



Lecture Slides for

INTRODUCTION TO

# Machine Learning

## 2nd Edition

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CHAPTER 13:

# Kernel Machines

# Kernel Machines

- Discriminant-based: No need to estimate densities first
- Define the discriminant in terms of support vectors
- The use of kernel functions, application-specific measures of similarity
- No need to represent instances as vectors
- Convex optimization problems with a unique solution

# Optimal Separating Hyperplane

$$\mathcal{X} = \{\mathbf{x}^t, r^t\}_t \text{ where } r^t = \begin{cases} +1 & \text{if } \mathbf{x}^t \in C_1 \\ -1 & \text{if } \mathbf{x}^t \in C_2 \end{cases}$$

find  $\mathbf{w}$  and  $w_0$  such that

$$\mathbf{w}^T \mathbf{x}^t + w_0 \geq +1 \text{ for } r^t = +1$$

$$\mathbf{w}^T \mathbf{x}^t + w_0 \leq -1 \text{ for } r^t = -1$$

which can be rewritten as

$$r^t (\mathbf{w}^T \mathbf{x}^t + w_0) \geq +1$$

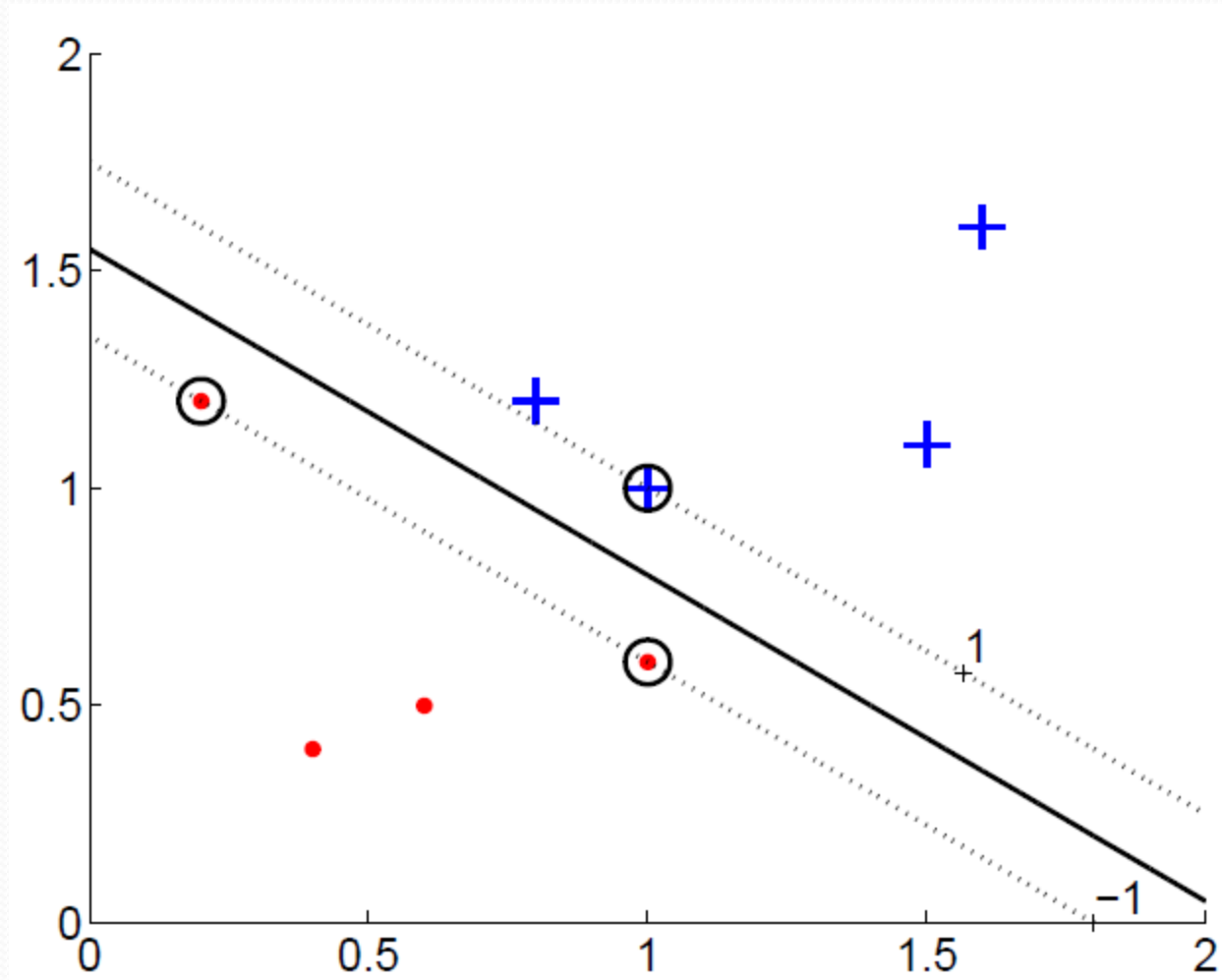
(Cortes and Vapnik, 1995; Vapnik, 1995)

# Margin

- Distance from the discriminant to the closest instances on either side
- Distance of  $\mathbf{x}$  to the hyperplane is  $\frac{|\mathbf{w}^T \mathbf{x}^t + w_0|}{\|\mathbf{w}\|}$
- We require  $\frac{r^t(\mathbf{w}^T \mathbf{x}^t + w_0)}{\|\mathbf{w}\|} \geq \rho, \forall t$
- For a unique sol'n, fix  $\rho \|\mathbf{w}\| = 1$ , and to max margin

$$\min \frac{1}{2} \|\mathbf{w}\|^2 \text{ subject to } r^t(\mathbf{w}^T \mathbf{x}^t + w_0) \geq +1, \forall t$$

# Margin



$$\min \frac{1}{2} \|\mathbf{w}\|^2 \text{ subject to } r^t (\mathbf{w}^T \mathbf{x}^t + w_0) \geq +1, \forall t$$

$$\begin{aligned} L_p &= \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{t=1}^N \alpha^t [r^t (\mathbf{w}^T \mathbf{x}^t + w_0) - 1] \\ &= \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{t=1}^N \alpha^t r^t (\mathbf{w}^T \mathbf{x}^t + w_0) + \sum_{t=1}^N \alpha^t \end{aligned}$$

$$\frac{\partial L_p}{\partial \mathbf{w}} = 0 \Rightarrow \mathbf{w} = \sum_{t=1}^N \alpha^t r^t \mathbf{x}^t$$

$$\frac{\partial L_p}{\partial w_0} = 0 \Rightarrow \sum_{t=1}^N \alpha^t r^t = 0$$

$$\begin{aligned}
L_d &= \frac{1}{2}(\mathbf{w}^T \mathbf{w}) - \mathbf{w}^T \sum_t \alpha^t r^t \mathbf{x}^t - w_0 \sum_t \alpha^t r^t + \sum_t \alpha^t \\
&= -\frac{1}{2}(\mathbf{w}^T \mathbf{w}) + \sum_t \alpha^t \\
&= -\frac{1}{2} \sum_t \sum_s \alpha^t \alpha^s r^t r^s (\mathbf{x}^t)^T \mathbf{x}^s + \sum_t \alpha^t \\
&\text{subject to } \sum_t \alpha^t r^t = 0 \text{ and } \alpha^t \geq 0, \forall t
\end{aligned}$$

Most  $\alpha^t$  are 0 and only a small number have  $\alpha^t > 0$ ; they are the support vectors



