

# Machine Learning

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## Session 7 Support Vector Machines

Optimal separating Hyperplanes

SVM: Primal and dual formulations

Example

The non separable case

Non Linear svm

Example

From

S. Theodoridis, K.Koutroumbas. Pattern Recognition Elsevier 2009, 3.7.{1,2}

Slides of Ricardo Gutierrez-Osuna

Bishop, 7, 7.1

# 'Optimal' Separating Hyperplane

- Problem Statement

- Consider the problem of finding an **optimal** separating hyperplane for a **linearly separable** dataset.

$$\{(\mathbf{x}^{(n)}, y^{(n)})\}, n = 1, \dots, N \quad \mathbf{x}^{(n)} \in \mathbb{R}^D, y^{(n)} \in \{+1, -1\}$$

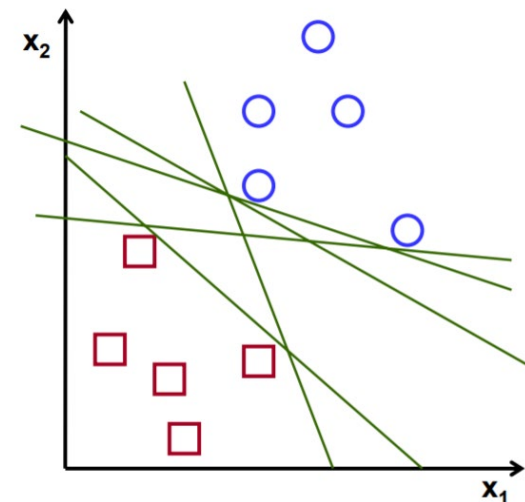
- Which hyperplane would you choose?

- The hyperplane is:

$$\mathbf{w}^T \mathbf{x} + b = 0$$

- The discriminant function is

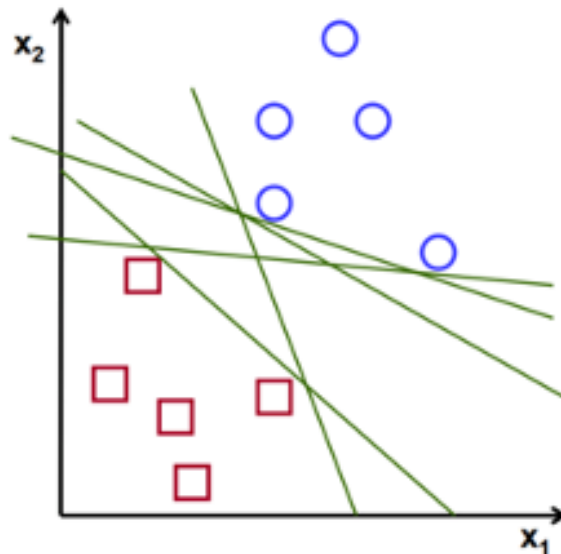
$$g(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b$$



# Optimal Separating Hyperplane

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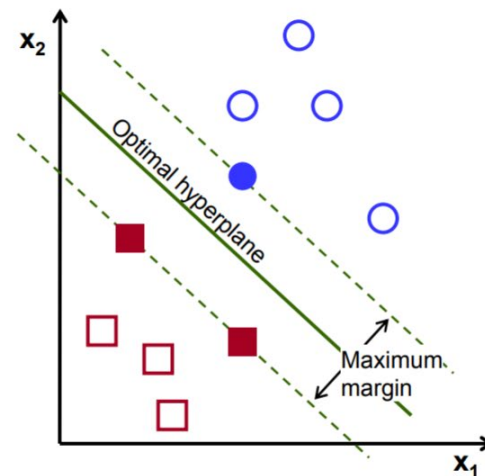
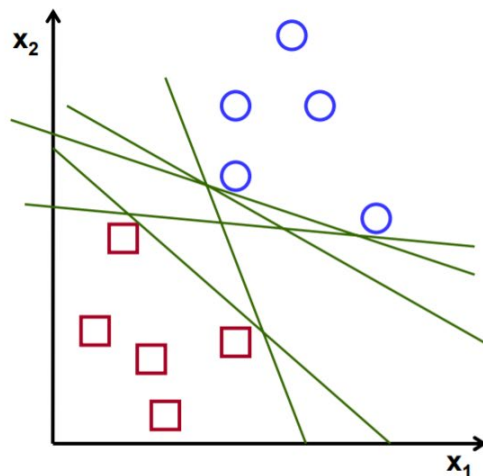
- Which hyperplane would you choose?
  - A hyperplane that passes too close to the training examples will be sensitive to noise and less likely to generalize well for unseen data
  - Instead, it seems reasonable to expect that a hyperplane that is farthest from all training examples will generalize better



# Optimal Separating Hyperplane

- Problem Statement

- Which hyperplane would you choose?
  - A hyperplane that passes too close to the training examples will be sensitive to noise and less likely to generalize well for unseen data
  - Instead, it seems reasonable to expect that a hyperplane that is farthest from all training examples will generalize better
- The optimal separating hyperplane will be the one with the largest **margin**, which is defined as **two times the minimum distance** of an example to the decision surface.

