

# Nomenclature

- Given  $x_1, x_2, \dots, x_n$  sample points, with true category labels:

$y_1, y_2, \dots, y_n$

$$\left. \begin{array}{l} y_i = 1 \\ y_i = -1 \end{array} \right\} \begin{array}{l} \text{if point } x_i \text{ is from class } \omega_1 \\ \text{if point } x_i \text{ is from class } \omega_2 \end{array}$$

- Decision are made according to:

*if*  $\mathbf{w}^t x_i' = w^t x_i + b > 0$  class  $\omega_1$  is chosen

*if*  $\mathbf{w}^t x_i' = w^t x_i + b < 0$  class  $\omega_2$  is chosen

- Now these decisions are wrong when  $\mathbf{w}^t \mathbf{x}_i$  is negative and belongs to class  $\omega_1$ .

Let  $z_i = \alpha_i x_i$  Then  $z_i > 0$  when correctly labelled,  
negative otherwise.

# Support Vector Machines

- Support vector machines differ from standard linear machines in three ways.
- **Discriminant function flexibility**
  - Linear
    - But with nonlinear preprocessing possible
    - efficient evaluation via kernel trick
- **Error function**
  - Max margin, constrained by misclassification errors
- **Optimization**
  - Choice of error function allows global solution
  - Nature of solution focuses on points on points on margin (the support vectors)

$$\mathbf{x} = \mathbf{x}_p + \frac{r\mathbf{w}}{\|\mathbf{w}\|}$$

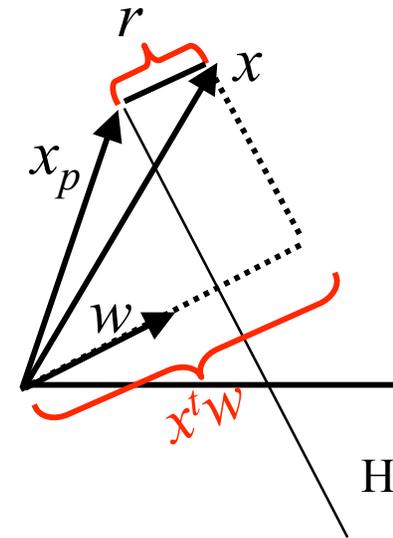
since  $g(\mathbf{x}_p) = 0$  and  $\mathbf{w}^t \mathbf{w} = \|\mathbf{w}\|^2$

$$g(\mathbf{x}) = \mathbf{w}^t \mathbf{x} + w_0 \Rightarrow \mathbf{w}^t \left( \mathbf{x}_p + \frac{r\mathbf{w}}{\|\mathbf{w}\|} \right) + w_0$$

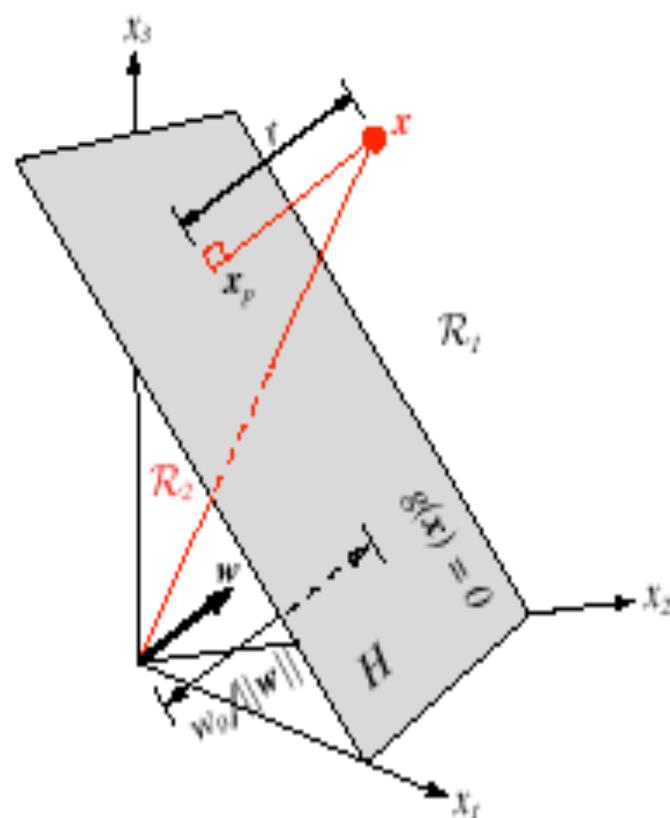
$$= g(\mathbf{x}_p) + \mathbf{w}^t \mathbf{w} \frac{r}{\|\mathbf{w}\|}$$

$$\Rightarrow r = \frac{g(x)}{\|\mathbf{w}\|}$$

in particular  $d([0,0], H) = \frac{w_0}{\|\mathbf{w}\|}$



- In conclusion, a linear discriminant function divides the feature space by a hyperplane decision surface
- The orientation of the surface is determined by the normal vector  $w$  and the location of the surface is determined by the bias



**FIGURE 5.2.** The linear decision boundary  $H$ , where  $g(\mathbf{x}) = \mathbf{w}^t \mathbf{x} + w_0 = 0$ , separates the feature space into two half-spaces  $\mathcal{R}_1$  (where  $g(\mathbf{x}) > 0$ ) and  $\mathcal{R}_2$  (where  $g(\mathbf{x}) < 0$ ). From: Richard O. Duda, Peter E. Hart, and David G. Stork, *Pattern Classification*. Copyright © 2001 by John Wiley & Sons, Inc.

# Support vector machines

We assign a value  $y \in \{+1, -1\}$  to each point in the training set and seek a  $\mathbf{w}$  for which  $y_i(\mathbf{w}^T \mathbf{x} + w_0) > 0$  for all  $i$ .

We want to have a margin, so :  $y_i(\mathbf{w}^T \mathbf{x} + w_0) \geq b$ .

If we scale  $|\mathbf{w}|$ ,  $w_0$  and  $b$ , nothing changes, so we set  $b = 1$ .

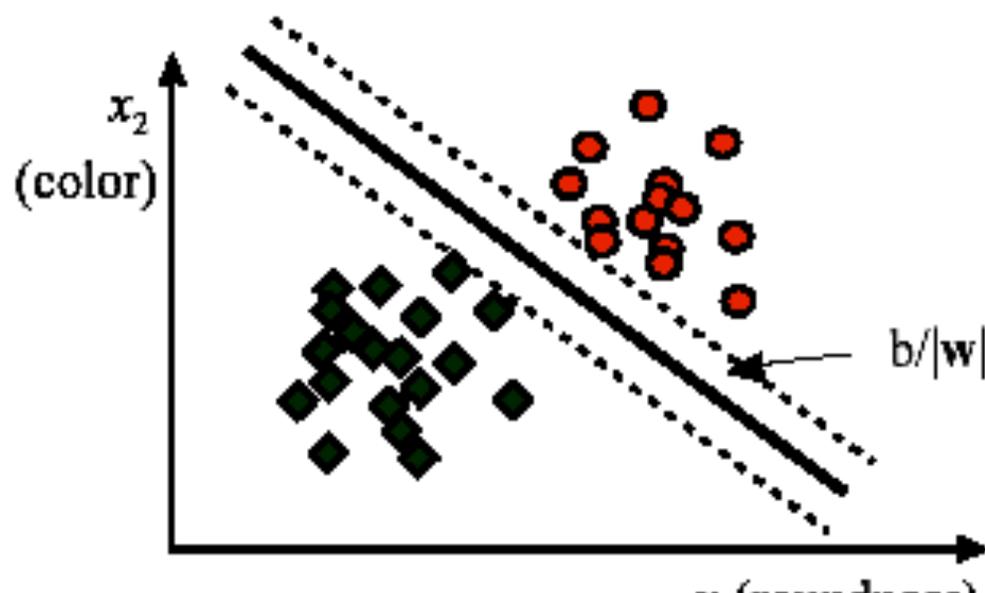
We get two hyperplanes :