# Soft Margin Hyperplane

- Not linearly separable

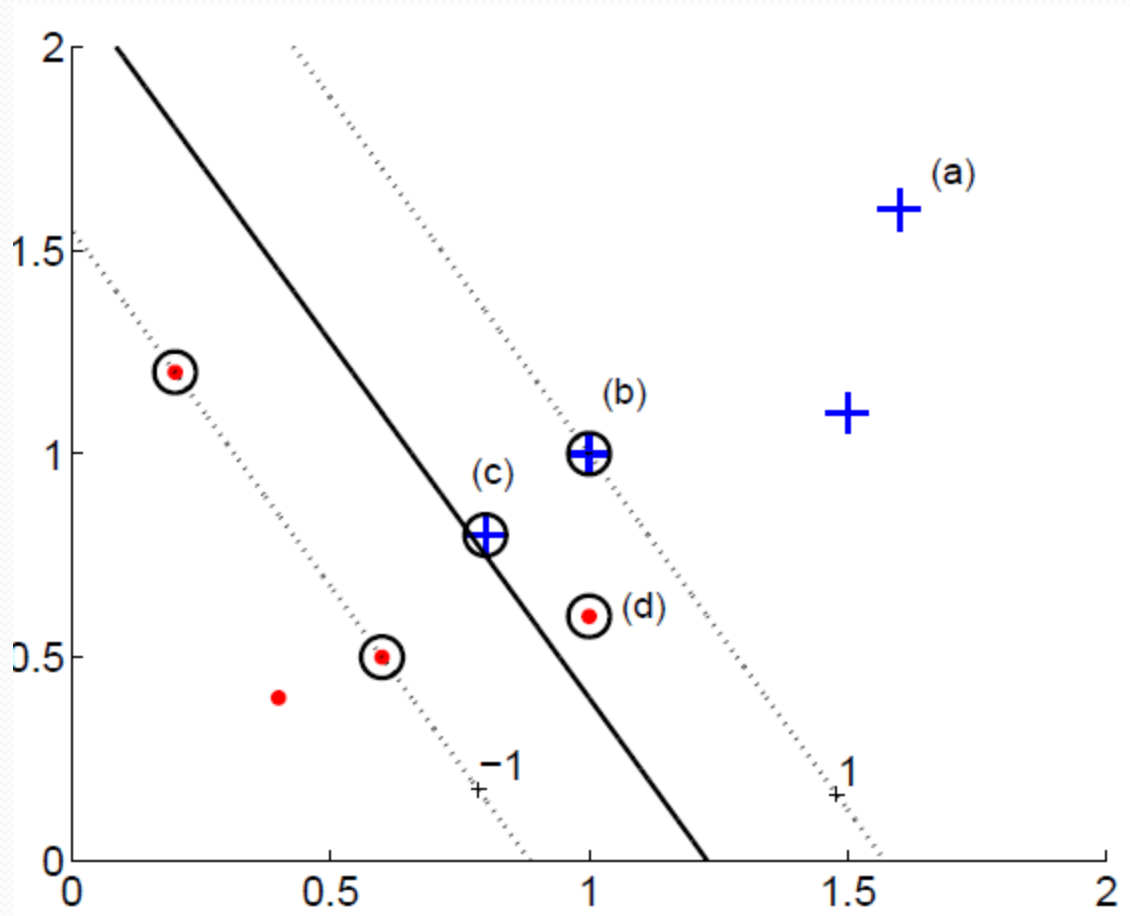
$$r^t(\mathbf{w}^T \mathbf{x}^t + w_0) \geq 1 - \xi^t$$

- Soft error

$$\sum_t \xi^t$$

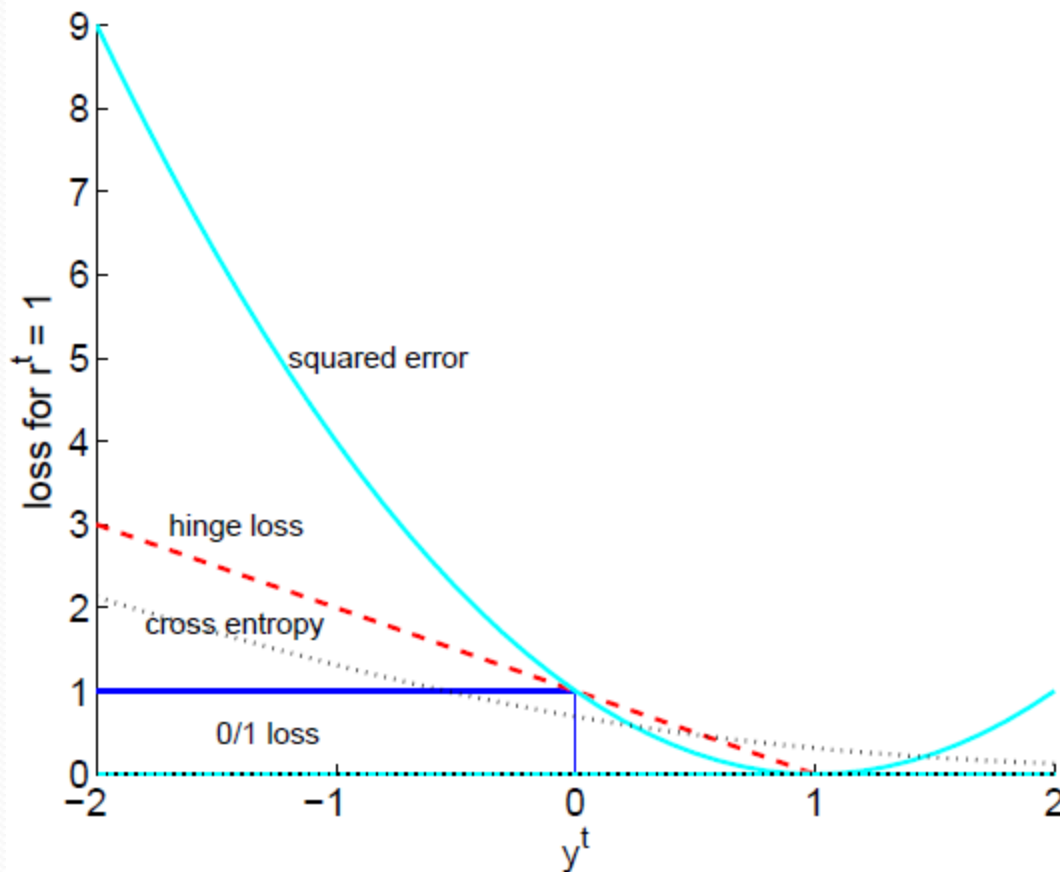
- New primal is

$$L_p = \frac{1}{2} \|\mathbf{w}\|^2 + c \sum_t \xi^t - \sum_t \alpha^t [r^t(\mathbf{w}^T \mathbf{x}^t + w_0) - 1 + \xi^t] - \sum_t \mu^t \xi^t$$



# Hinge Loss

$$L_{\text{hinge}}(y^t, r^t) = \begin{cases} 0 & \text{if } y^t r^t \geq 1 \\ 1 - y^t r^t & \text{otherwise} \end{cases}$$



# $\nu$ -SVM

$$\min \frac{1}{2} \|\mathbf{w}\|^2 - \nu \rho + \frac{1}{N} \sum_t \xi^t$$

subject to

$$r^t (\mathbf{w}^T \mathbf{x}^t + w_0) \geq \rho - \xi^t, \xi^t \geq 0, \rho \geq 0$$

$$L_d = -\frac{1}{2} \sum_{t=1}^N \sum_s \alpha^t \alpha^s r^t r^s (x^t)^T x^s$$

subject to

$$\sum_t \alpha^t r^t = 0, 0 \leq \alpha^t \leq \frac{1}{N}, \sum_t \alpha^t \geq \nu$$

*$\nu$  controls the fraction of support vectors*

# Kernel Trick

- Preprocess input  $\mathbf{x}$  by basis functions

$$\mathbf{z} = \boldsymbol{\varphi}(\mathbf{x})$$

$$g(\mathbf{z}) = \mathbf{w}^T \mathbf{z}$$

$$g(\mathbf{x}) = \mathbf{w}^T \boldsymbol{\varphi}(\mathbf{x})$$

- The SVM solution

$$\mathbf{w} = \sum_t \alpha^t r^t \mathbf{z}^t = \sum_t \alpha^t r^t \boldsymbol{\varphi}(\mathbf{x}^t)$$

$$g(\mathbf{x}) = \mathbf{w}^T \boldsymbol{\varphi}(\mathbf{x}) = \sum_t \alpha^t r^t \boldsymbol{\varphi}(\mathbf{x}^t)^T \boldsymbol{\varphi}(\mathbf{x})$$

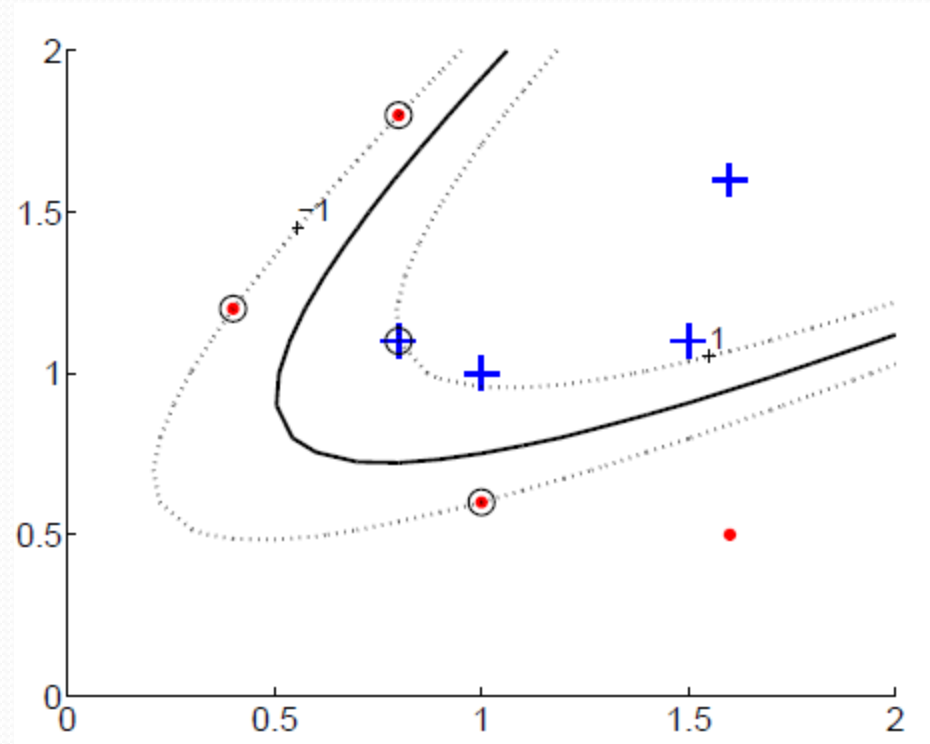
$$g(\mathbf{x}) = \sum_t \alpha^t r^t K(\mathbf{x}^t, \mathbf{x})$$