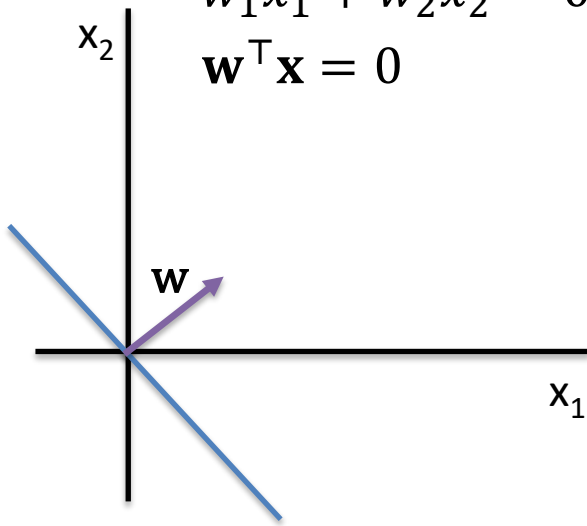


# Optimal Separating Hyperplane

- Geometry:** let's express the margin as a function of the weight vector and bias of the separating hyperplane

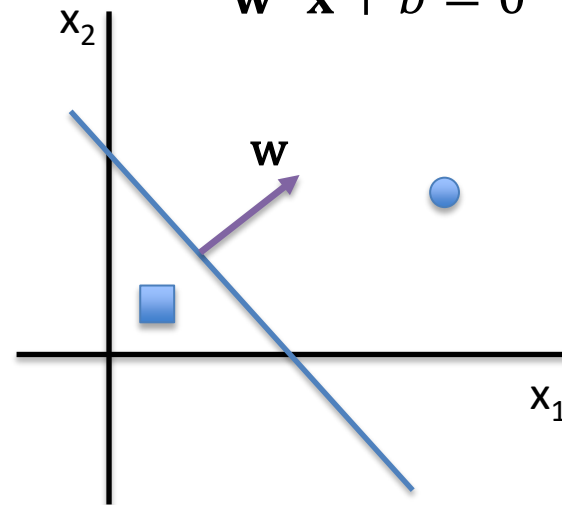
**Remember:**

$$w_1x_1 + w_2x_2 = 0$$
$$\mathbf{w}^T \mathbf{x} = 0$$



$\mathbf{x}$  are the points orthogonal to  $\mathbf{w}$

$$w_1x_1 + w_2x_2 + b = 0$$
$$\mathbf{w}^T \mathbf{x} + b = 0$$



The **discriminant** is  $g(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b$   
 $g(\bullet) > 0$  class +1  
 $g(\blacksquare) < 0$  class -1

With this language  $\mathbf{x}$  could be of  $D$  dimensions

# Optimal Separating Hyperplane

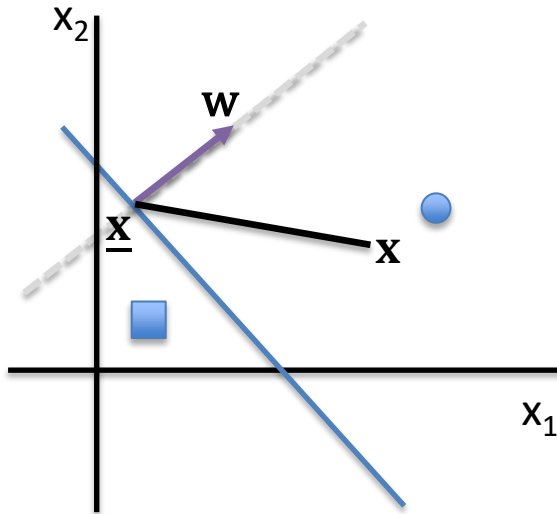
- **Geometry:** let's express the margin as a function of the weight vector and bias of the separating hyperplane.
- Step 1: The distance between a point  $\mathbf{x}$  and a hyperplane  $(\mathbf{w}, b)$  is

$$\frac{|\mathbf{w}^\top \mathbf{x} + b|}{\|\mathbf{w}\|}$$

Project the difference between  $\mathbf{x}$  and a point  $\underline{\mathbf{x}}$  in the hyperplane

$$\frac{\mathbf{w}^\top}{\|\mathbf{w}\|} (\mathbf{x} - \underline{\mathbf{x}}) = \frac{\mathbf{w}^\top \mathbf{x}}{\|\mathbf{w}\|} - \frac{\mathbf{w}^\top \underline{\mathbf{x}}}{\|\mathbf{w}\|} = \frac{\mathbf{w}^\top \mathbf{x}}{\|\mathbf{w}\|} + \frac{b}{\|\mathbf{w}\|} = \frac{\mathbf{w}^\top \mathbf{x} + b}{\|\mathbf{w}\|}$$