$$H_1 : \mathbf{w}^T \mathbf{x} + w_0 = +1$$

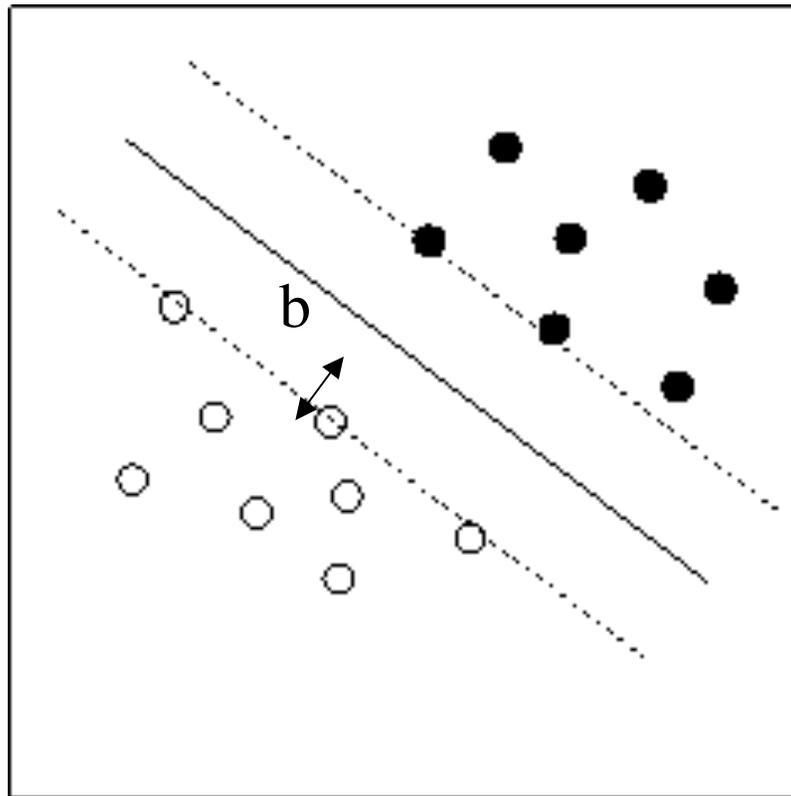
$$H_2 : \mathbf{w}^T \mathbf{x} + w_0 = -1.$$

The size of the margin is  $1/|\mathbf{w}|$

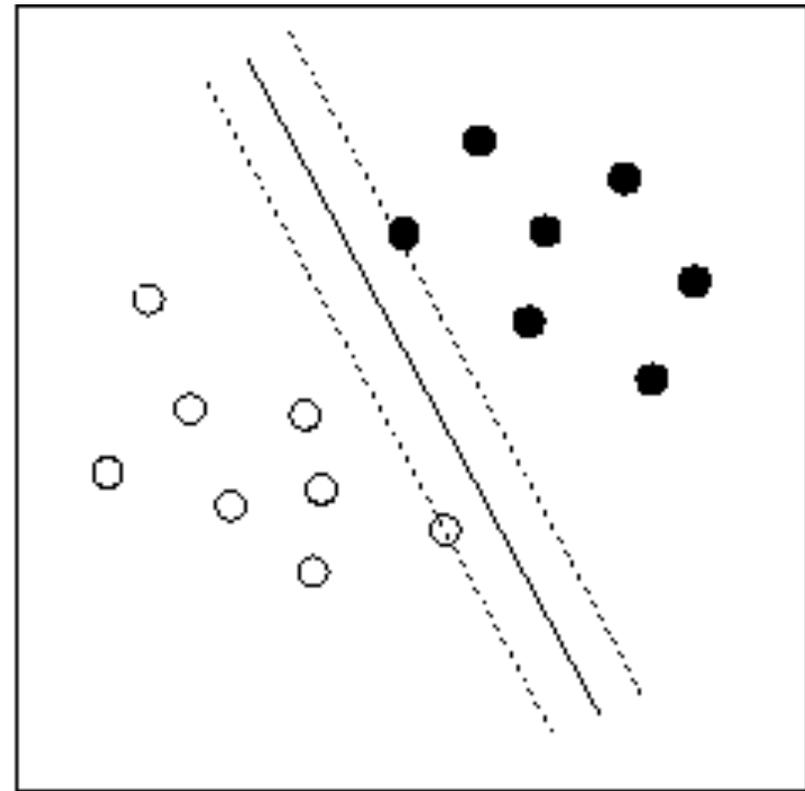
The points that lie on the hyperplanes are called *support vectors*.



# Margins in data space



(a) Larger margin



(b) Smaller margin

Larger margins promote uniqueness for underconstrained problems

- Therefore, the problem of maximizing the margin is equivalent to

$$\begin{array}{ll} \text{minimize} & J(w) = \frac{1}{2} \|w\|^2 \\ \text{subject to} & y_i (w^T x_i + b) \geq 1 \quad \forall i \end{array}$$

- Notice that  $J(w)$  is a quadratic function, which means that there exists a single global minimum and no local minima
- **To solve this problem, we will use classical Lagrangian optimization techniques**
  - We first present the Kuhn-Tucker Theorem, which provides an essential result for the interpretation of Support Vector Machines

# (Kuhn-Tucker Theorem)

---

- Given an optimization problem with convex domain  $\Omega \subseteq \mathbb{R}^N$

$$\begin{aligned} &\text{minimize} && f(z) && z \in \Omega \\ &\text{subject to} && g_i(z) \leq 0 && i = 1, \dots, k \\ &&& h_i(z) = 0 && i = 1, \dots, m \end{aligned}$$

- with  $f \in C^1$  convex and  $g_i, h_i$  affine, necessary and sufficient conditions for a normal point  $z^*$  to be an optimum are the existence of  $\alpha^*, \beta^*$  such that

$$\begin{aligned} \frac{\partial L(z^*, \alpha^*, \beta^*)}{\partial z} &= 0 \\ \alpha_i^* g_i(z^*) &= 0 && i = 1, \dots, k \\ g_i(z^*) &\leq 0 && i = 1, \dots, k \\ \alpha_i^* &\geq 0 && i = 1, \dots, k \end{aligned} \quad \text{where} \quad L(z, \alpha, \beta) = f(z) + \sum_{i=1}^k \alpha_i g_i(z) + \sum_{i=1}^m \beta_i h_i(z)$$

- $L(z, \alpha, \beta)$  is known as a *generalized Lagrangian function*
- The third condition is known as the Karush-Kuhn-Tucker (KKT) complementary condition. It implies that for active constraints  $\alpha_i \geq 0$ ; and for inactive constraints  $\alpha_i = 0$ 
  - As we will see in a minute, the KKT condition allows us to identify the training examples that define the largest margin hyperplane. These examples will be known as **Support Vectors**.

# Constrained Optimization Problems

Minimize enforcing Equality Constraints

Find:  $\vec{x}^* = \vec{x}_{\min}$  such that  $h(\vec{x}^*) = 0$

Lagrange Multiplier

$$\min f(x_1, x_2) \quad s.t. \quad h(x_1, x_2) = 0$$

$$L(x_1, x_2, v) = f(x_1, x_2) + v h(x_1, x_2) \leftarrow \begin{pmatrix} L : \text{Lagrange func} \\ v : \text{Lagrange multiplier} \end{pmatrix}$$

$$\frac{\partial L(x_1^*, x_2^*)}{\partial x_1} = \frac{\partial f(x_1^*, x_2^*)}{\partial x_1} + v \frac{\partial h(x_1^*, x_2^*)}{\partial x_1} = 0$$

$$\frac{\partial L(x_1^*, x_2^*)}{\partial x_2} = \frac{\partial f(x_1^*, x_2^*)}{\partial x_2} + v \frac{\partial h(x_1^*, x_2^*)}{\partial x_2} = 0$$

$$\nabla L(x^*) = \nabla f(x^*) + \nu \nabla h(x^*) = \underline{0}$$

$$\nabla f(x^*) = -\nu \nabla h(x^*) \longrightarrow \text{geometrical meaning}$$

At the candidate minimum point, gradients of the cost and constraint func are along the same line.