# Vectorial Kernels

- Polynomials of degree  $q$ :

$$K(\mathbf{x}^t, \mathbf{x}) = (\mathbf{x}^T \mathbf{x}^t + 1)^q$$

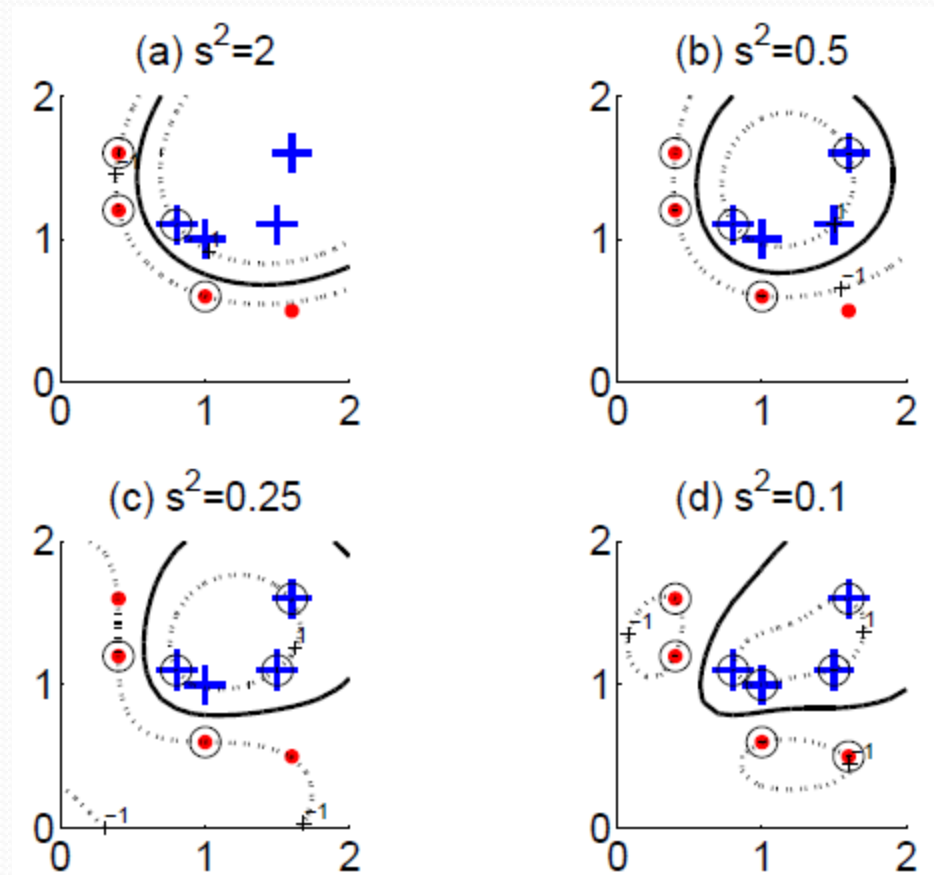
$$\begin{aligned} K(\mathbf{x}, \mathbf{y}) &= (\mathbf{x}^T \mathbf{y} + 1)^2 \\ &= (x_1 y_1 + x_2 y_2 + 1)^2 \\ &= 1 + 2x_1 y_1 + 2x_2 y_2 + 2x_1 x_2 y_1 y_2 + x_1^2 y_1^2 + x_2^2 y_2^2 \\ \phi(\mathbf{x}) &= [1, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1 x_2, x_1^2, x_2^2]^T \end{aligned}$$



# Vectorial Kernels

- Radial-basis functions:

$$K(\mathbf{x}^t, \mathbf{x}) = \exp\left[-\frac{\|\mathbf{x}^t - \mathbf{x}\|^2}{2s^2}\right]$$



# Defining kernels

- Kernel “engineering”
- Defining good measures of similarity
- String kernels, graph kernels, image kernels, ...
- Empirical kernel map: Define a set of templates  $\mathbf{m}_i$  and score function  $s(\mathbf{x}, \mathbf{m}_i)$

$$\phi(\mathbf{x}^t) = [s(\mathbf{x}^t, \mathbf{m}_1), s(\mathbf{x}^t, \mathbf{m}_2), \dots, s(\mathbf{x}^t, \mathbf{m}_M)]$$

and

$$K(\mathbf{x}, \mathbf{x}^t) = \phi(\mathbf{x})^T \phi(\mathbf{x}^t)$$



# Multiple Kernel Learning

- Fixed kernel combination

$$K(\mathbf{x}, \mathbf{y}) = \begin{cases} cK(\mathbf{x}, \mathbf{y}) \\ K_1(\mathbf{x}, \mathbf{y}) + K_2(\mathbf{x}, \mathbf{y}) \\ K_1(\mathbf{x}, \mathbf{y})K_2(\mathbf{x}, \mathbf{y}) \end{cases}$$

- Adaptive kernel combination

$$K(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^m \eta_i K_i(\mathbf{x}, \mathbf{y})$$

$$L_d = \sum_t \alpha^t - \frac{1}{2} \sum_t \sum_s \alpha^t \alpha^s r^t r^s \sum_i \eta_i K_i(\mathbf{x}^t, \mathbf{x}^s)$$

$$g(\mathbf{x}) = \sum_t \alpha^t r^t \sum_i \eta_i K_i(\mathbf{x}^t, \mathbf{x})$$

- Localized kernel combination

$$g(\mathbf{x}) = \sum_t \alpha^t r^t \sum_i \eta_i(\mathbf{x} | \theta) K_i(\mathbf{x}^t, \mathbf{x})$$

# Multiclass Kernel Machines

- 1-vs-all
- Pairwise separation
- Error-Correcting Output Codes (section 17.5)
- Single multiclass optimization

$$\min \frac{1}{2} \sum_{i=1}^K \|\mathbf{w}_i\|^2 + c \sum_i \sum_t \xi_i^t$$

subject to

$$\mathbf{w}_{z^t}^T \mathbf{x}^t + w_{z^t 0} \geq \mathbf{w}_i^T \mathbf{x}^t + w_{i0} + 2 - \xi_i^t, \forall i \neq z^t, \xi_i^t \geq 0$$

# SVM for Regression

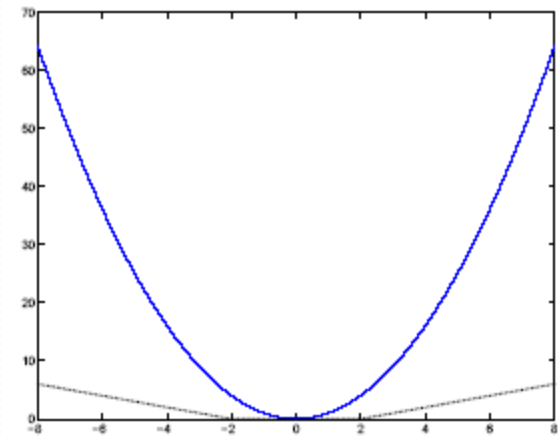
- Use a linear model (possibly kernelized)

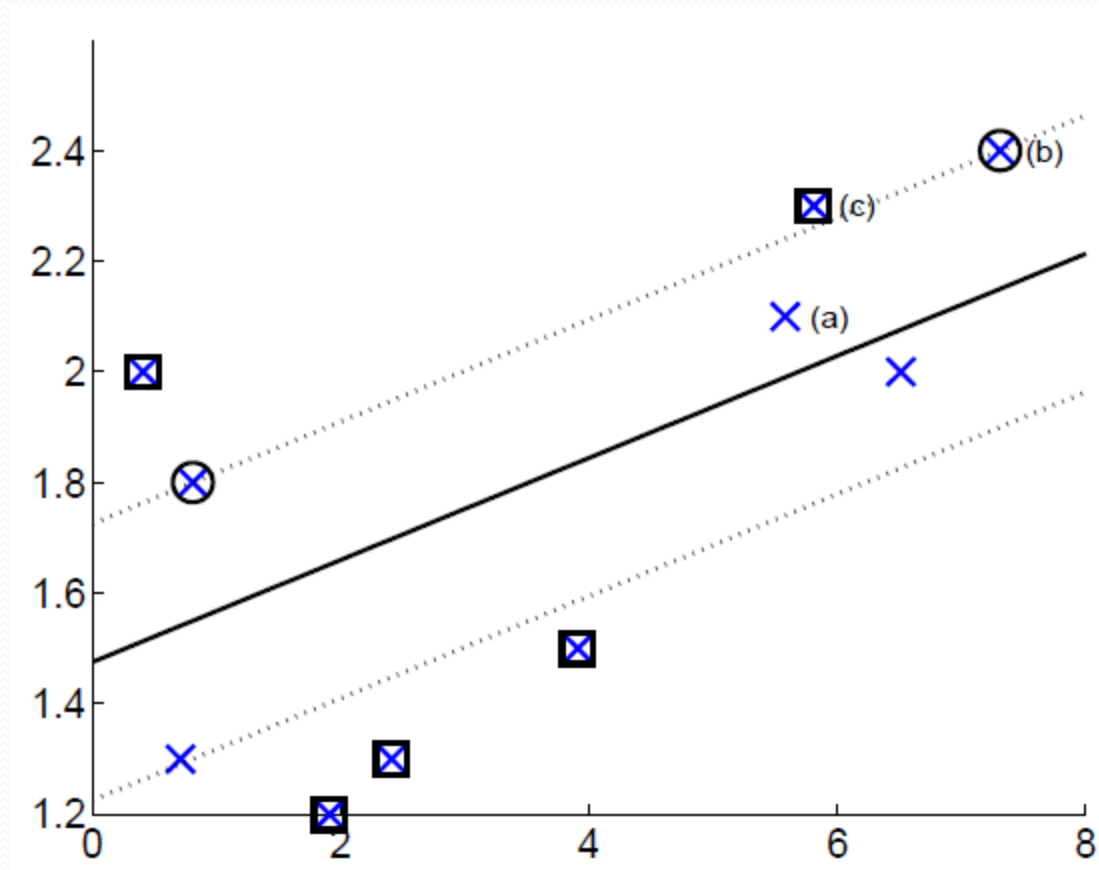
$$f(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + w_0$$