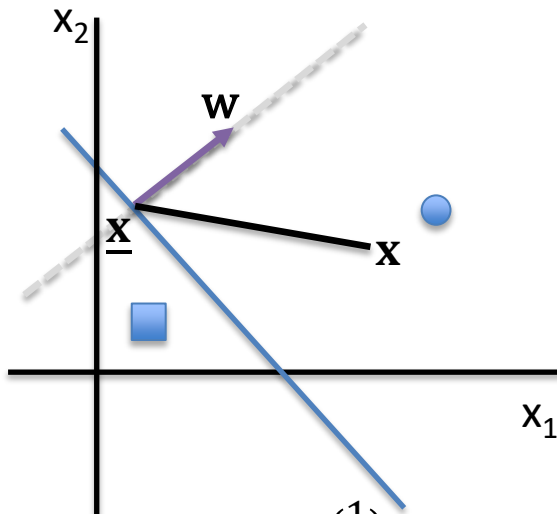
$\underline{\mathbf{x}}$  in the hyperplane  $\mathbf{w}^\top \underline{\mathbf{x}} + b = 0$ , then:  $\mathbf{w}^\top \underline{\mathbf{x}} = -b$



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$\underline{\mathbf{x}}$  in the hyperplane  $\mathbf{w}^\top \underline{\mathbf{x}} + b = 0$ , then:  $\mathbf{w}^\top \underline{\mathbf{x}} = -b$

For example  $\mathbf{x}^{(1)} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$  and the hyperplane  $x_1 + x_2 - 1 = 0$ ;

$$\text{dist}(\mathbf{x}^{(1)}, x_1 + x_2 - 1 = 0) = \left| \frac{(1,1) \begin{pmatrix} 1 \\ 1 \end{pmatrix} - 1}{\sqrt{1^2 + 1^2}} \right| = \left| \frac{1}{\sqrt{2}} \right| = \left| \frac{\sqrt{2}}{2} \right|$$

And  $\mathbf{x}^{(2)} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$  and the same hyperplane,  $\text{dist}(\mathbf{x}^{(2)}, x_1 + x_2 - 1 = 0) = \left| \frac{(1,1) \begin{pmatrix} 0 \\ 0 \end{pmatrix} - 1}{\sqrt{1^2 + 1^2}} \right| = \left| -\frac{\sqrt{2}}{2} \right|$   
(do the figure!)

# Optimal Separating Hyperplane

- **Geometry:** let's express the margin as a function of the weight vector and bias of the separating hyperplane.
- Step 1: The distance point  $\mathbf{x}$  and a hyperplane  $(\mathbf{w}, b)$  is  $\frac{|\mathbf{w}^\top \mathbf{x} + b|}{\|\mathbf{w}\|}$
- Step 2: the distance point-hyperplane is unique, but we can use several equations for the hyperplane. We impose that for the closest points to the hyperplane, we get  $\mathbf{w}^\top \mathbf{x} + b = 1$ . This is the **Canonical Hyperplane**



# Optimal Separating Hyperplane

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For example, if the closest point to  $x_1 + x_2 - 1 = 0$  is  $\mathbf{x}^{(n)} = \begin{pmatrix} 2 \\ 2 \end{pmatrix}$ , what would be the canonical hyperplane?

–  $(1, 1) \begin{pmatrix} 2 \\ 2 \end{pmatrix} - 1 = 3$  and we want 1 as the result. We take:

$$\left(\frac{1}{3}, \frac{1}{3}\right) \begin{pmatrix} 2 \\ 2 \end{pmatrix} - \frac{1}{3} = \frac{3}{3}$$

The canonical hyperplane will be

$$\frac{1}{3}x_1 + \frac{1}{3}x_2 - \frac{1}{3} = 0$$

- With these two steps, the two closest points to this canonical hyperplane will have distance  $\frac{1}{\|\mathbf{w}\|}$  and the margin will be:  $m = \frac{2}{\|\mathbf{w}\|}$