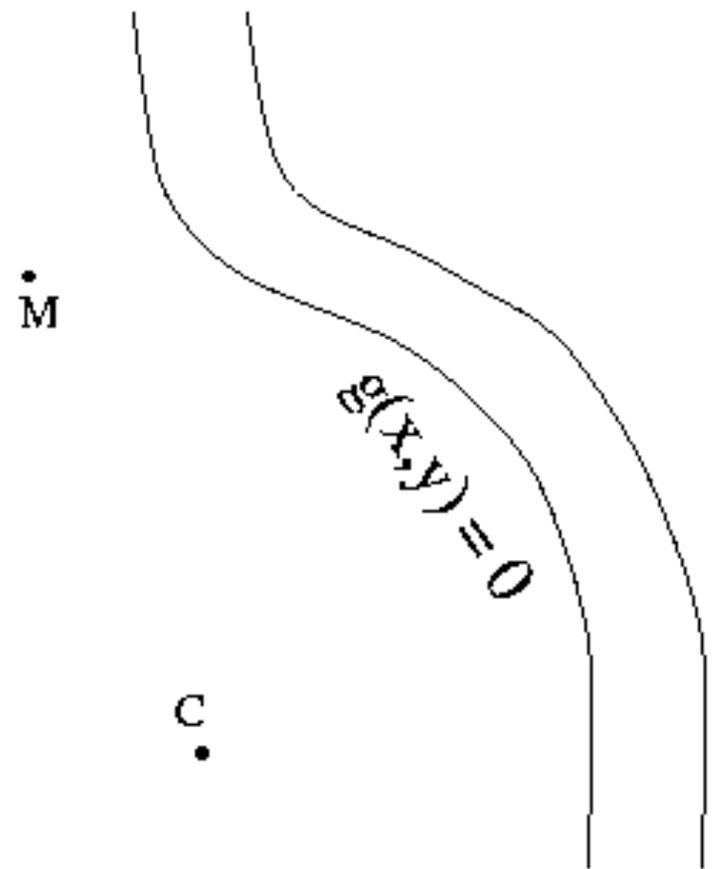
(In other words,  $\nabla f$  is a linear combination of  $\nabla h$ )

$$L(x, \nu) = f(x) + \nu^T h(x)$$

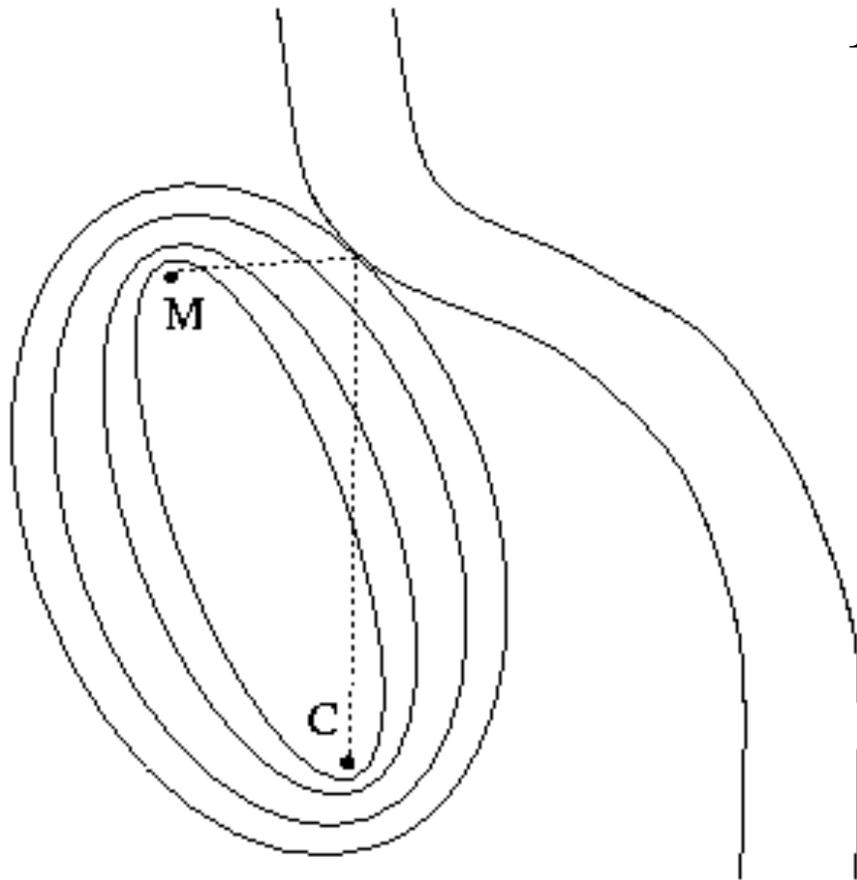
Therefore constrained optimization is converted to unconstrained optimization.

$$\nabla L(x^*, \nu^*) = 0$$

- The "Milkmaid problem"
- It's milking time at the farm, and the milkmaid has been sent to the field to get the day's milk. She is in quite a hurry, because she has a date, so she wants to finish her job as quickly as possible. However, before she gathers the milk, she has to rinse out her bucket in the nearby river.
- Just when she reaches point M, our heroine spots the cow, at point C. She is in a hurry, so she wants to take the shortest possible path from where she is to the river and then to the cow. If the near bank of the river is a curve satisfying the function  $g(x,y) = 0$ , what is the shortest path for the milkmaid to take? (Assume that the field is flat and uniform and that all points on the river bank are equally good.)



- Problem:
- Minimize  $f(P) = d(M,P) + d(P,C)$ ,  
 – such that  $g(P) = 0$ .



$$F(P, \alpha) = f(P) - \alpha g(P).$$

$$\nabla F = 0$$

$$\frac{\partial f}{\partial P} + \alpha \frac{\partial g}{\partial P} = 0$$

$$\frac{\partial F}{\partial \alpha} = 0 \quad \rightarrow \quad g(P) = 0$$

# Constrained Optimization

Instead of solving

$$\left( \frac{\partial f(\mathbf{w})}{\partial w_1}, \frac{\partial f(\mathbf{w})}{\partial w_2} \right) = (0, 0)$$

deal with **Lagrangian**

$$L(\mathbf{w}, \alpha, \beta) = f(\mathbf{w}) + \alpha \cdot g(\mathbf{w}) + \beta \cdot h(\mathbf{w})$$

and solve the **dual problem** by reasoning about the **dual variables**  $\alpha, \beta$ .

Primal problem:

minimize  $f(\mathbf{w})$

subject to  $g(\mathbf{w}) \leq 0, \quad h(\mathbf{w}) = 0$

Dual problem:

$\theta(\alpha, \beta)$  is minimal value of

$$L(\mathbf{w}, \alpha, \beta) = f(\mathbf{w}) + \alpha \cdot g(\mathbf{w}) + \beta \cdot h(\mathbf{w})$$

w.r.t.  $\mathbf{w}$

maximize  $\theta(\alpha, \beta)$

subject to  $\alpha \geq 0$

# Kuhn-Tucker Example

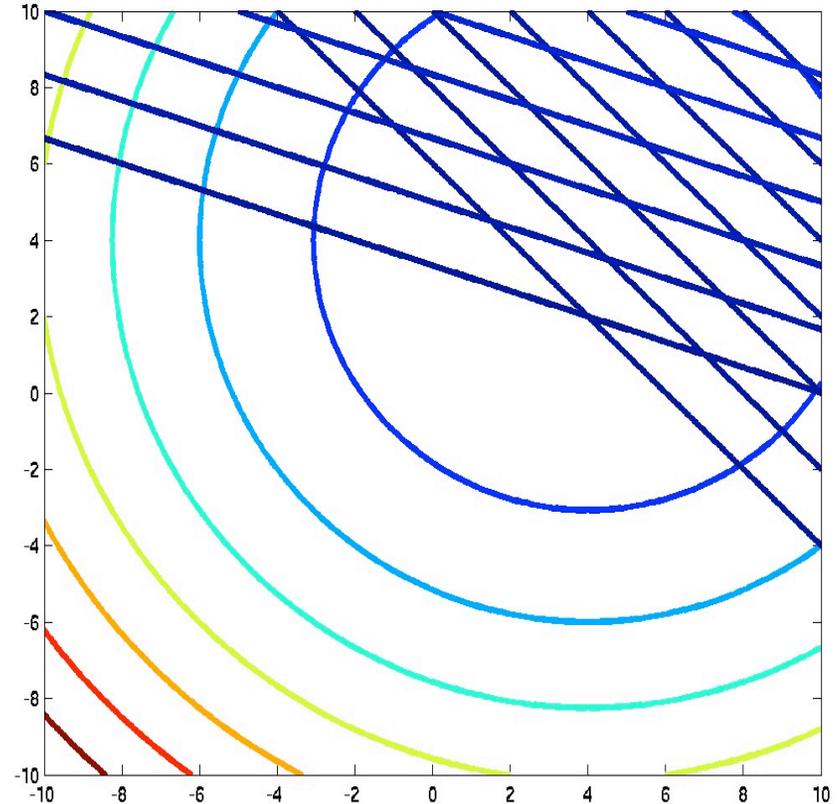
Consider the problem

$$\min \left\{ f(\vec{x}) = (x_1 - 4)^2 + (x_2 - 4)^2 \right\},$$

such that

$$g_1(\vec{x}) = x_1 + x_2 \leq 6 \quad \text{and}$$

$$g_2(\vec{x}) = x_1 + 3x_2 \leq 4$$



We form a new function for minimization :