- Use the  $\epsilon$ -sensitive error function

$$e_{\epsilon}(r^t, f(\mathbf{x}^t)) = \begin{cases} 0 & \text{if } |r^t - f(\mathbf{x}^t)| < \epsilon \\ |r^t - f(\mathbf{x}^t)| - \epsilon & \text{otherwise} \end{cases}$$

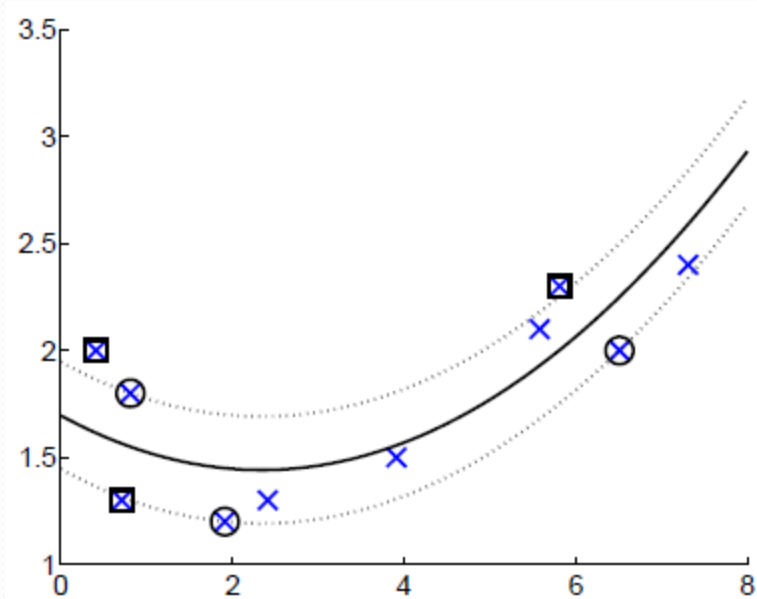
- $$\min \frac{1}{2} \|\mathbf{w}\|^2 + c \sum_t (\xi_+^t + \xi_-^t)$$
$$r^t - (\mathbf{w}^T \mathbf{x} + w_0) \leq \epsilon + \xi_+^t$$
$$(\mathbf{w}^T \mathbf{x} + w_0) - r^t \leq \epsilon + \xi_-^t$$
$$\xi_+^t, \xi_-^t \geq 0$$



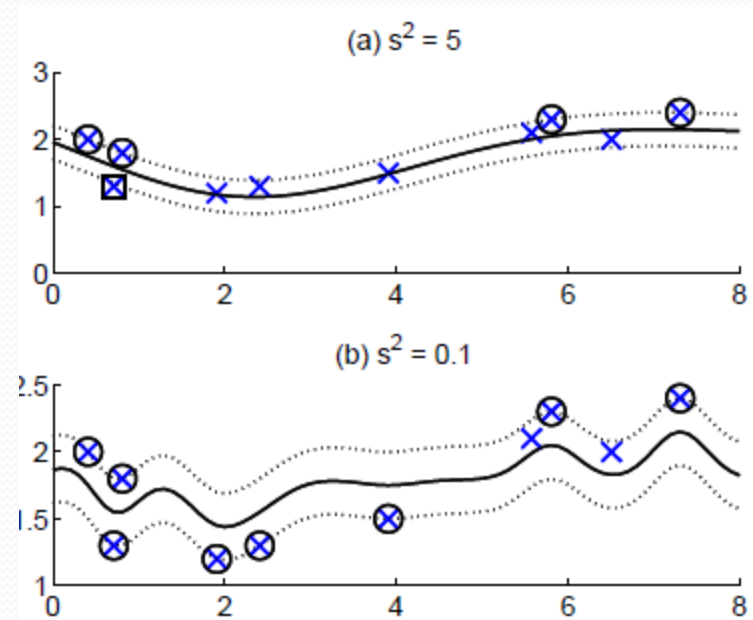


# Kernel Regression

- Polynomial kernel



- Gaussian kernel



# One-Class Kernel Machines

- Consider a sphere with center  $\mathbf{a}$  and radius  $R$

$$\min R^2 + C \sum_t \xi^t$$

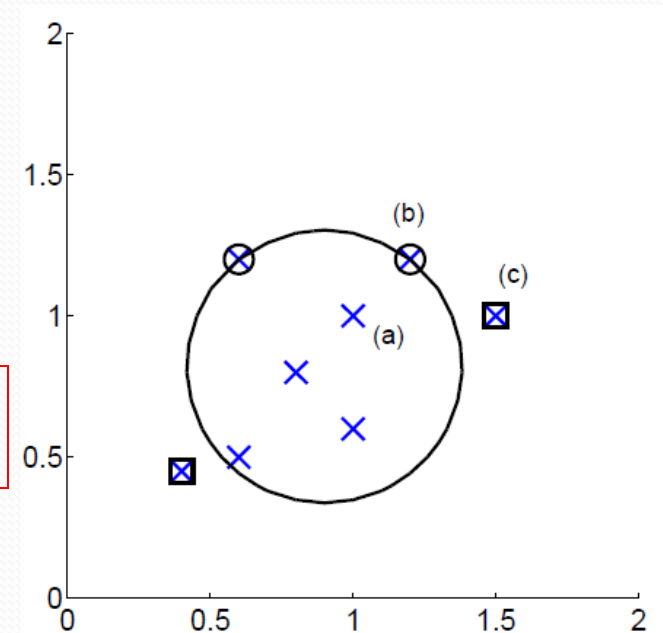
subject to

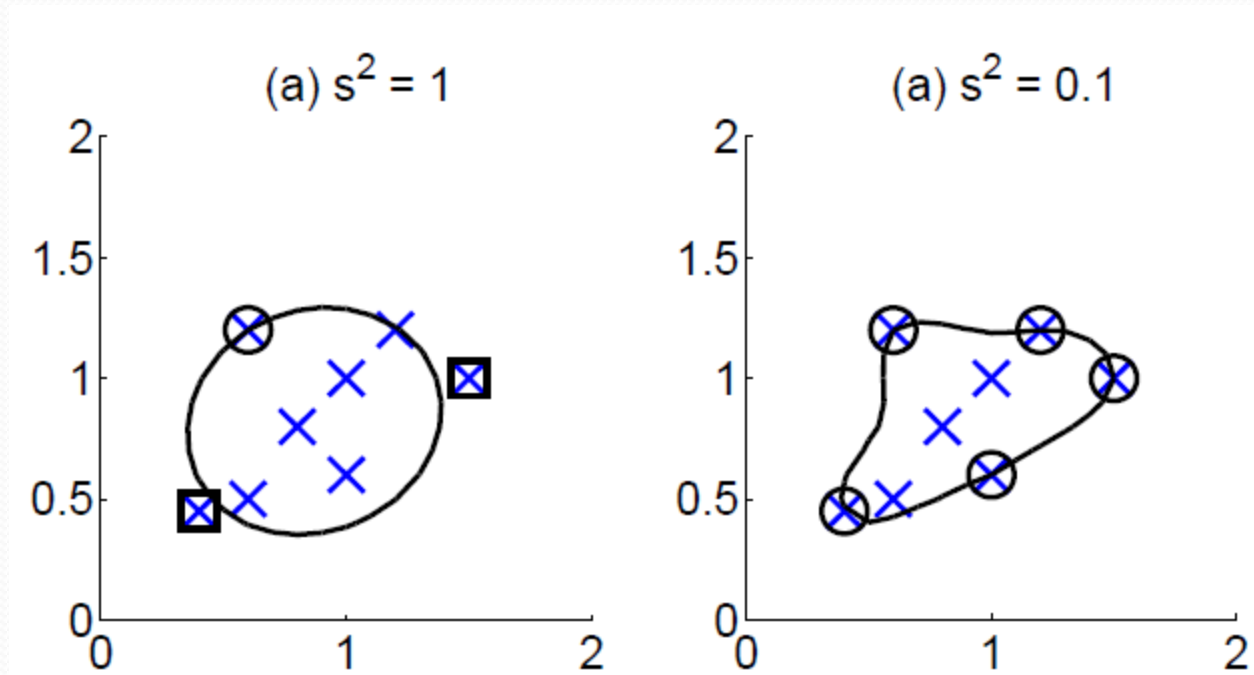
$$\|\mathbf{x}^t - \mathbf{a}\| \leq R^2 + \xi^t, \xi^t \geq 0$$