# Optimal Separating Hyperplane

- Geometry

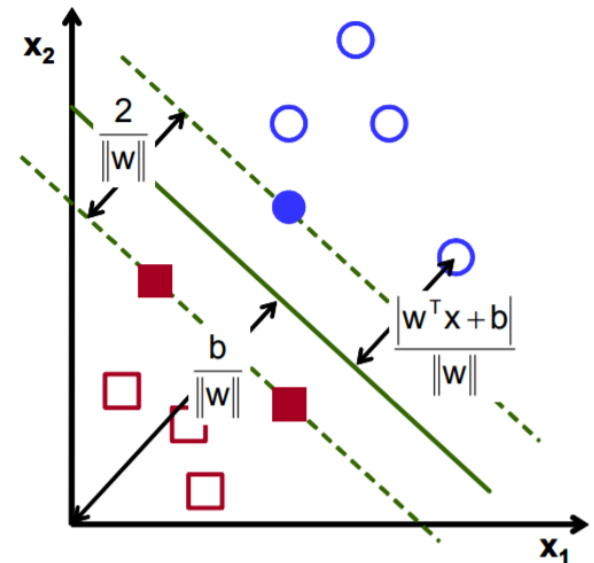
- We choose the solution for which the discriminant function becomes one for the training examples closest to the boundary

$$|\mathbf{w}^T \mathbf{x} + b| = 1$$

This is known as the **canonical hyperplane**

- Therefore, the distance from the closest example to the boundary is  $\frac{|\mathbf{w}^T \mathbf{x} + b|}{\|\mathbf{w}\|} = \frac{1}{\|\mathbf{w}\|}$ ,
- And the **margin becomes**

$$m = \frac{2}{\|\mathbf{w}\|}$$



We estimate  $\mathbf{w}$  in such a way that the margin becomes largest.

Equivalently: **minimize  $\|\mathbf{w}\|$**  such that it classifies well all the points

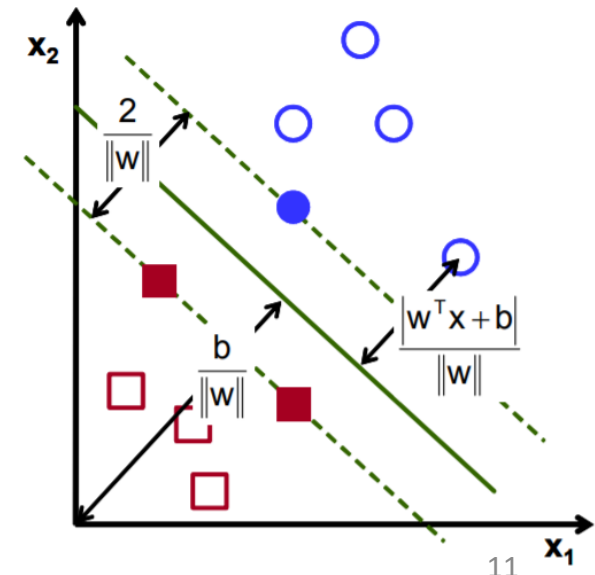
# Optimal Separating Hyperplane

- **Geometry** We want a  $\mathbf{w}$  minimum such that classifies well all the points.
- Step 3: Convert each point in a restriction:
  - If  $y^{(n)} = +1$ , we want  $\mathbf{w}^\top \mathbf{x}^{(n)} + b \geq +1$ , so we impose:  $y^{(n)}(\mathbf{w}^\top \mathbf{x}^{(n)} + b) \geq 1$
  - If  $y^{(n)} = -1$ , we want  $\mathbf{w}^\top \mathbf{x}^{(n)} + b \leq -1$ , so we impose:  $y^{(n)}(\mathbf{w}^\top \mathbf{x}^{(n)} + b) \geq 1$

We want the minimum of  $\|\mathbf{w}\| = \sqrt{x_1^2 + \dots + x_D^2}$  subject to a constraint (one constraint for each point)

$$y^{(n)}(\mathbf{w}^\top \mathbf{x}^{(n)} + b) \geq 1, \quad n = 1 \dots N$$

Once found  $\mathbf{w}$ , the **canonical** hyperplane is calculated and this discriminant function is our classifier



# The Optimization Problem

- The problem of maximizing the margin  $m = \frac{2}{||\mathbf{w}||}$  is equivalent to

$$\text{minimize } J(\mathbf{w}) = \frac{1}{2} ||\mathbf{w}||^2$$

$$\text{subject to } y^{(n)}(\mathbf{w}^\top \mathbf{x}^{(n)} + b) \geq 1, \quad \forall n = 1, \dots, N$$

- $J(\mathbf{w})$  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  $\Omega \subset \mathbb{R}^D$

$$\begin{array}{lll} \text{minimize} & f(\mathbf{z}) & \mathbf{z} \in \Omega \\ \text{subject to} & g_n(\mathbf{z}) \leq 0 & n \in 1, \dots, N \\ & h_m(\mathbf{z}) = 0 & m \in 1, \dots, M \end{array}$$

