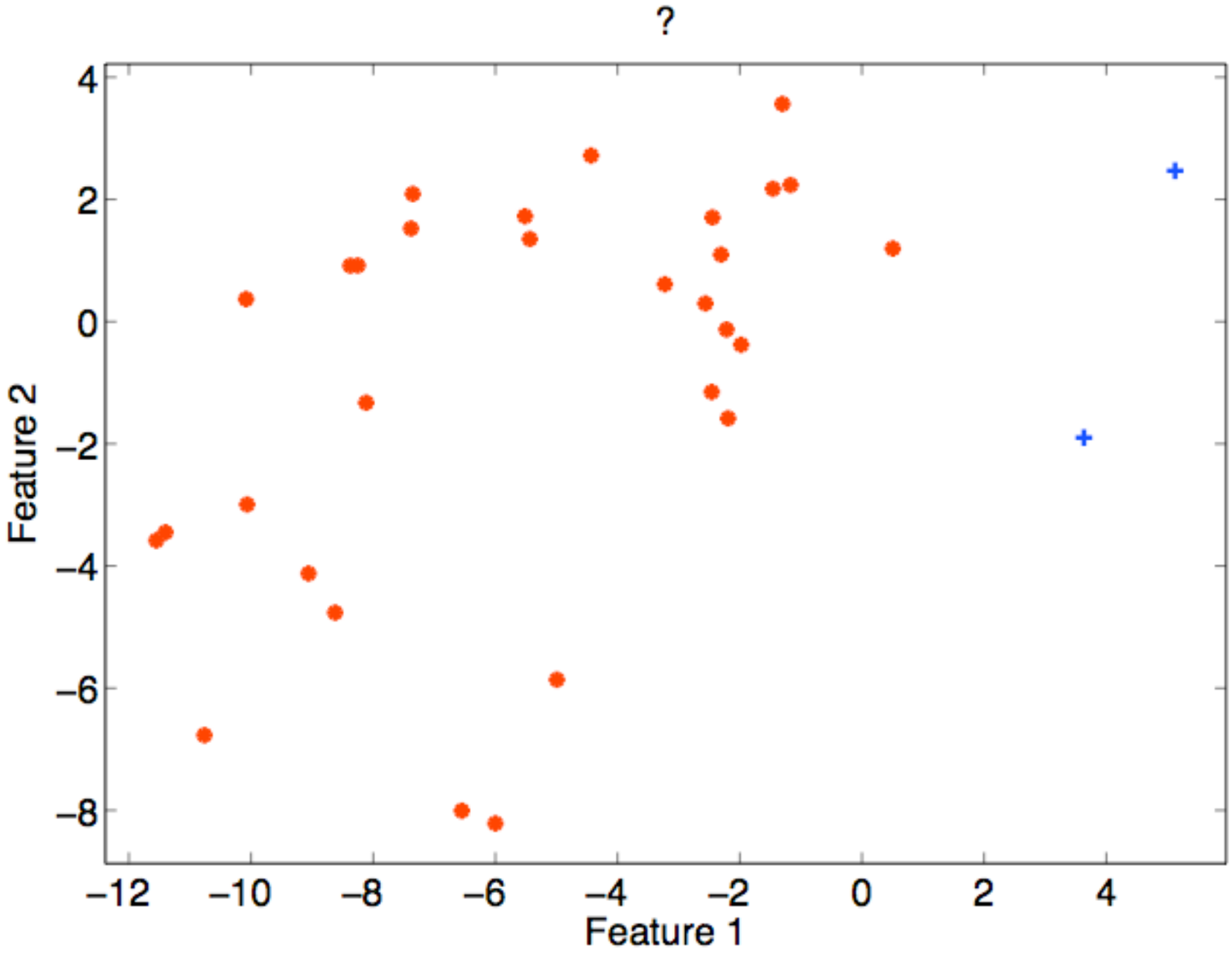
Classification problem

BONUS