$$L(\vec{x}) = f(\vec{x}) + \nu_1 g_1(\vec{x}) + \nu_2 g_2(\vec{x})$$

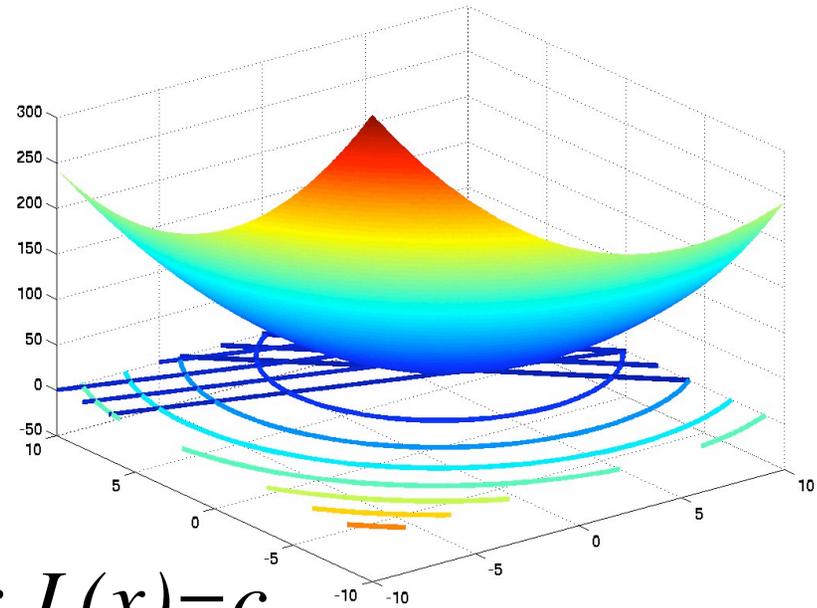
$$L(\vec{x}) = (x_1 - 4)^2 + (x_2 - 4)^2 + \nu_1(x_1 + x_2 - 6) + \nu_2(x_1 + 3x_2 - 4)$$

The Kuhn - Tucker conditions are :

$$\nabla L(\vec{x}) = 0, \quad \nu_i \geq 0, \quad \nu_i g_i(\vec{x}) = 0$$

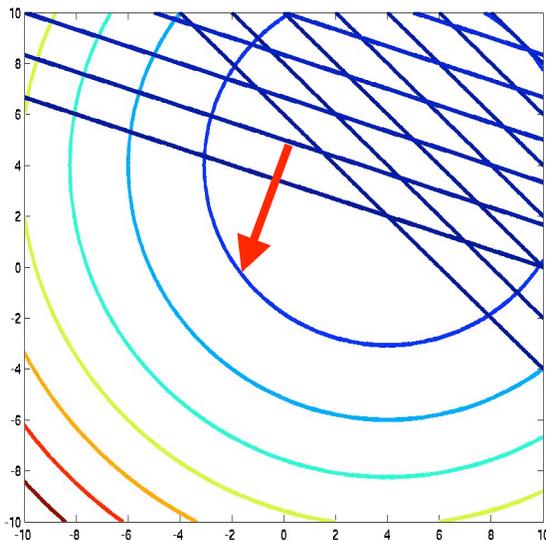
# What do the multipliers do?

Adding constraint shifts  $L(x)$  in direction of constraint normal

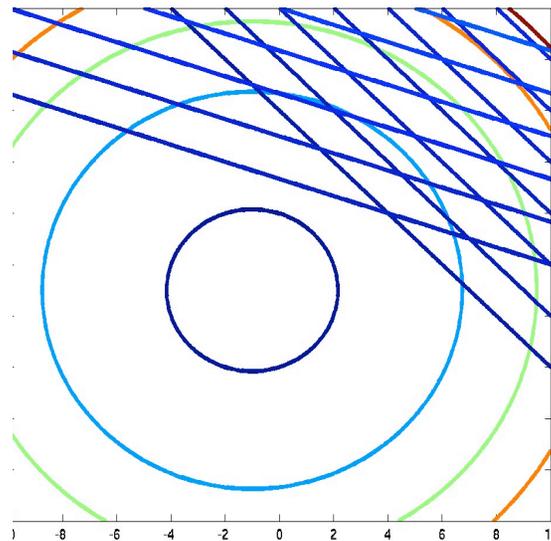


Circles:  $L(x) = c$

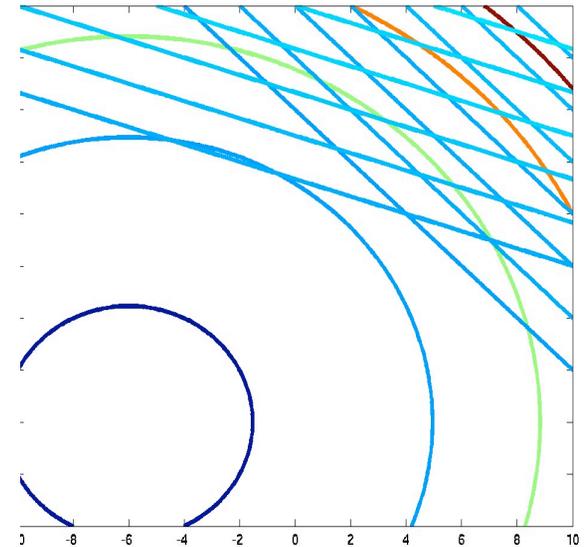
$$v_1 = 0, v_2 = 0$$



$$v_1 = 5, v_2 = 0$$



$$v_1 = 10, v_2 = 0$$



Kuhn-Tucker conditions:

$$\nabla L(\vec{x}) = \left[ \begin{array}{l} \frac{\partial L(\vec{x})}{\partial x_1} = 2(x_1 - 4) + v_1 + v_2 = 0 \\ \frac{\partial L(\vec{x})}{\partial x_2} = 2(x_2 - 4) + v_1 + 3v_2 = 0 \\ \frac{\partial L(\vec{x})}{\partial v_1} = (x_1 + x_2 - 6) \leq 0 \\ \frac{\partial L(\vec{x})}{\partial v_2} = (x_1 + 3x_2 - 4) \leq 0 \end{array} \right]$$

$$v_1 \geq 0$$

$$v_2 \geq 0$$

$$v_1(x_1 + x_2 - 6) = 0$$

$$v_2(x_1 + 3x_2 - 4) = 0$$

Solve for  $x$  in terms of  $v_1, v_2$   
Then substitute and solve for  
 $v_1, v_2$

$$x_1 = -(v_1 + v_2)/2 + 4$$

$$x_2 = -(v_1 + 3v_2)/2 + 4$$

Plugging in :