- With  $f \in C^1$  convex and  $g_n, h_m$  affine, necessary and sufficient conditions for a normal point  $\mathbf{z}^*$  to be an optimum are the existence of  $\boldsymbol{\alpha}^*, \boldsymbol{\beta}^*$  such that

$$\frac{\partial \mathcal{L}(\mathbf{z}^*, \boldsymbol{\alpha}^*, \boldsymbol{\beta}^*)}{\partial \mathbf{z}} = 0$$

$$\frac{\partial \mathcal{L}(\mathbf{z}^*, \boldsymbol{\alpha}^*, \boldsymbol{\beta}^*)}{\partial \boldsymbol{\beta}} = 0$$

$$\alpha_n^* g_n(\mathbf{z}^*) = 0 \quad n \in 1, \dots, N$$

$$g_n(\mathbf{z}^*) \leq 0 \quad n \in 1, \dots, N$$

$$\alpha_n^* \geq 0 \quad n \in 1, \dots, N$$

where  $\mathcal{L}(\mathbf{z}, \boldsymbol{\alpha}, \boldsymbol{\beta}) = f(\mathbf{z}) + \sum_{n=1}^N \alpha_n g_n(\mathbf{z}) + \sum_{m=1}^M \beta_m h_m(\mathbf{z})$  is known as *generalized Lagrangian function*

# Kuhn-Tucker Theorem

- The third condition:  $\alpha_n^* g_n(\mathbf{z}^*) = 0, \quad n \in 1, \dots, N$

is known as the Karush-Kuhn-Tucker (KKT) complementary condition. It implies that

for active constraints  $\rightarrow \alpha_n^* \geq 0$

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for inactive constraints  $\rightarrow \alpha_n^* = 0$

- The KKT condition will allows us to identify the training examples that define the largest margin hyperplane
  - For these examples,  $\alpha_n^* \geq 0$  and they are known as **Support Vectors**
  - For the rest of examples,  $\alpha_n^* = 0$

# The Lagrangian dual problem (1/4)

- Constrained minimization of  $J(\mathbf{w}) = \frac{1}{2} \|\mathbf{w}\|^2$  is solved by introducing the Lagrangian

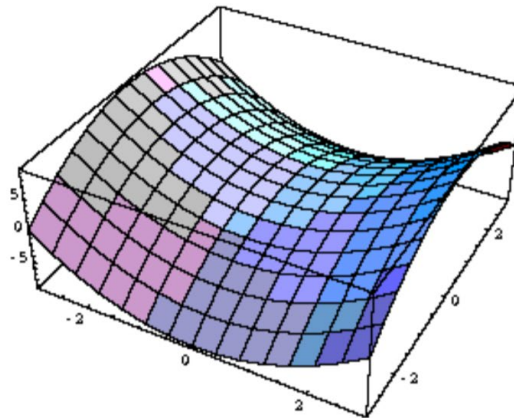
$$L_p(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{n=1}^N \alpha_n (y^{(n)} (\mathbf{w}^\top \mathbf{x}^{(n)} + b) - 1)$$

Which yields an unconstrained optimization problem that is solved by:

- Minimizing  $L_p$  with respect to the primal variables  $\mathbf{w}, b$  AND
- Maximizing  $L_p$  with respect to the dual variables  $\alpha_n$

Thus, the optimum is defined by a saddle point (see below for illustration)

This is known as the  
**Lagrangian primal problem**



**A saddle point**



# The Lagrangian dual problem (2/4)

- To simplify the primal problem, we eliminate the primal variables  $\mathbf{w}, b$  using the first Kuhn-Tucker condition  $\frac{\partial \mathcal{L}}{\partial \mathbf{z}} = 0$  on:

$$L_p(\mathbf{w}, b, \alpha) = \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{n=1}^N \alpha_n (y^{(n)} (\mathbf{w}^\top \mathbf{x}^{(n)} + b) - 1)$$

- Expansion of  $L_p$  yields

$$L_p(\mathbf{w}, b, \alpha) = \frac{1}{2} \mathbf{w}^\top \mathbf{w} - \sum_{n=1}^N \alpha_n y^{(n)} \mathbf{w}^\top \mathbf{x}^{(n)} - b \sum_{n=1}^N \alpha_n y^{(n)} + \sum_{n=1}^N \alpha_n$$

- Differentiating  $L_p(\mathbf{w}, b, \alpha)$  with respect to  $\mathbf{w}, b$ , and setting to zero yields

$$\frac{\partial L_p(\mathbf{w}, b, \alpha)}{\partial \mathbf{w}} = 0 \rightarrow \mathbf{w} = \sum_{n=1}^N \alpha_n y^{(n)} \mathbf{x}^{(n)}$$

$$\frac{\partial L_p(\mathbf{w}, b, \alpha)}{\partial b} = 0 \rightarrow \sum_{n=1}^N \alpha_n y^{(n)} = 0$$