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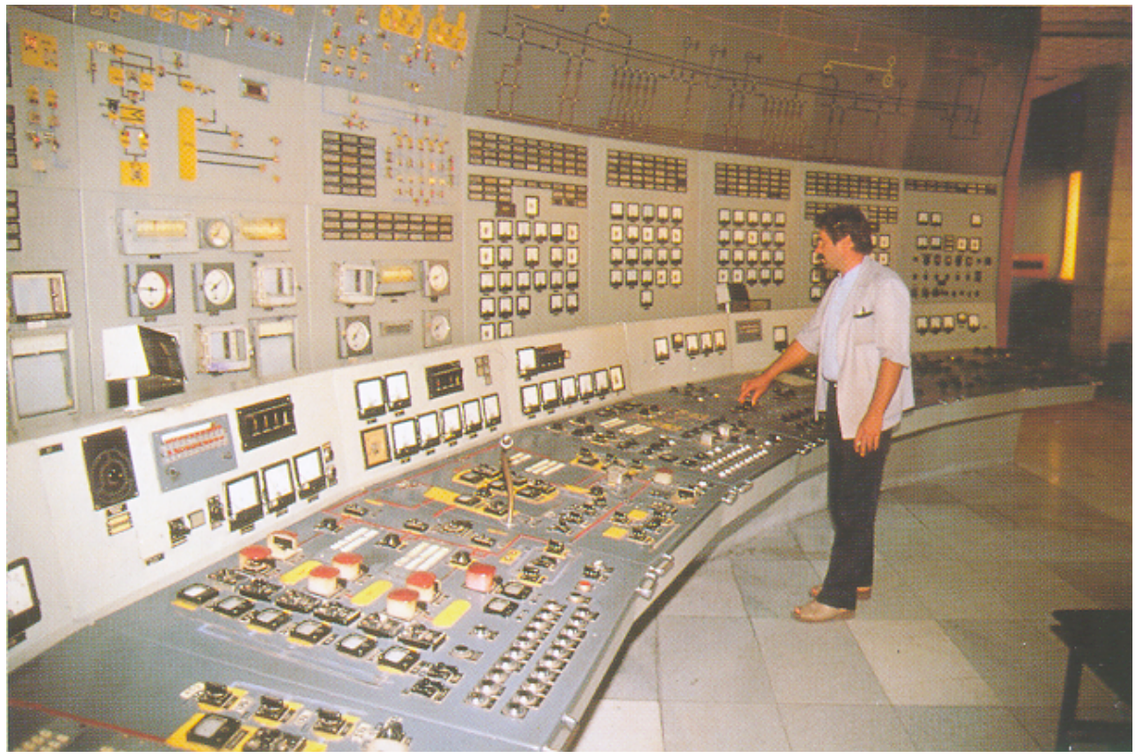
One-class classification