$$L_d = \sum_t \alpha^t \boxed{(\mathbf{x}^t)^T \mathbf{x}^s} - \sum_{t=1}^N \sum_s \alpha^t \alpha^s r^t r^s \boxed{(\mathbf{x}^t)^T \mathbf{x}^s}$$

subject to

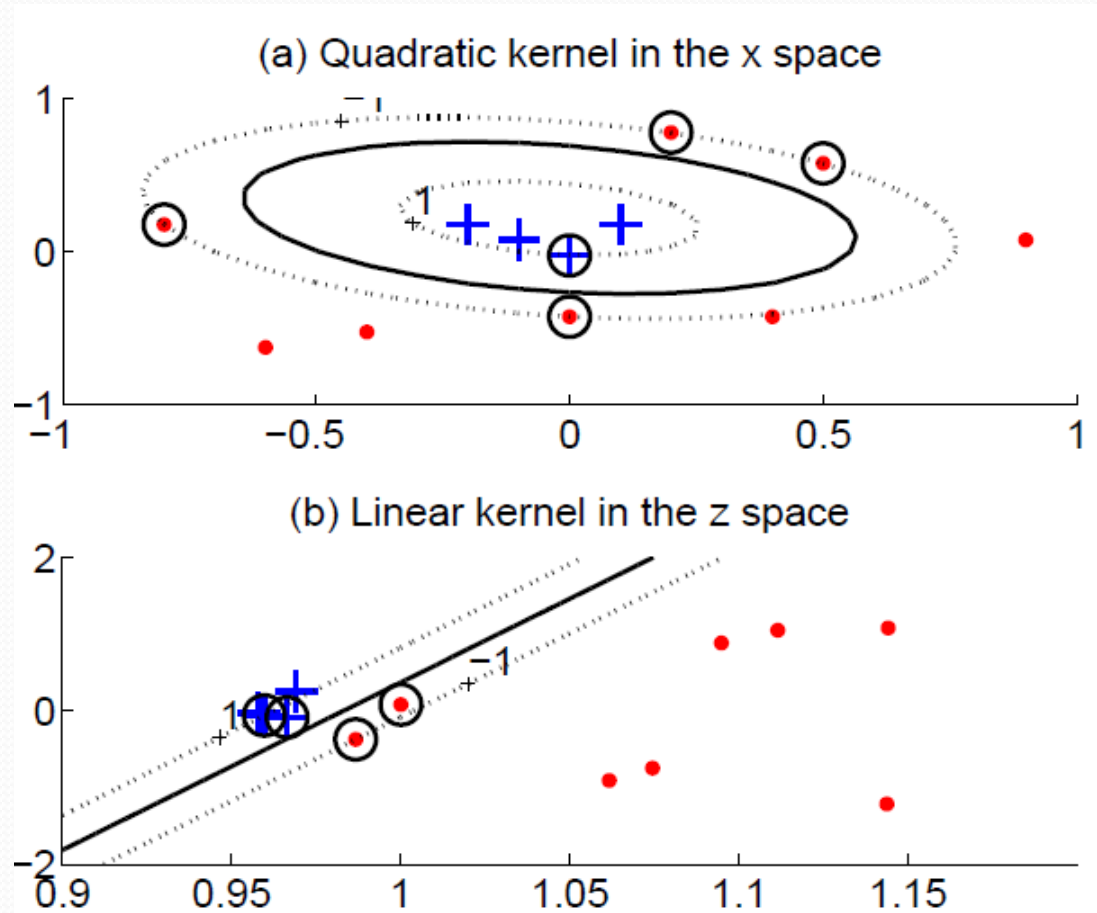
$$0 \leq \alpha^t \leq C, \sum_t \alpha^t = 1$$





# Kernel Dimensionality Reduction

- Kernel PCA does PCA on the kernel matrix (equal to canonical PCA with a linear kernel)
- Kernel LDA





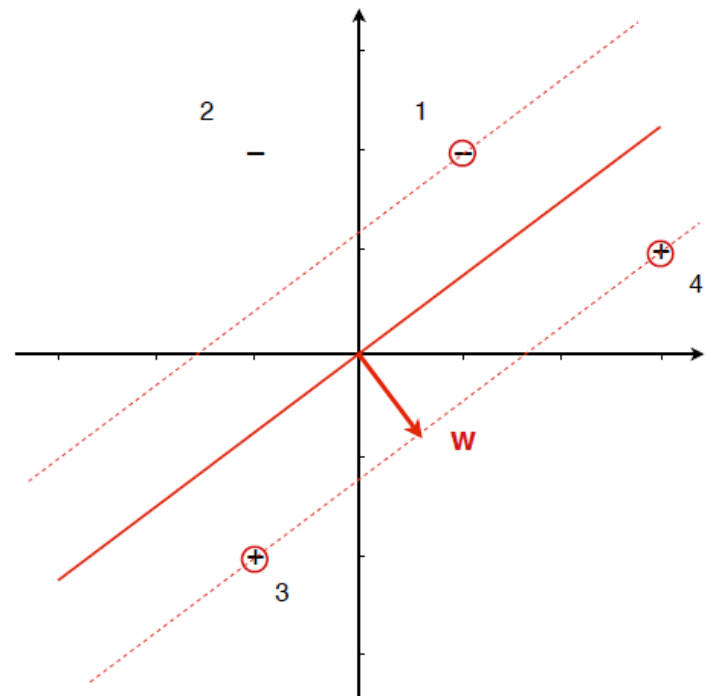
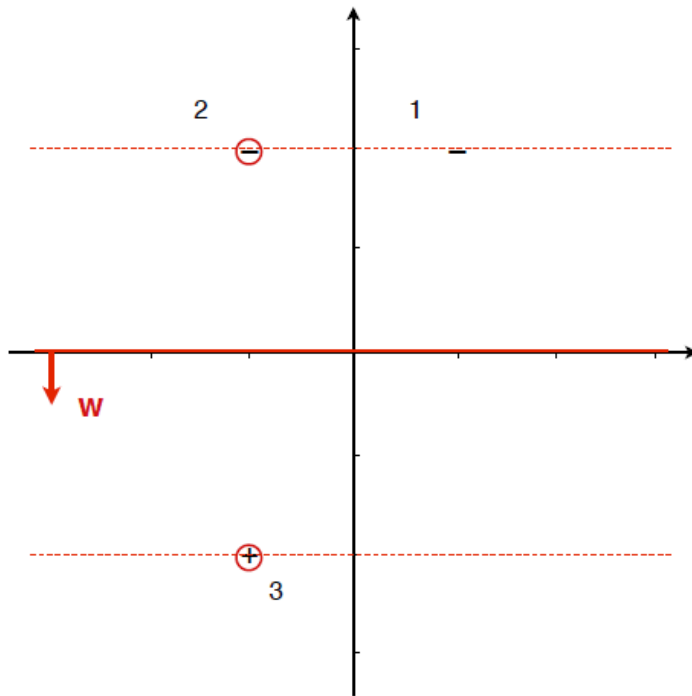
# Numerical Example

The dual optimisation problem for support vector machines is to maximise the dual Lagrangian under positivity constraints and one equality constraint:

$$\alpha_1^*, \dots, \alpha_n^* = \arg \max_{\alpha_1, \dots, \alpha_n} -\frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j + \sum_{i=1}^n \alpha_i$$

subject to  $\alpha_i \geq 0, 1 \leq i \leq n$  and  $\sum_{i=1}^n \alpha_i y_i = 0$

- This example and following slides are obtained from «**Machine Learning The Art and Science of Algorithms that Make Sense of Data**» book.
- <http://people.cs.bris.ac.uk/~flach/mlbook/>



**(left)** A maximum-margin classifier built from three examples, with  $\mathbf{w} = (0, -1/2)$  and margin 2. The circled examples are the support vectors: they receive non-zero Lagrange multipliers and define the decision boundary. **(right)** By adding a second positive the decision boundary is rotated to  $\mathbf{w} = (3/5, -4/5)$  and the margin decreases to 1.