$$v_1(- (v_1 + v_2)/2 + 4 +$$

$$- (v_1 + 3v_2)/2 + 4 - 6) = 0$$

$$\Rightarrow v_1 = 0 \quad \text{or} \quad v_1 = 2 - 2v_2$$

$$v_2(- (v_1 + v_2)/2 + 4 +$$

$$3(- (v_1 + 3v_2)/2 + 4) - 4) = 0$$

$$v_2 = 0, \quad v_1 = (12 - 5v_2)/2$$

$$\text{if } v_1 = 0$$

$$v_2 = 12/5$$

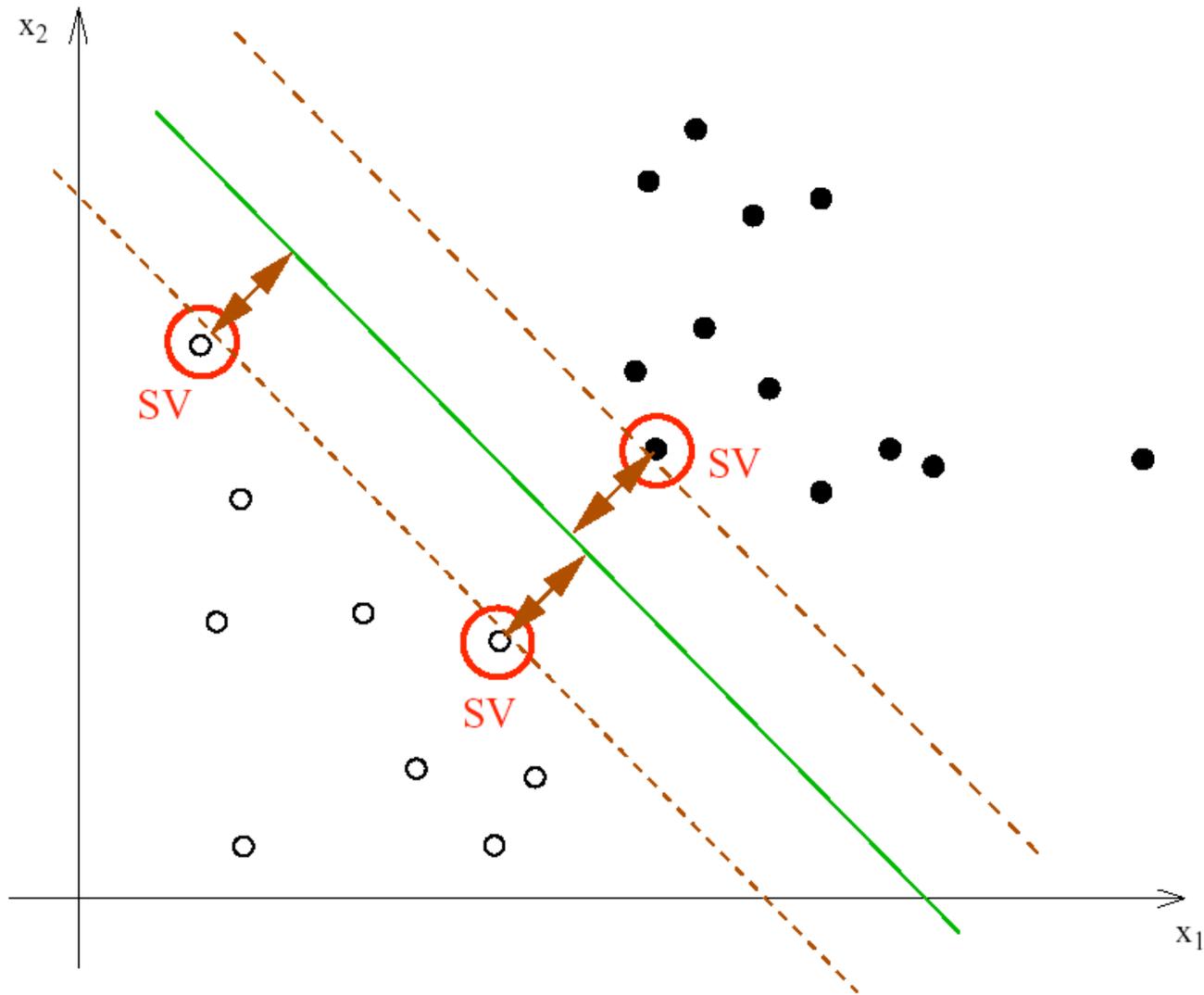
$$\text{if } v_1 = 2 - 2v_2$$

$$v_2 = 8$$

$$\text{but if } v_2 = 0$$

$$\Rightarrow v_1 = 2$$

# Support Vectors



# Now solve SVM problem

Maximizing the margin means minimizing  $|\mathbf{w}|$ .

But, subject to the inequality constraints :

$$C1: \quad y_i(\mathbf{w}^T \mathbf{x}_i + w_0) \geq 1 \quad i = 1, \dots, n.$$

This is constrained optimization and Khun - Tucker gives

$$L_p(\mathbf{w}, \boldsymbol{\alpha}) = \frac{1}{2} \mathbf{w}^T \mathbf{w} - \sum_{i=1}^n \alpha_i (y_i (\mathbf{w}^T \mathbf{x}_i + w_0) - 1).$$

Taking the derivatives with respect to  $w_0, w_1, \dots, w_p$  and set to zero :

# Now solve SVM problem

$$\frac{\partial L_P}{\partial w_j} = \frac{\partial}{\partial w_j} \left[ \frac{1}{2} \mathbf{w}^T \mathbf{w} - \sum_{t=1}^n \alpha_i (y_t (\mathbf{w}^T \mathbf{x}_t + w_0) - 1) \right] = 0 \quad \text{gives}$$

$$\sum_{t=1}^n \alpha_i y_t = 0, \quad \leftarrow \left( \frac{\partial L}{\partial w_0} \right)$$

$$\left. \begin{aligned} w_1 - \sum_{t=1}^n \alpha_i y_t x_{1,t} &= 0 \\ w_2 - \sum_{t=1}^n \alpha_i y_t x_{2,t} &= 0 \\ &\square \\ w_p - \sum_{t=1}^n \alpha_i y_t x_{p,t} &= 0 \end{aligned} \right\} \mathbf{w} = \sum_{t=1}^n \alpha_i y_t \mathbf{x}_t$$

*Kernel trick*

Substitute this in the Lagrangian, to get the *dual form* :

$$L_D = \sum_{t=1}^n \alpha_i - \frac{1}{2} \sum_{t=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_t y_j \mathbf{x}_t^T \mathbf{x}_j$$

*All we need is inner products!*

this quadratic function of  $\mathbf{a}$  has to be maximized subject to:  $\alpha_i \geq 0 \quad \sum_{t=1}^n \alpha_i y_t = 0.$

Actual optimization is done by standard general purpose quadratic programming package.

A point is not allowed to lie within the margin :

$$y_i(\mathbf{w}^T \mathbf{x}_i + w_0) - 1 \geq 0 \quad i = 1, \dots, n.$$

In the optimal situation we have :

$$\alpha_i (y_i(\mathbf{w}^T \mathbf{x}_i + w_0) - 1) = 0 \quad i = 1, \dots, n..$$

The Lagrange multipliers  $\alpha_i$  are non - negative, so :

if

$$y_i(\mathbf{w}^T \mathbf{x}_i + w_0) - 1 = 0 \quad (\text{point on the margin})$$

then  $\alpha_i \geq 0$ , (*active constraint*) otherwise

$\alpha_i = 0$  (*inactive constraint*).

Points with  $\alpha_i \geq 0$  are called *support vectors*

# Classification with support vector machines

---

Once the  $\alpha_i$ 's have been determined the value of  $\mathbf{w}$  can be determined

$$\mathbf{w} = \sum_{t=1}^n \alpha_i y_t \mathbf{x}_t = \sum_{t \in SV} \alpha_i y_t \mathbf{x}_t$$

and the value of  $w_0$  can be determined from

$\alpha_i y_t (\mathbf{w}^T \mathbf{x}_t + w_0) - 1 = 0$  for any  $t$  as support vector or as the average :

$$n_{sv} w_0 + \mathbf{w}^T \sum_{t \in SV} \mathbf{x}_t = \sum_{t \in SV} y_t$$

A new pattern is classified according to the sign of

$$\mathbf{w}^T \mathbf{x} + w_0.$$

Substituting  $\mathbf{w}$  and  $w_0$  gives : assign  $\mathbf{x}$  to class  $\omega_1$  if

$$\sum_{t \in SV} \alpha_i y_t \mathbf{x}_t^T \mathbf{x} - \frac{1}{n_{sv}} \sum_{t \in SV} \sum_{j \in SV} \alpha_i y_t \mathbf{x}_t^T \mathbf{x}_j + \frac{1}{n_{sv}} \sum_{t \in SV} y_t > 0$$

*note* : only first term depends on new data pattern  $\mathbf{x}$ !

## Why it is Good to Have Few SVs

---

Leave out an example that does not become SV  $\longrightarrow$  same solution.

**Theorem [66]:** Denote  $\#SV(m)$  the number of SVs obtained by training on  $m$  examples randomly drawn from  $P(\mathbf{x}, y)$ , and  $\mathbf{E}$  the expectation. Then

$$\mathbf{E} [\text{Prob}(\text{test error})] \leq \frac{\mathbf{E} [\#SV(m)]}{m}$$

Here,  $\text{Prob}(\text{test error})$  refers to the expected value of the risk, where the expectation is taken over training the SVM on samples of size  $m - 1$ .

# Nonlinear support vector machines

---

We seek a discriminant function

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

with decision rule:

$$\mathbf{w}^T \phi(\mathbf{x}) + w_0 \begin{cases} > 0 \\ < 0 \end{cases} \Rightarrow \mathbf{x} \in \begin{cases} \omega_1 \text{ with corresponding value } y_i = +1 \\ \omega_2 \text{ with corresponding value } y_i = -1 \end{cases}$$