- 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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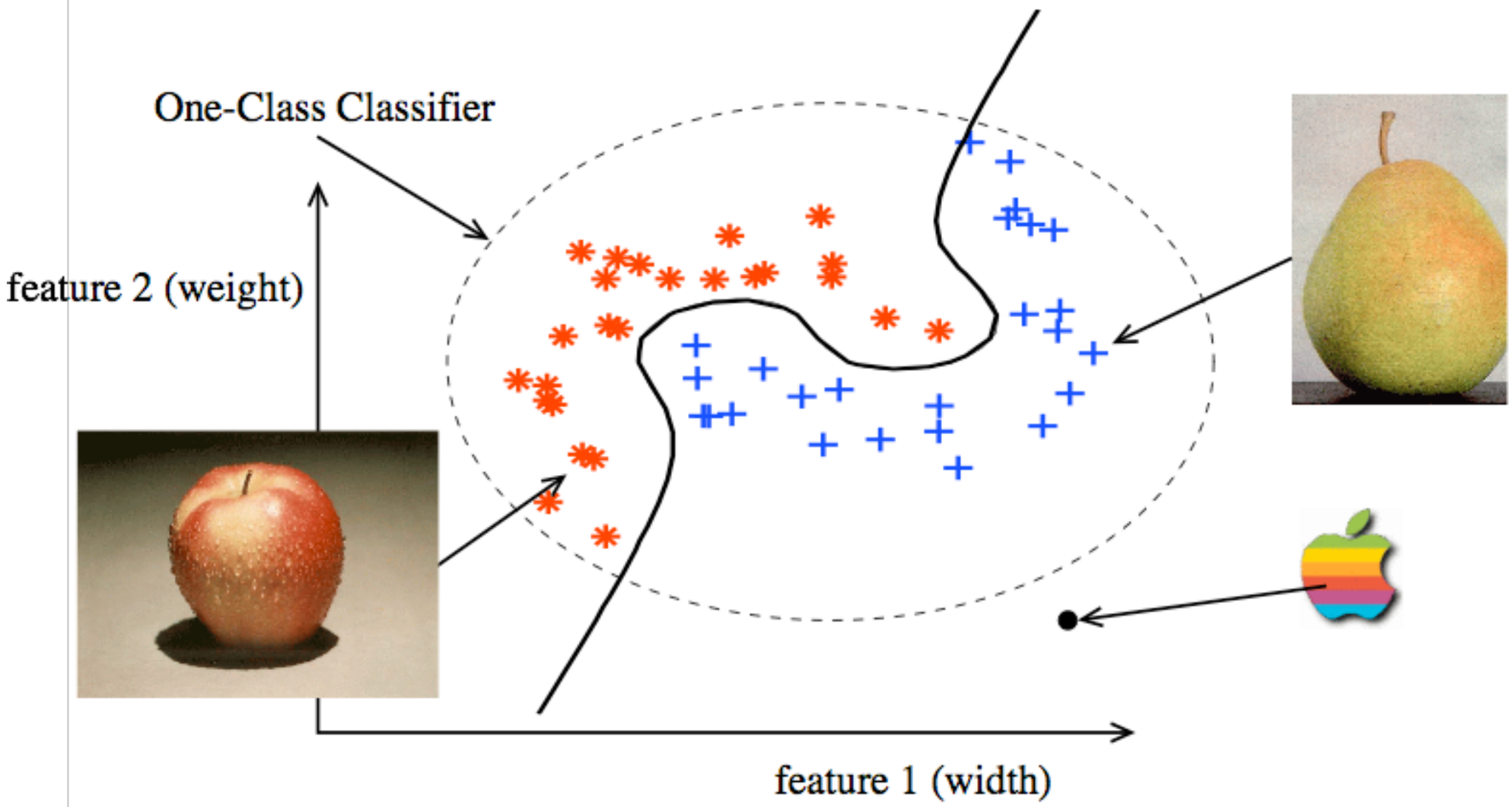
One-class classification



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

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From classifiers to outlier detection

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

generative classifiers:

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

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

discriminative classifiers:

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

?

- Outlier detection without density estimation?