- From «**Machine Learning The Art and Science of Algorithms that Make Sense of Data**» book. <http://people.cs.bris.ac.uk/~flach/mlbook/>

$$\mathbf{X} = \begin{pmatrix} 1 & 2 \\ -1 & 2 \\ -1 & -2 \end{pmatrix} \quad \mathbf{y} = \begin{pmatrix} -1 \\ -1 \\ +1 \end{pmatrix} \quad \mathbf{X}' = \begin{pmatrix} -1 & -2 \\ 1 & -2 \\ -1 & -2 \end{pmatrix}$$

The matrix  $\mathbf{X}'$  on the right incorporates the class labels; i.e., the rows are  $y_i \mathbf{x}_i$ .  
The Gram matrix is (without and with class labels):

$$\mathbf{XX}^T = \begin{pmatrix} 5 & 3 & -5 \\ 3 & 5 & -3 \\ -5 & -3 & 5 \end{pmatrix} \quad \mathbf{X}'\mathbf{X}'^T = \begin{pmatrix} 5 & 3 & 5 \\ 3 & 5 & 3 \\ 5 & 3 & 5 \end{pmatrix}$$

The dual optimisation problem is thus

$$\begin{aligned} & \arg \max_{\alpha_1, \alpha_2, \alpha_3} -\frac{1}{2} \left( 5\alpha_1^2 + 3\alpha_1\alpha_2 + 5\alpha_1\alpha_3 + 3\alpha_2\alpha_1 + 5\alpha_2^2 + 3\alpha_2\alpha_3 + 5\alpha_3\alpha_1 + 3\alpha_3\alpha_2 + 5\alpha_3^2 \right) + \alpha_1 + \alpha_2 + \alpha_3 \\ & = \arg \max_{\alpha_1, \alpha_2, \alpha_3} -\frac{1}{2} \left( 5\alpha_1^2 + 6\alpha_1\alpha_2 + 10\alpha_1\alpha_3 + 5\alpha_2^2 + 6\alpha_2\alpha_3 + 5\alpha_3^2 \right) + \alpha_1 + \alpha_2 + \alpha_3 \end{aligned}$$

subject to  $\alpha_1 \geq 0, \alpha_2 \geq 0, \alpha_3 \geq 0$  and  $-\alpha_1 - \alpha_2 + \alpha_3 = 0$ .

- From «**Machine Learning The Art and Science of Algorithms that Make Sense of Data**» book. <http://people.cs.bris.ac.uk/~flach/mlbook/>

- ✎ Using the equality constraint we can eliminate one of the variables, say  $\alpha_3$ , and simplify the objective function to

$$\arg \max_{\alpha_1, \alpha_2, \alpha_3} -\frac{1}{2} (20\alpha_1^2 + 32\alpha_1\alpha_2 + 16\alpha_2^2) + 2\alpha_1 + 2\alpha_2$$

- ✎ Setting partial derivatives to 0 we obtain  $-20\alpha_1 - 16\alpha_2 + 2 = 0$  and  $-16\alpha_1 - 16\alpha_2 + 2 = 0$  (notice that, because the objective function is quadratic, these equations are guaranteed to be linear).
- ✎ We therefore obtain the solution  $\alpha_1 = 0$  and  $\alpha_2 = \alpha_3 = 1/8$ . We then have  $\mathbf{w} = 1/8(\mathbf{x}_3 - \mathbf{x}_2) = \begin{pmatrix} 0 \\ -1/2 \end{pmatrix}$ , resulting in a margin of  $1/\|\mathbf{w}\| = 2$ .
- ✎ Finally,  $t$  can be obtained from any support vector, say  $\mathbf{x}_2$ , since  $y_2(\mathbf{w} \cdot \mathbf{x}_2 - t) = 1$ ; this gives  $-1 \cdot (-1 - t) = 1$ , hence  $t = 0$ .

- From «**Machine Learning The Art and Science of Algorithms that Make Sense of Data**» book. <http://people.cs.bris.ac.uk/~flach/mlbook/>

We now add an additional positive at (3, 1). This gives the following data matrices:

$$\mathbf{X}' = \begin{pmatrix} -1 & -2 \\ 1 & -2 \\ -1 & -2 \\ 3 & 1 \end{pmatrix} \quad \mathbf{X}'\mathbf{X}'^T = \begin{pmatrix} 5 & 3 & 5 & -5 \\ 3 & 5 & 3 & 1 \\ 5 & 3 & 5 & -5 \\ -5 & 1 & -5 & 10 \end{pmatrix}$$

- It can be verified by similar calculations to those above that the margin decreases to 1 and the decision boundary rotates to  $\mathbf{w} = \begin{pmatrix} 3/5 \\ -4/5 \end{pmatrix}$ .
- The Lagrange multipliers now are  $\alpha_1 = 1/2$ ,  $\alpha_2 = 0$ ,  $\alpha_3 = 1/10$  and  $\alpha_4 = 2/5$ . Thus, only  $\mathbf{x}_3$  is a support vector in both the original and the extended data set.

- From «**Machine Learning The Art and Science of Algorithms that Make Sense of Data**» book. <http://people.cs.bris.ac.uk/~flach/mlbook//>

# SVM with Hinge Loss

Learning an SVM has been formulated as a **constrained** optimization problem over  $\mathbf{w}$  and  $\xi$

$$\min_{\mathbf{w} \in \mathbb{R}^d, \xi_i \in \mathbb{R}^+} \|\mathbf{w}\|^2 + C \sum_i^N \xi_i \text{ subject to } y_i (\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 - \xi_i \text{ for } i = 1 \dots N$$

The constraint  $y_i (\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 - \xi_i$ , can be written more concisely as

$$y_i f(\mathbf{x}_i) \geq 1 - \xi_i$$

which, together with  $\xi_i \geq 0$ , is equivalent to

$$\xi_i = \max(0, 1 - y_i f(\mathbf{x}_i))$$

Hence the learning problem is equivalent to the **unconstrained** optimization problem over  $\mathbf{w}$

$$\min_{\mathbf{w} \in \mathbb{R}^d} \underbrace{\|\mathbf{w}\|^2}_{\text{regularization}} + C \sum_i^N \underbrace{\max(0, 1 - y_i f(\mathbf{x}_i))}_{\text{loss function}}$$

- Slides are adopted from A. Zisserman

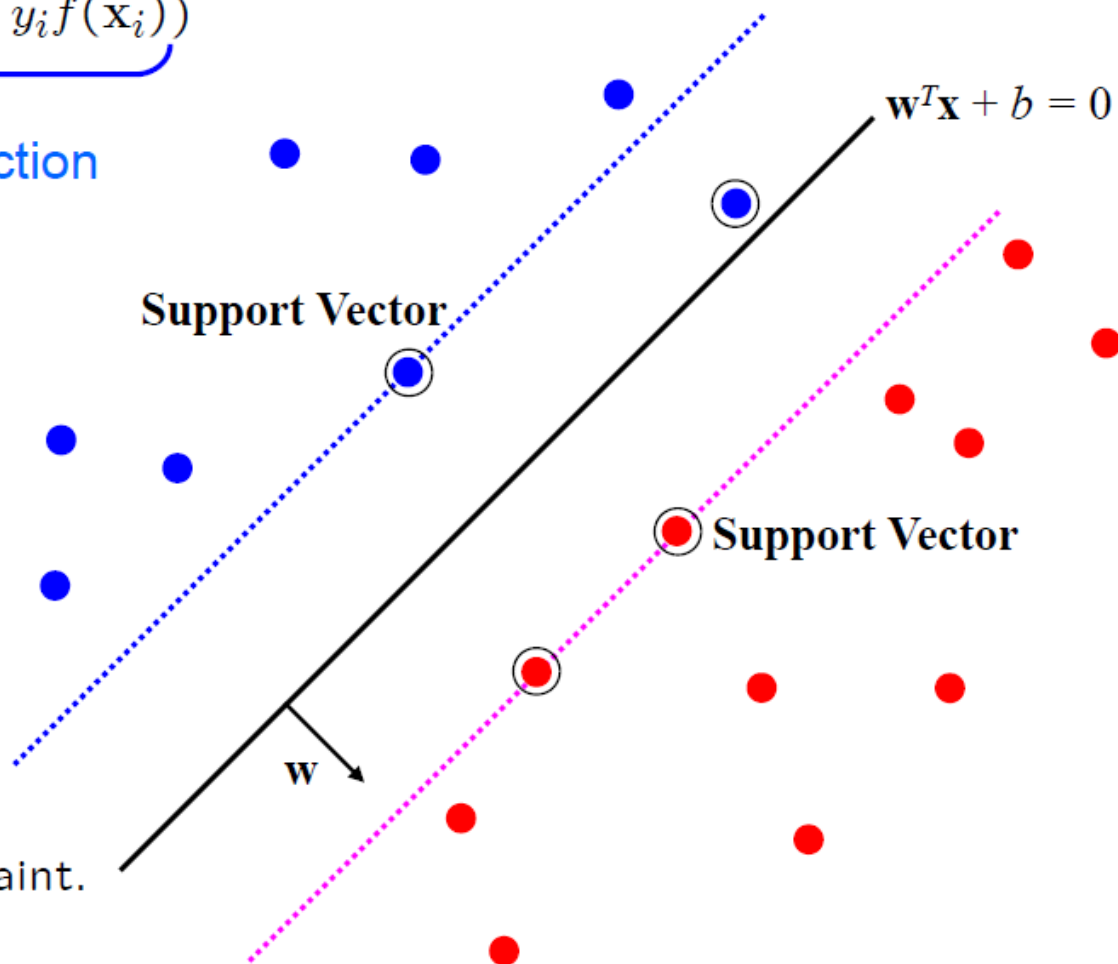
# Loss function

$$\min_{\mathbf{w} \in \mathbb{R}^d} \|\mathbf{w}\|^2 + C \sum_i^N \underbrace{\max(0, 1 - y_i f(\mathbf{x}_i))}_{\text{loss function}}$$