# The Lagrangian dual problem (3/4)

$$L_p(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2} \mathbf{w}^\top \mathbf{w} - \sum_{n=1}^N \alpha_n y^{(n)} \mathbf{w}^\top \mathbf{x}^{(n)} - b \sum_{n=1}^N \alpha_n y^{(n)} + \sum_{n=1}^N \alpha_n$$

- Using the optimality condition  $\frac{\partial J}{\partial \mathbf{w}} = 0$ , the **first** term in  $L_p$  can be expressed as

$$\mathbf{w}^\top \mathbf{w} = \mathbf{w}^\top \sum_{n=1}^N \alpha_n y^{(n)} \mathbf{x}^{(n)} = \sum_{n=1}^N \alpha_n y^{(n)} \mathbf{w}^\top \mathbf{x}^{(n)}$$

$$\mathbf{w} = \sum_{m=1}^N \alpha_m y^{(m)} \mathbf{x}^{(m)}$$

$$= \sum_{n=1}^N \alpha_n y^{(n)} \left( \sum_{m=1}^N \alpha_m y^{(m)} \mathbf{x}^{(m)} \right)^\top \mathbf{x}^{(n)} = \sum_{n=1}^N \sum_{m=1}^N \alpha_n \alpha_m y^{(n)} y^{(m)} \mathbf{x}^{(m)\top} \mathbf{x}^{(n)}$$

- The second term in  $L_p$  can be expressed in the same way
- The third term in  $L_p$  is zero by virtue of the optimality condition  $\frac{\partial J}{\partial b} = 0$

# The Lagrangian dual problem (4/4)

- Merging these expressions together we obtain

$$L_D(\boldsymbol{\alpha}) = \sum_{n=1}^N \alpha_n - \frac{1}{2} \sum_{n=1}^N \sum_{m=1}^N \alpha_n \alpha_m y^{(n)} y^{(m)} \mathbf{x}^{(m)\top} \mathbf{x}^{(n)}$$

Subject to the simpler constraints  $\alpha_n \geq 0$  and  $\sum_{n=1}^N \alpha_n y^{(n)} = 0$

[the 1st term is the previous 3rd term and the 2nd one comes from  $(1/2 - 1)\mathbf{w}^\top \mathbf{w}$ ]

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- Remarks:
  - We have transformed the problem of finding a saddle point for  $L_p(\mathbf{w}, b, \boldsymbol{\alpha})$  into the easier one of maximizing  $L_D(\boldsymbol{\alpha})$ . Notice that  $L_D(\boldsymbol{\alpha})$  depends on the Lagrange multipliers  $\boldsymbol{\alpha}$ , but it **does not** depend on  $(\mathbf{w}, b)$

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  - The **primal problem scales with dimensionality  $D$**  ( $\mathbf{w}$  has one coefficient for each dimension), whereas **the dual problem scales with  $N$** , the amount of training data (there is one Lagrange multiplier  $\alpha_n$  per example)

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  - Moreover, the training data appears only as dot products  $\mathbf{x}_n^\top \mathbf{x}_m$

# Support Vectors

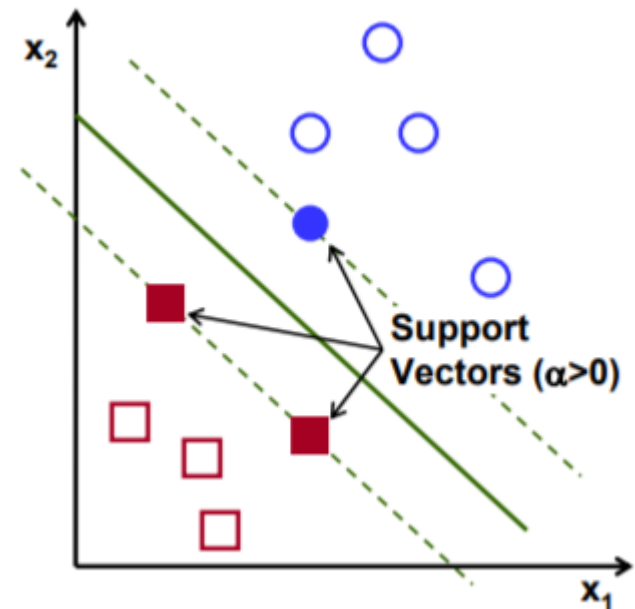
- The KKT complementary condition states that, for every point in the training set, the following equality must hold

$$\alpha_n (y^{(n)} (\mathbf{w}^\top \mathbf{x}^{(n)} + b) - 1) = 0 \quad \forall n = 1, \dots, N$$