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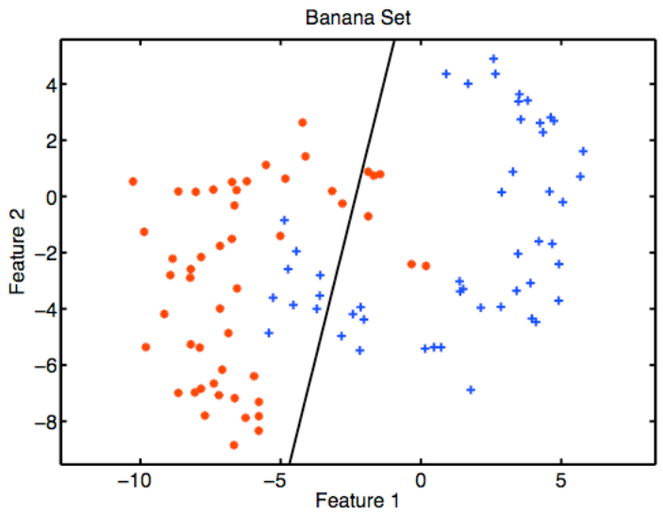
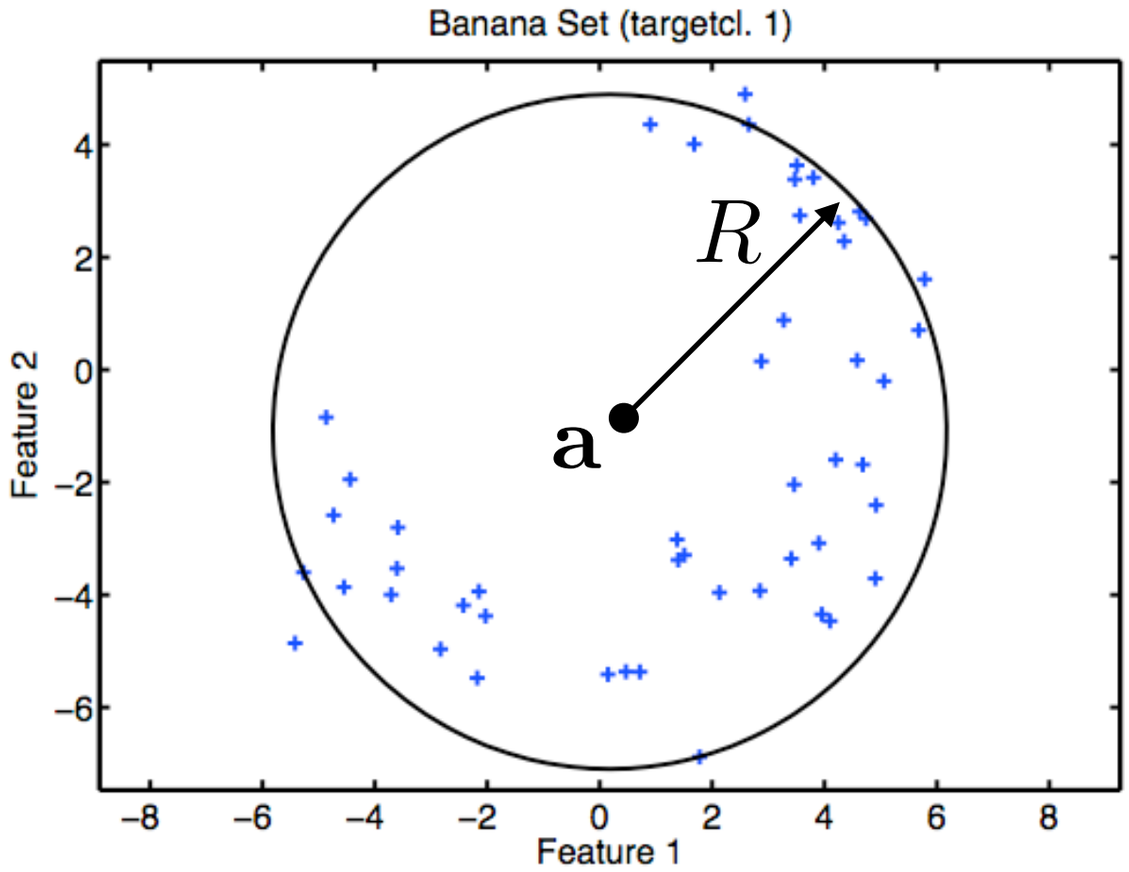
Decision boundary OCC





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

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Support Vector Data Description