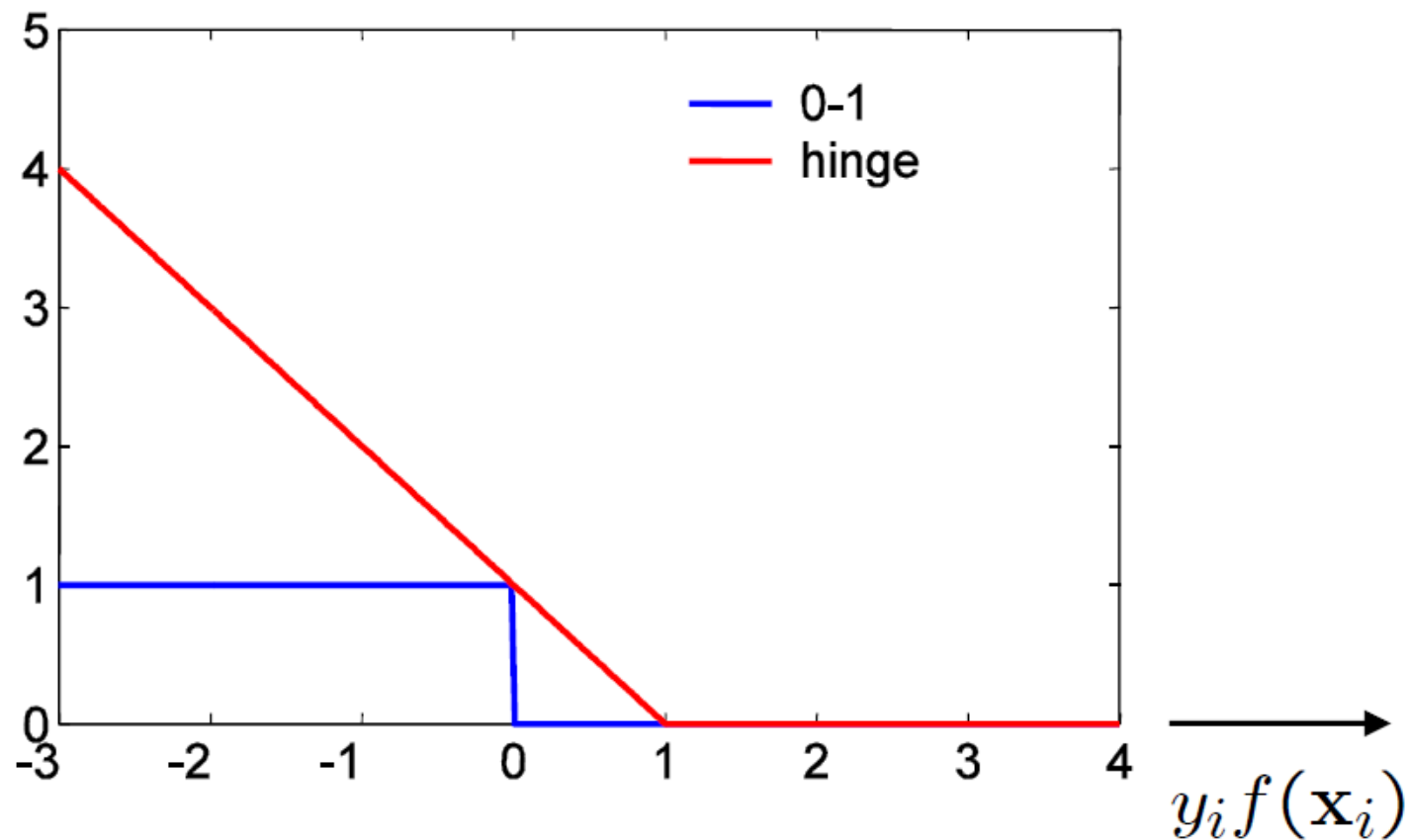
loss function

Points are in three categories:

1.  $y_i f(x_i) > 1$   
Point is outside margin.  
No contribution to loss
2.  $y_i f(x_i) = 1$   
Point is on margin.  
No contribution to loss.  
As in hard margin case.
3.  $y_i f(x_i) < 1$   
Point violates margin constraint.  
Contributes to loss



# Loss functions



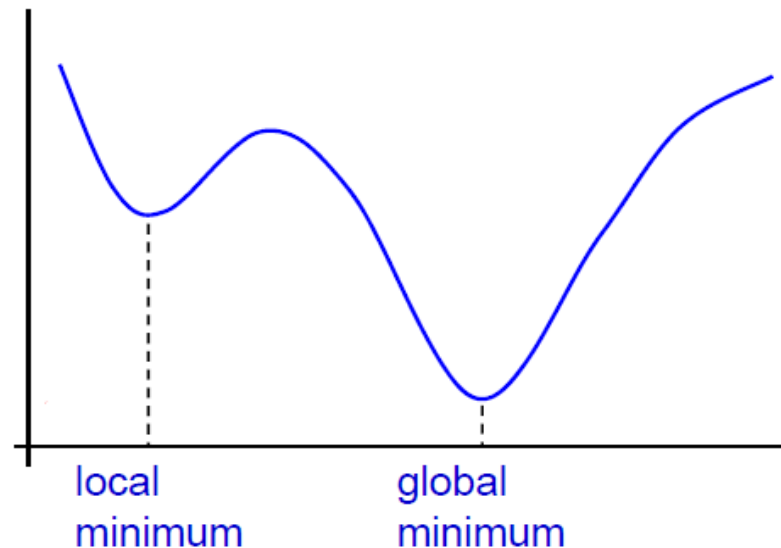
- SVM uses “hinge” loss  $\max(0, 1 - y_i f(\mathbf{x}_i))$
- an approximation to the 0-1 loss



# Optimization continued

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$$\min_{\mathbf{w} \in \mathbb{R}^d} C \sum_i^N \max(0, 1 - y_i f(\mathbf{x}_i)) + \|\mathbf{w}\|^2$$



- Does this cost function have a unique solution?
- Does the solution depend on the starting point of an iterative optimization algorithm (such as gradient descent)?

If the cost function is **convex**, then a locally optimal point is globally optimal (provided the optimization is over a convex set, which it is in our case)

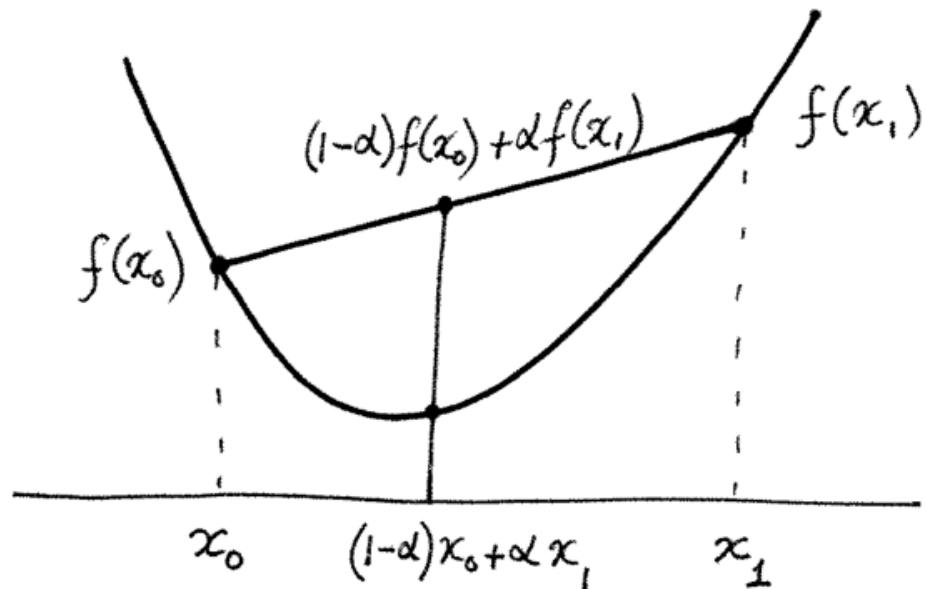
# Convex functions

$D$  – a domain in  $\mathbb{R}^n$ .