- Therefore, for each example, either  $\alpha_n = 0$  or  $y^{(n)} (\mathbf{w}^\top \mathbf{x}^{(n)} + b - 1) = 0$  must hold
- Those points for which  $\alpha_n > 0$  must then lie on one of the two hyperplanes that define the largest margin (only at these hyperplanes the term  $y^{(n)} (\mathbf{w}^\top \mathbf{x}^{(n)} + b - 1)$  becomes zero)

These points are known as **Support Vectors**

- All the other must have  $\alpha_n = 0$



# Support Vectors

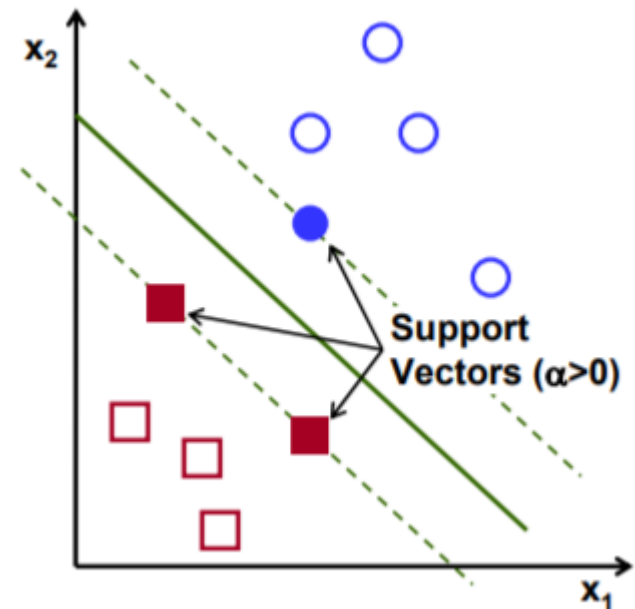
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- Therefore, for each example, either  $\alpha_n = 0$  or  $y^{(n)} (\mathbf{w}^\top \mathbf{x}^{(n)} + b) - 1 = 0$  must hold
- Note that only the support vectors contribute to defining the optimal hyperplane

$$\frac{\partial J(\mathbf{w}, b, \boldsymbol{\alpha})}{\partial \mathbf{w}} = 0 \rightarrow \mathbf{w} = \sum_{n=1}^N \alpha_n y^{(n)} \mathbf{x}^{(n)}$$

- The bias  $b$  is found from the KKT complementary condition on the support vectors
- Therefore, the complete dataset could be replaced by only the support vectors





# Example

- **Example:**  $\{(x^{(1)} = 1, y^{(1)} = +1), (x^{(2)} = -1, y^{(2)} = -1)\}$

We want the the maxim margin hyperplane that separate both classes.

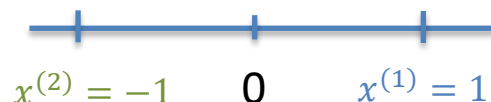
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- Plot the situation



- Model of the classifier for this case:  $g(x) = wx + b$

- $w$  will be the solution to:  $\min_w \frac{1}{2} ||\mathbf{w}\|^2 \rightarrow \min_w \frac{w^2}{2}$

subject to:  $y^{(n)}(\mathbf{w}^\top \mathbf{x}^{(n)} + b) \geq 1$  for  $n = 1$  and  $n = 2$

$$+1(w \cdot 1 + b) \geq 1 \rightarrow w + b - 1 \geq 0$$

$$-1(w \cdot (-1) + b) \geq 1 \rightarrow w - b - 1 \geq 0$$

- Primal

$$L_p(w, b, \alpha_1, \alpha_2) = \frac{w^2}{2} - \alpha_1(w + b - 1) - \alpha_2(w - b - 1) \quad (\text{note we put minus – before all constraints})$$

$$\frac{\partial L_p}{\partial w} = w - \alpha_1 - \alpha_2 = 0 \Rightarrow w = \alpha_1 + \alpha_2 \quad (\text{in general : } \mathbf{w} = \sum_{m=1}^N \alpha_m y^{(m)} \mathbf{x}^{(m)})$$

$$\frac{\partial L_p}{\partial b} = -\alpha_1 + \alpha_2 = 0 \Rightarrow \alpha_1 = \alpha_2$$

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We have:  $w = \alpha_1 + \alpha_2$  and  $\alpha_1 = \alpha_2$  and  $w = 2\alpha_1$

To obtain the dual  $L_D(\alpha_1, \alpha_2)$  we need to substitute the previous result in

$$L_p(w, b, \alpha_1, \alpha_2) = \frac{w^2}{2} - \alpha_1(w + b - 1) - \alpha_2(w - b - 1)$$

$$L_D(\alpha_1, \alpha_2) = \frac{2\alpha_1}{2} - \alpha_1(2\alpha_1 + b - 1) - \alpha_1(2\alpha_1 - b - 1) = 2\alpha_1^2 - 4\alpha_1 + 2\alpha_1 = -2\alpha_1^2 + 2\alpha_1$$

$$\frac{\partial L_D(\alpha_1, \alpha_2)}{\partial \alpha_1} = -4\alpha_1 + 2 = 0 \rightarrow \alpha_1 = \frac{1}{2}$$