The dual form of the Lagrangian now becomes:

$$L_D = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j \phi^T(\mathbf{x}_i) \phi(\mathbf{x}_j)$$

solution (expressed in support vectors):

$$\mathbf{w} = \sum_{i \in SV} \alpha_i y_i \phi(\mathbf{x}_i)$$

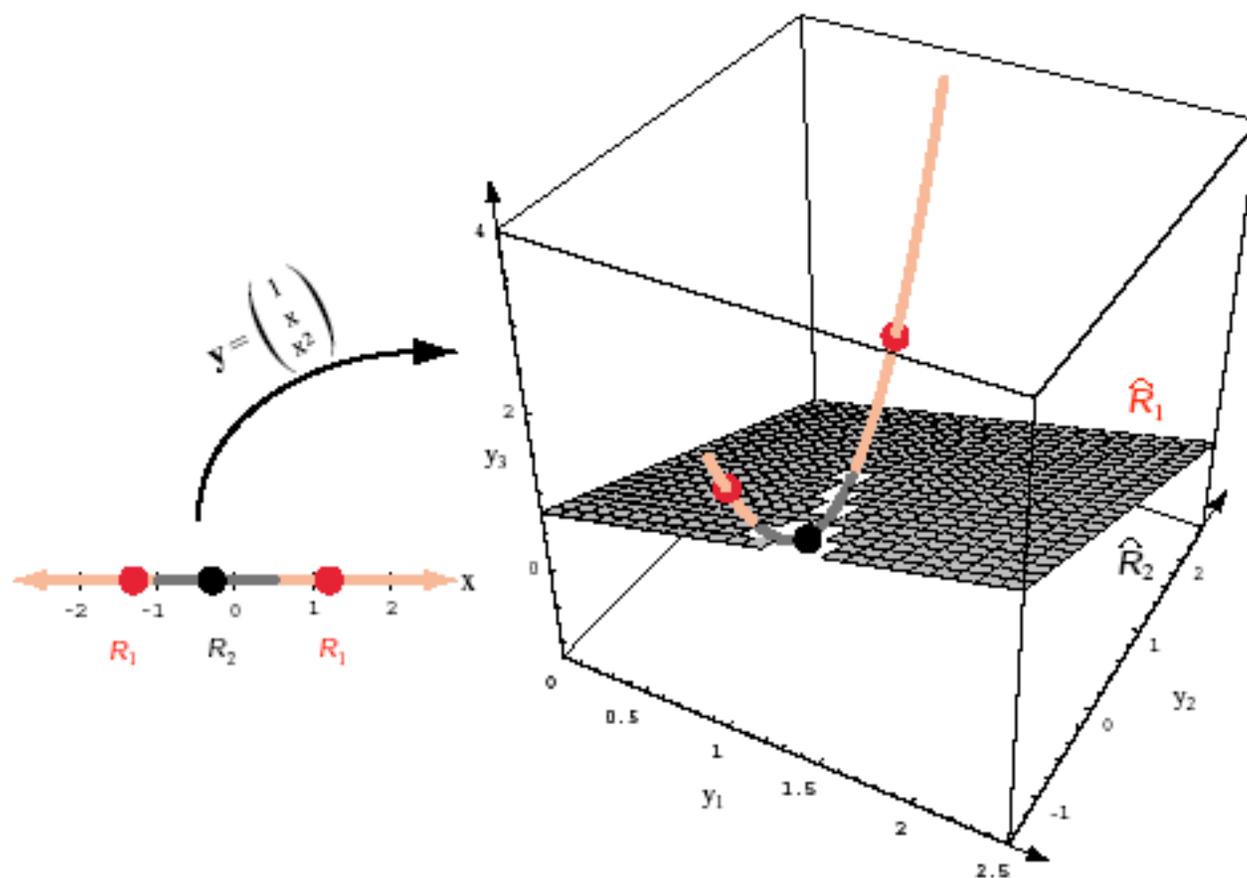


Figure 5.5: The mapping  $\mathbf{y} = (1, x, x^2)^t$  takes a line and transforms it to a parabola in three dimensions. A plane splits the resulting  $\mathbf{y}$  space into regions corresponding to two categories, and this in turn gives a non-simply connected decision region in the one-dimensional  $x$  space.

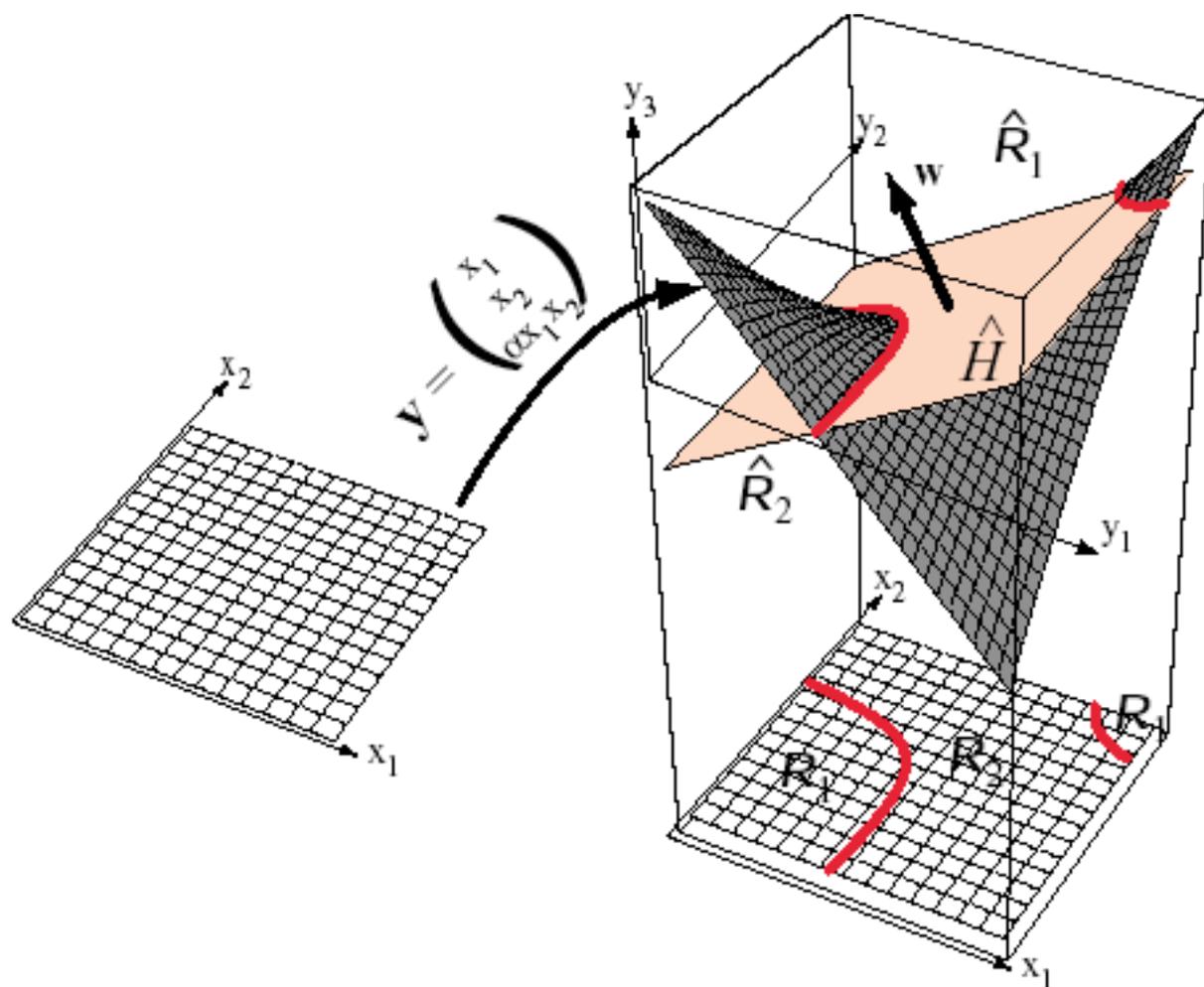


Figure 5.6: The two-dimensional input space  $\mathbf{x}$  is mapped through a polynomial function  $f$  to  $\mathbf{y}$ . Here the mapping is  $y_1 = x_1$ ,  $y_2 = x_2$  and  $y_3 \propto x_1 x_2$ . A linear discriminant in this transformed space is a hyperplane, which cuts the surface. Points to the positive side of the hyperplane  $\hat{H}$  correspond to category  $\omega_1$ , and those beneath it  $\omega_2$ . Here, in terms of the  $\mathbf{x}$  space,  $\mathcal{R}_1$  is a not simply connected.