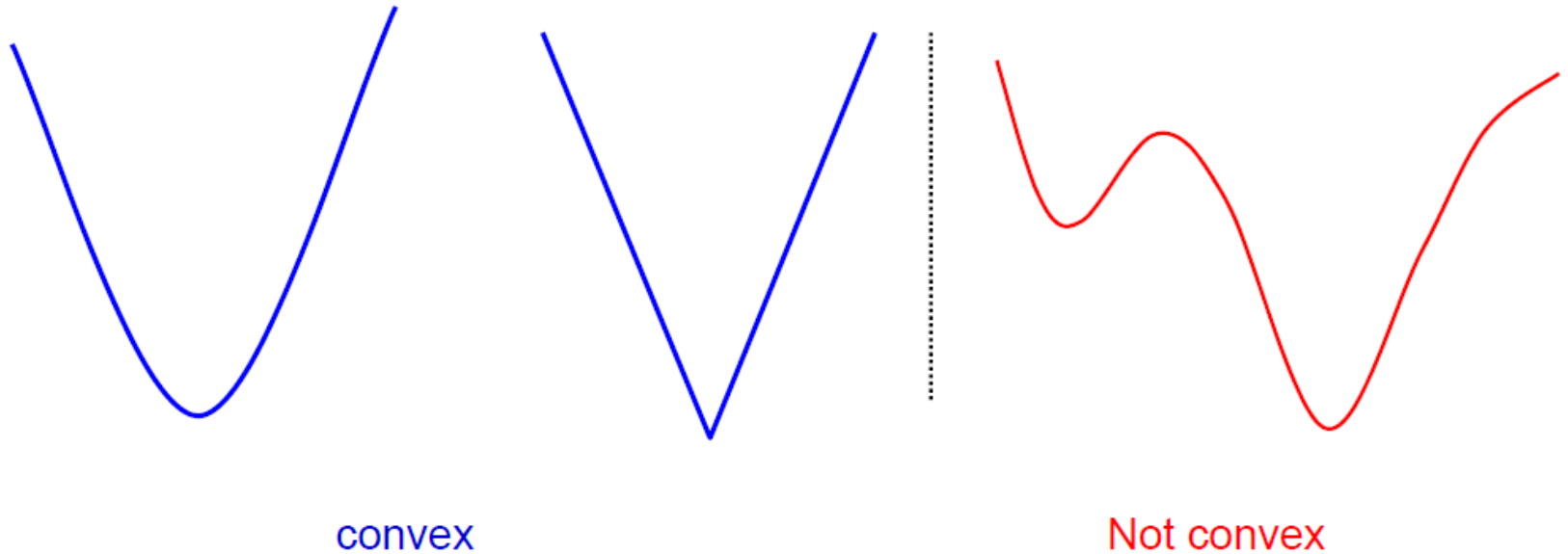
A **convex function**  $f : D \rightarrow \mathbb{R}$  is one that satisfies, for any  $x_0$  and  $x_1$  in  $D$ :

$$f((1 - \alpha)x_0 + \alpha x_1) \leq (1 - \alpha)f(x_0) + \alpha f(x_1) .$$

Line joining  $(x_0, f(x_0))$   
and  $(x_1, f(x_1))$  lies  
above the function graph.



# Convex function examples

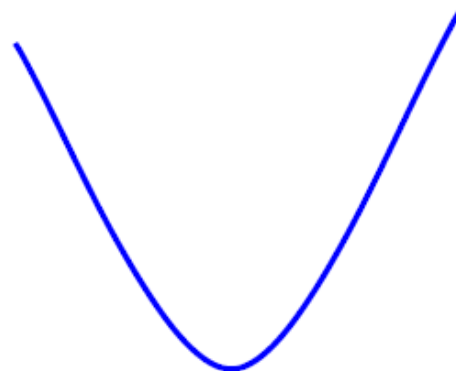


A non-negative sum of convex functions is convex

- Adopted from A. Zisserman



+



SVM

$$\min_{\mathbf{w} \in \mathbb{R}^d} C \sum_i^N \max(0, 1 - y_i f(\mathbf{x}_i)) + \|\mathbf{w}\|^2$$

convex

- Adopted from A. Zisserman

# Gradient (or steepest) descent algorithm for SVM

---

To minimize a cost function  $\mathcal{C}(\mathbf{w})$  use the iterative update

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t - \eta_t \nabla_{\mathbf{w}} \mathcal{C}(\mathbf{w}_t)$$

where  $\eta$  is the learning rate.

First, rewrite the optimization problem as an **average**

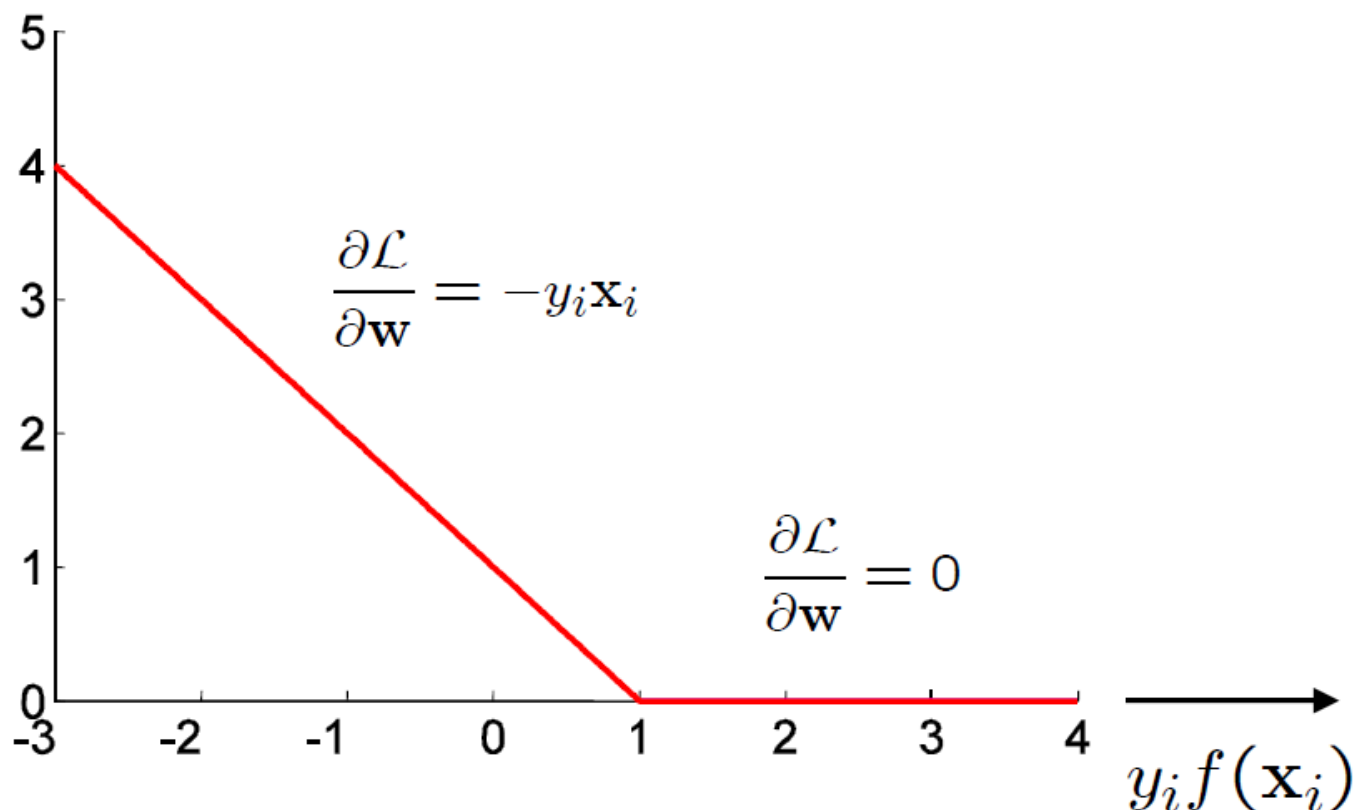
$$\begin{aligned} \min_{\mathbf{w}} \mathcal{C}(\mathbf{w}) &= \frac{\lambda}{2} \|\mathbf{w}\|^2 + \frac{1}{N} \sum_i^N \max(0, 1 - y_i f(\mathbf{x}_i)) \\ &= \frac{1}{N} \sum_i^N \left( \frac{\lambda}{2} \|\mathbf{w}\|^2 + \max(0, 1 - y_i f(\mathbf{x}_i)) \right) \end{aligned}$$

(with  $\lambda = 2/(NC)$  up to an overall scale of the problem) and  $f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$

Because the hinge loss is not differentiable, a **sub-gradient** is computed

# Sub-gradient for hinge loss

$$\mathcal{L}(\mathbf{x}_i, y_i; \mathbf{w}) = \max(0, 1 - y_i f(\mathbf{x}_i)) \quad f(\mathbf{x}_i) = \mathbf{w}^\top \mathbf{x}_i + b$$



# Sub-gradient descent algorithm for SVM

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$$\mathcal{C}(\mathbf{w}) = \frac{1}{N} \sum_i^N \left( \frac{\lambda}{2} \|\mathbf{w}\|^2 + \mathcal{L}(\mathbf{x}_i, y_i; \mathbf{w}) \right)$$

The iterative update is

$$\begin{aligned} \mathbf{w}_{t+1} &\leftarrow \mathbf{w}_t - \eta \nabla_{\mathbf{w}_t} \mathcal{C}(\mathbf{w}_t) \\ &\leftarrow \mathbf{w}_t - \eta \frac{1}{N} \sum_i^N (\lambda \mathbf{w}_t + \nabla_{\mathbf{w}} \mathcal{L}(\mathbf{x}_i, y_i; \mathbf{w}_t)) \end{aligned}$$

where  $\eta$  is the learning rate.

Then each iteration  $t$  involves cycling through the training data with the updates:

$$\begin{aligned} \mathbf{w}_{t+1} &\leftarrow \mathbf{w}_t - \eta(\lambda \mathbf{w}_t - y_i \mathbf{x}_i) && \text{if } y_i f(\mathbf{x}_i) < 1 \\ &\leftarrow \mathbf{w}_t - \eta \lambda \mathbf{w}_t && \text{otherwise} \end{aligned}$$

In the Pegasos algorithm the learning rate is set at  $\eta_t = \frac{1}{\lambda t}$

- Adopted from A. Zisserman