	Support Vector cl.	**Support vector DD**
model	hyperplane $\mathbf{w}, b$	hypersphere $\mathbf{a}, R$
complexity	$\|\mathbf{w}\|^2$	R^2
error	$\|\mathbf{w}\|^2 + C\sum_i \xi_i$	$R^2 + C\sum_i \xi_i$
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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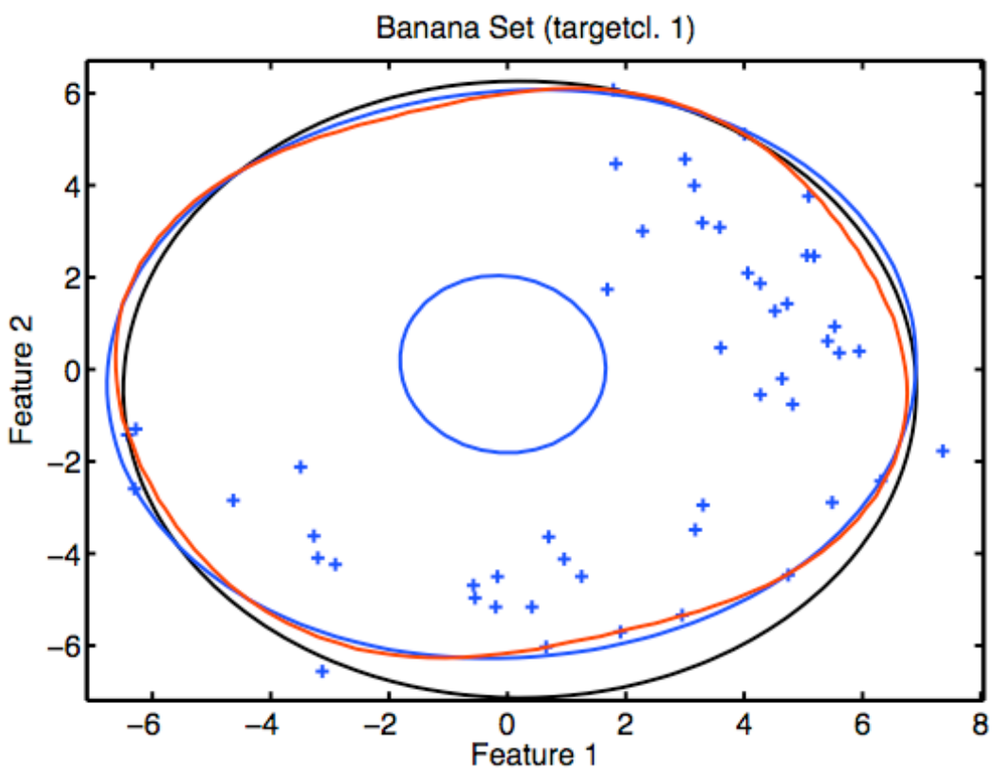
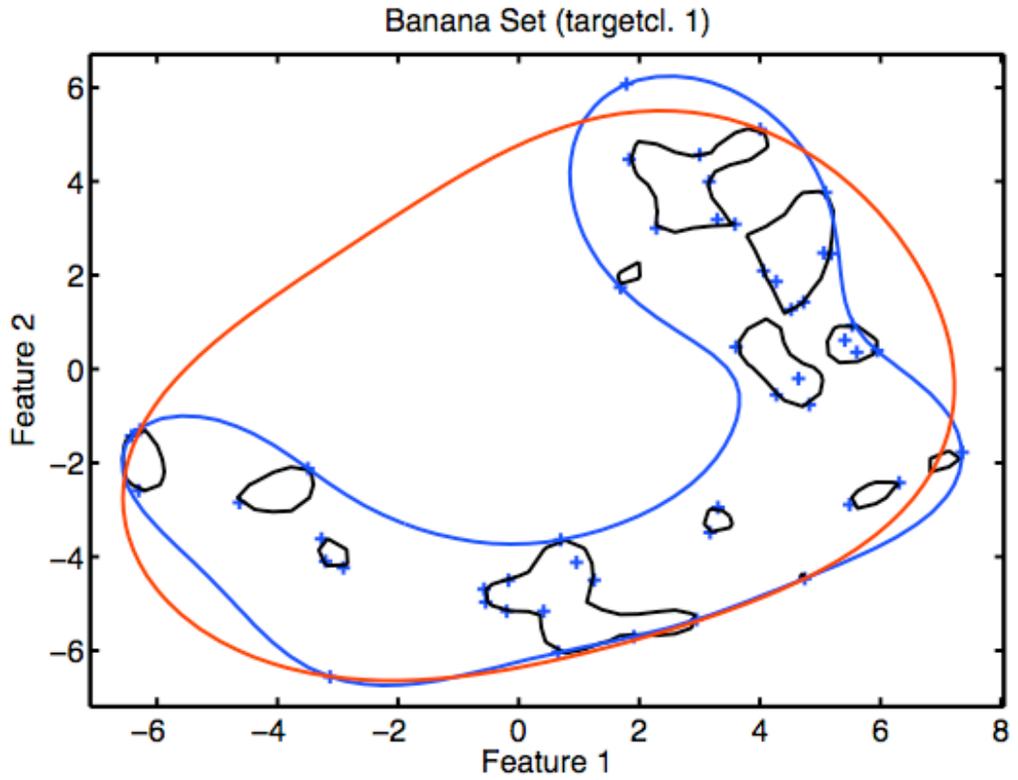
Different kernels





Polynomial

$$K(\mathbf{z}, \mathbf{x}) = (\mathbf{x}^T \mathbf{z} + 1)^d$$

Radial basis (Gaussian)