# Kernels and Feature Spaces

---

Preprocess the data with

$$\begin{aligned}\Phi : \mathcal{X} &\rightarrow \mathcal{H} \\ x &\mapsto \Phi(x),\end{aligned}$$

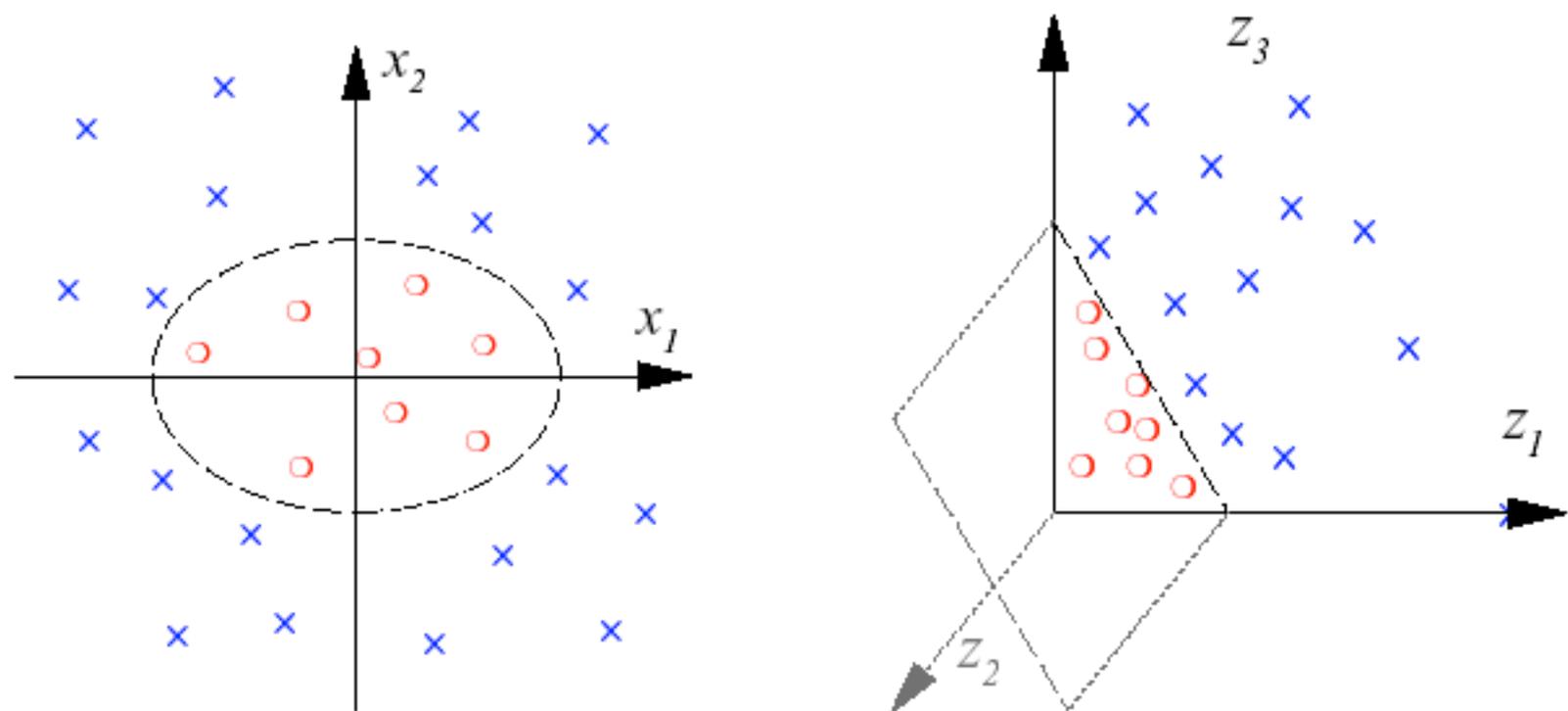
where  $\mathcal{H}$  is a dot product space, and learn the mapping from  $\Phi(x)$  to  $y$ .

- usually,  $\dim(\mathcal{X}) \ll \dim(\mathcal{H})$
- “Curse of Dimensionality”?
- crucial issue: *capacity*, not *dimensionality*

## Example: All Degree 2 Monomials

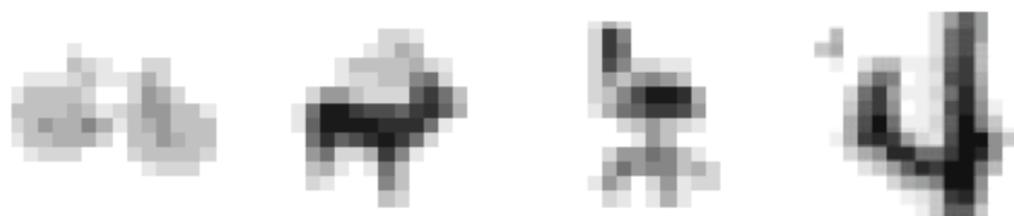
---

$$\Phi : \mathbb{R}^2 \rightarrow \mathbb{R}^3$$
$$(x_1, x_2) \mapsto (z_1, z_2, z_3) := (x_1^2, \sqrt{2} x_1 x_2, x_2^2)$$



## General Product Feature Space

---



How about patterns  $x \in \mathbb{R}^N$  and product features of order  $d$ ?

Here,  $\dim(\mathcal{H})$  grows like  $N^d$ .

E.g.  $N = 16 \times 16$ , and  $d = 5 \longrightarrow$  dimension  $10^{10}$

# The Kernel Trick, $N=2$ , $d=2$

---

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

$$\begin{aligned} (\langle x, z \rangle)^2 &= (x_1z_1 + x_2z_2)^2 \\ &= (x_1^2z_1^2 + 2x_1z_1x_2z_2 + x_2^2z_2^2) \\ &= \left\langle [x_1^2, \sqrt{2}x_1x_2, x_2^2], [z_1^2, \sqrt{2}z_1z_2, z_2^2] \right\rangle \\ &= \langle \Phi(\vec{x}), \Phi(\vec{z}) \rangle \\ &= K(\vec{x}, \vec{z}) \end{aligned}$$

- Thus the dot product in the non-linear feature space can be computed in  $\mathfrak{R}^2$  via the kernel function.

## The Kernel Trick, II

---

More generally:  $x, x' \in \mathbb{R}^N$ ,  $d \in \mathbb{N}$ :

$$\begin{aligned}\langle x, x' \rangle^d &= \left( \sum_{j=1}^N x_j \cdot x'_j \right)^d \\ &= \sum_{j_1, \dots, j_d=1}^N x_{j_1} \cdots x_{j_d} \cdot x'_{j_1} \cdots x'_{j_d} = \langle \Phi(x), \Phi(x') \rangle,\end{aligned}$$

where  $\Phi$  maps into the space spanned by all ordered products of  $d$  input directions

## The Kernel Trick — Summary

---

- *any* algorithm that only depends on dot products can benefit from the kernel trick
- this way, we can apply linear methods to vectorial as well as *non-vectorial data*
- think of the kernel as a nonlinear *similarity measure*
- examples of common kernels:

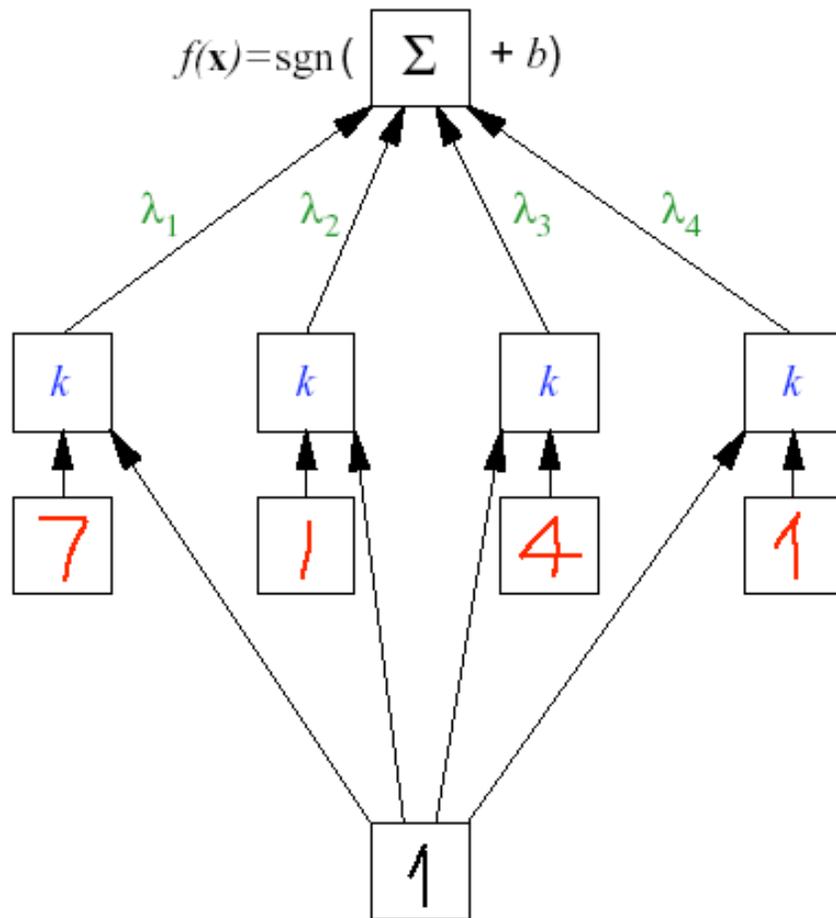
$$\text{Polynomial } k(x, x') = (\langle x, x' \rangle + c)^d$$

$$\text{Sigmoid } k(x, x') = \tanh(\kappa \langle x, x' \rangle + \Theta)$$

$$\text{Gaussian } k(x, x') = \exp(-\|x - x'\|^2 / (2\sigma^2))$$

- Kernel are studied also in the Gaussian Process prediction community (covariance functions) [71, 68, 72, 40] —  
course

# The SVM Architecture



classification

weights

comparison:  $k(x, x_i)$ , e.g.  $k(x, x_i) = (x \cdot x_i)^d$

support vectors  
 $x_1 \dots x_4$

input vector  $x$

$$f(\mathbf{x}) = \text{sgn}(\sum \lambda_i k(\mathbf{x}, \mathbf{x}_i) + b)$$

$$k(\mathbf{x}, \mathbf{x}_i) = \exp(-\|\mathbf{x} - \mathbf{x}_i\|^2 / c)$$

$$k(\mathbf{x}, \mathbf{x}_i) = \tanh(\kappa(\mathbf{x} \cdot \mathbf{x}_i) + \theta)$$

# Classification

---

A new pattern is classified according to the sign of  $\mathbf{w}^T \phi(\mathbf{x}) + w_0$ .

Substituting  $\mathbf{w}$  gives :

$$g(\mathbf{x}) = \sum_{i \in SV} \alpha_i y_i \phi^T(\mathbf{x}_i) \phi(\mathbf{x}) + w_0, \text{ in which}$$

$$w_0 = \frac{1}{N_{\tilde{SV}}} \left\{ \sum_{i \in SV} y_i - \sum_{i \in SV, j \in SV} \alpha_i y_i \phi^T(\mathbf{x}_i) \phi(\mathbf{x}_j) \right\}.$$

Note that classification depends only on inner products of transformed feature vectors  $\phi(\mathbf{x})$ .

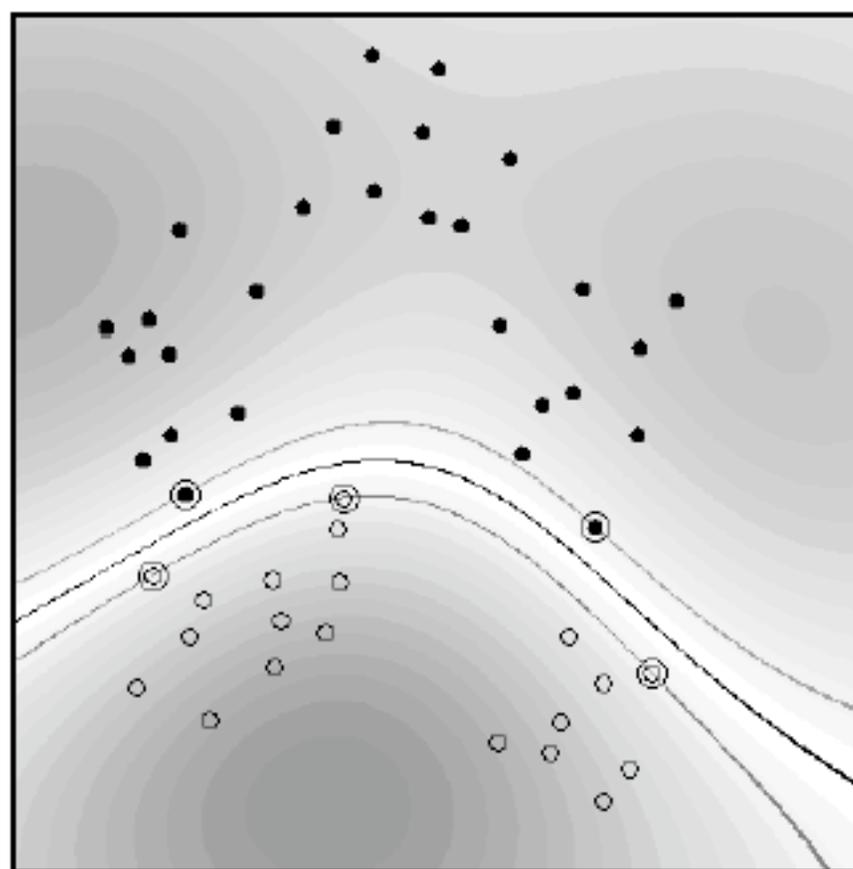
Some feature spaces come with a kernel  $\mathbf{K}$  (or vice versa) such that :

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

## Toy Example with Gaussian Kernel

---

$$k(x, x') = \exp\left(-\|x - x'\|^2\right)$$



# Simple example (XOR problem)

$$\Phi(w) = \frac{1}{2} w^T w$$

$$L(w, b, \alpha) = \frac{1}{2} w^T w - \sum_{i=1}^N \alpha_i [y_i (w^T x_i + b) - 1]$$

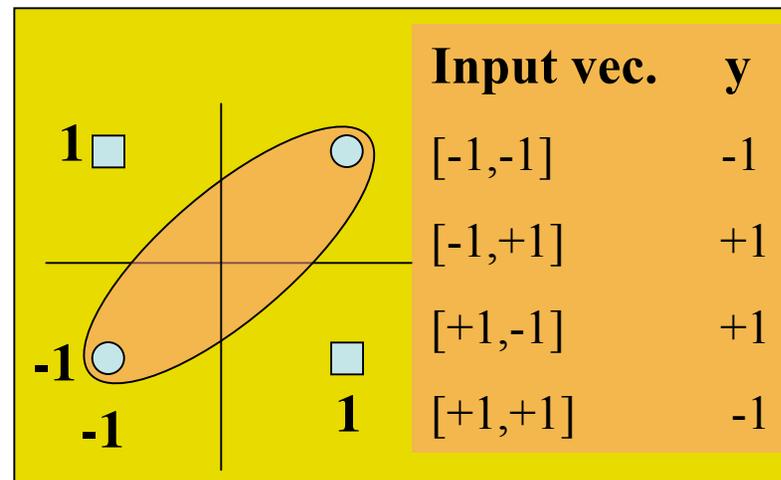
$$Q(\alpha) = \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j y_i y_j \varphi(x_i)^T \varphi(x_j)$$

$$Q(\alpha) = \sum_{i=1}^N \alpha_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j y_i y_j K(x_i, x_j)$$

$$\varphi(x) = [1, x_1^2, \sqrt{2}x_1 x_2, x_2^2, \sqrt{2}x_1, \sqrt{2}x_2]^T$$

$$K(x, x_i) = (1 + x^T x_i)^2$$

$$= 1 + x_1^2 x_{i1}^2 + 2x_1 x_{i1} x_2 x_{i2} + x_2^2 x_{i2}^2 + 2x_1 x_{i1} + 2x_2 x_{i2}$$



$K$  evaluated for all pairs of inputs:

$$K = \begin{bmatrix} 9 & 1 & 1 & 1 \\ 1 & 9 & 1 & 1 \\ 1 & 1 & 9 & 1 \\ 1 & 1 & 1 & 9 \end{bmatrix}$$

# Simple example(cont.)

## Dual formulation

$$Q(\alpha) = \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 \\ - \frac{1}{2}(9\alpha_1^2 - 2\alpha_1\alpha_2 - 2\alpha_1\alpha_3 + 2\alpha_1 + 9\alpha_2^2 \\ + 2\alpha_2\alpha_3 - 2\alpha_2\alpha_4 + 9\alpha_3^2 - 2\alpha_3\alpha_4 + 9\alpha_4^2)$$

$$9\alpha_1 - \alpha_2 - \alpha_3 + \alpha_4 = 1 \\ -\alpha_1 + 9\alpha_2 + \alpha_3 - \alpha_4 = 1 \\ -\alpha_1 + \alpha_2 + 9\alpha_3 - \alpha_4 = 1 \\ \alpha_1 - \alpha_2 - \alpha_3 + 9\alpha_4 = 1$$

$$\alpha_{o,1} = \alpha_{o,2} = \alpha_{o,3} = \alpha_{o,4} = \frac{1}{8}$$

$$Q_o(\alpha) = \frac{1}{4} \text{ Four Input vectors are} \\ \text{All support vectors}$$

$$\frac{1}{2} \|w_o\|^2 = \frac{1}{4}, \|w_o\| = \frac{1}{\sqrt{2}}$$

$$w_o = \sum_{i=1}^N \alpha_i y_i \varphi(x_i)$$

# Nonseparable Problems

---

If  $y_i \cdot (\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \geq 1$  cannot be satisfied, then  $\alpha_i \rightarrow \infty$ .

Modify the constraint to

$$y_i \cdot (\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \geq 1 - \xi_i$$

with

$$\xi_i \geq 0$$

(“*soft margin*”) and add

$$C \cdot \sum_{i=1}^m \xi_i$$

in the objective function.