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

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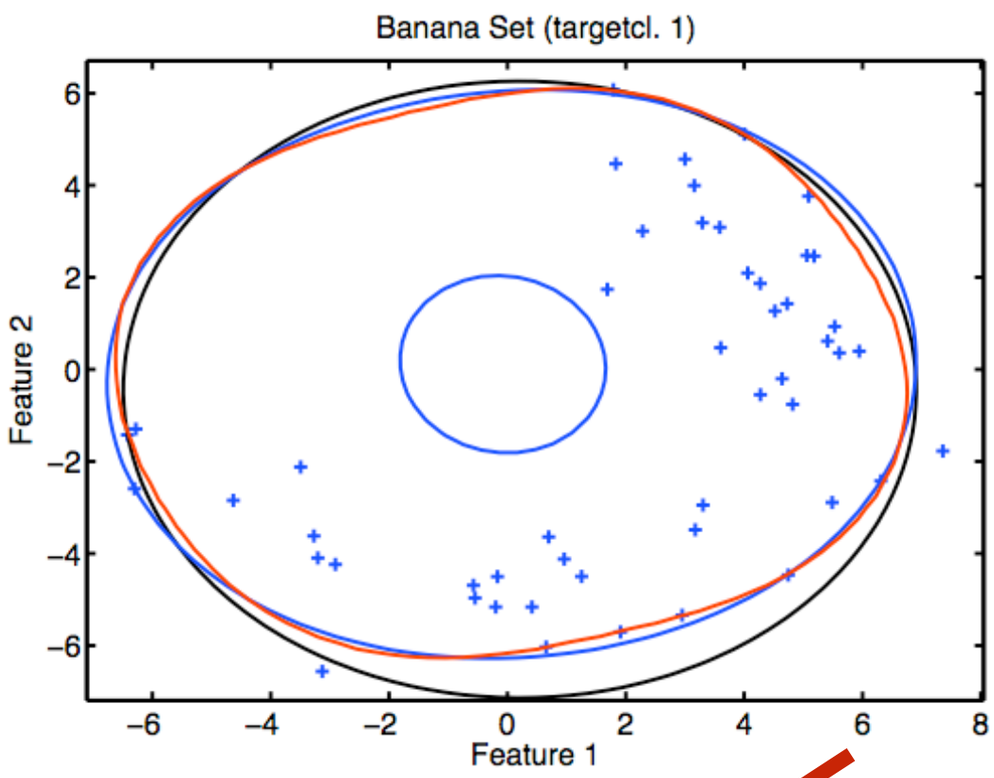
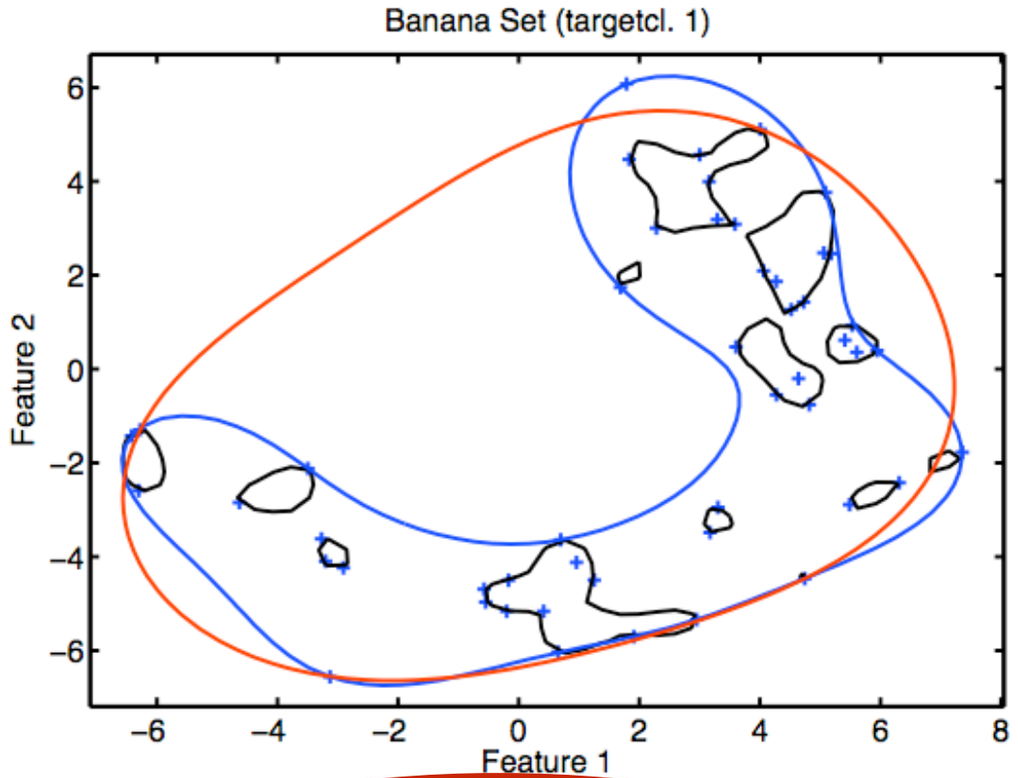
Different kernels





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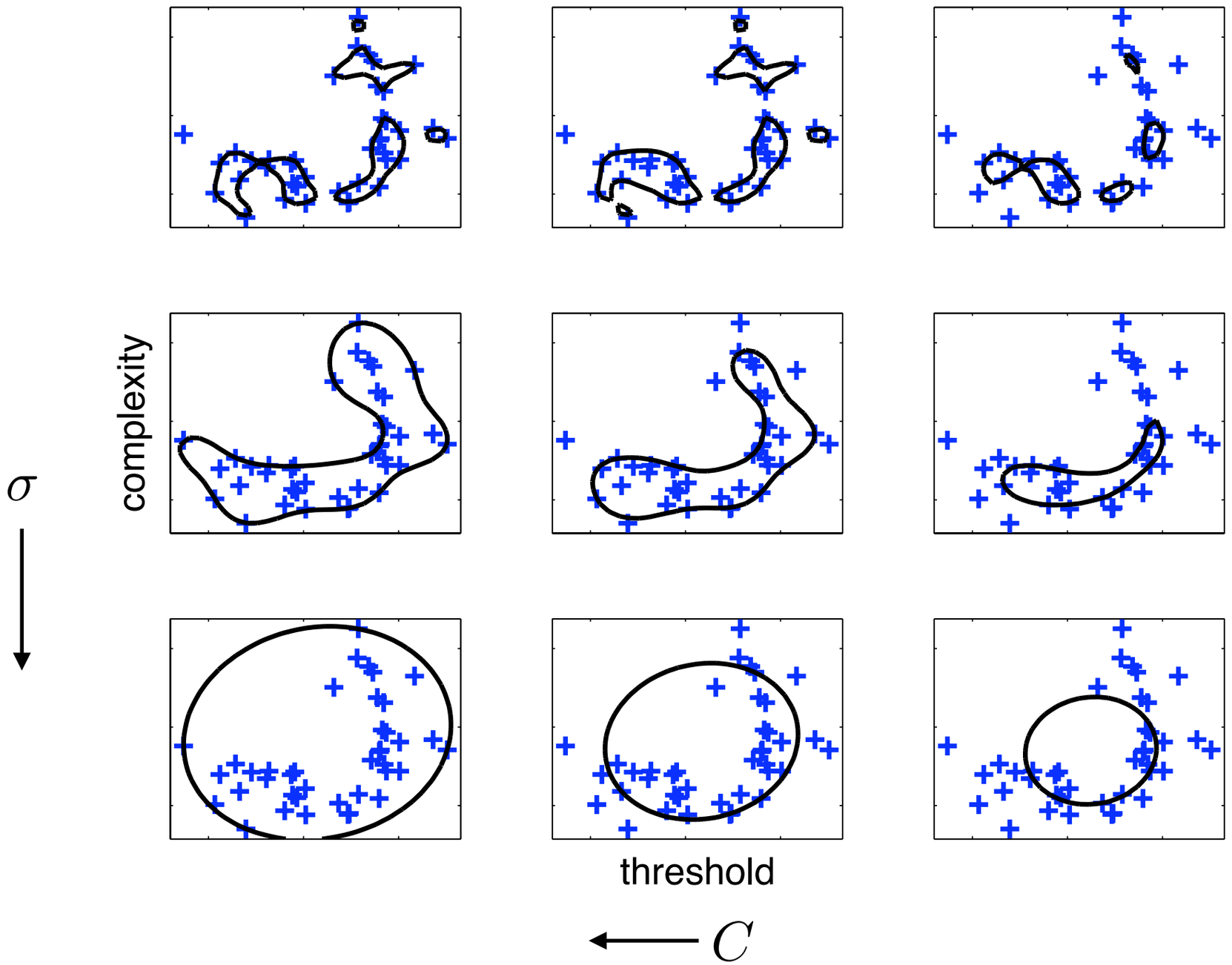
Complexity and threshold



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Bonus conclusions

- Avoiding density estimations is also useful in other applications (outlier detection, regression)
- Requires a formulation where (training data) only occurs in the form of inner products

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