Then  $w = \alpha_1 + \alpha_2 = \frac{1}{2} + \frac{1}{2} = 1 \Rightarrow$  both points are Support Vectors

- The classifier will be  $g(x) = 1x + b$

over the support  $x^{(1)} : g(x^{(1)}) = g(1) = 1 + b = 1$

over the support  $x^{(2)} : g(x^{(2)}) = g(-1) = -1 + b = -1$

} Then b=0

The classifier will be  $g(x) = x$  and the Margin  $\frac{2}{||1||} = 2$

# Example

- Example:**  $\{(x^{(1)} = 1, y^{(1)} = +1), (x^{(2)} = -1, y^{(2)} = -1)\}$

We want the the maxim margin hyperplane that separate both classes

- Plot the situation



There is an alternative way to obtain the result, using only the dual and the two results of the primal

From the primal we know:

$$\begin{aligned} \mathbf{w} &= \sum_{n=1}^N \alpha_n y^{(n)} x^{(n)} = (+1)\alpha_1(+1) + (-1)\alpha_2(-1) = \alpha_1 + \alpha_2 \\ \sum_{n=1}^N \alpha_n y^{(n)} &= 0 \Rightarrow \alpha_1 - \alpha_2 = 0 \end{aligned}$$

The dual (in matrix notation):

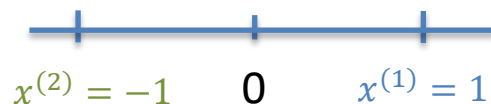
$$\begin{aligned} L_D(\boldsymbol{\alpha}) &= \sum_{n=1}^N \alpha_n - \frac{1}{2} \sum_{n=1}^N \sum_{m=1}^N \alpha_n \alpha_m y^{(n)} y^{(m)} \mathbf{x}^{(m)\top} \mathbf{x}^{(n)} = \\ &= (\alpha_1 \dots \alpha_N) \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} - \frac{1}{2} (\alpha_1 \dots \alpha_N) \begin{pmatrix} y^{(1)} \mathbf{x}^{(1)\top} \mathbf{x}^{(1)} y^{(1)} & \dots & y^{(1)} \mathbf{x}^{(1)\top} \mathbf{x}^{(N)} y^{(N)} \\ \vdots & \dots & \vdots \\ y^{(N)} \mathbf{x}^{(N)\top} \mathbf{x}^{(1)} y^{(1)} & \dots & y^{(N)} \mathbf{x}^{(N)\top} \mathbf{x}^{(N)} y^{(N)} \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_N \end{pmatrix} = \\ &= (\alpha_1 \dots \alpha_N) \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} - \frac{1}{2} (\alpha_1 \dots \alpha_N) \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} \end{aligned}$$

# Example

- Example:**  $\{(x^{(1)} = 1, y^{(1)} = +1), (x^{(2)} = -1, y^{(2)} = -1)\}$

We want the the maxim margin hyperplane that separate both classes

- Plot the situation



There is an alternative way to obtain the result, using only the dual and the two results of the primal

$$L_D(\alpha_1, \alpha_2) = (\alpha_1, \alpha_2) \begin{pmatrix} 1 \\ 1 \end{pmatrix} - \frac{1}{2} = (\alpha_1, \alpha_2) \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}$$

$$\frac{\partial L_D}{\partial \alpha} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} - \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Rightarrow 1 = \alpha_1 + \alpha_2$$

From the primal we know:

- $\mathbf{w} = \alpha_1 + \alpha_2$
- $\alpha_1 - \alpha_2 = 0$

Then:  $\alpha_1 = \alpha_2$   $1 = 2 \alpha_1$  and  $\alpha_1 = \alpha_2 = 1/2$   
 $w=1$

**The classifier will be**  $g(x) = x$  **and the Margin**  $\frac{2}{\|1\|} = 2$

Using

$$\frac{\partial \mathbf{a}^\top \mathbf{x}}{\partial \mathbf{x}} = \mathbf{a}$$

and for  $\mathbf{A}$  symmetric matrix

$$\frac{\partial \mathbf{x}^\top \mathbf{A} \mathbf{x}}{\partial \mathbf{x}} = 2\mathbf{A}\mathbf{x}$$

# Example (recap)

From the set learning points

- plot the points and write the model  $g(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + b$
- For each point, create the constraints, formulate the primal and obtain:
  - $\mathbf{w} = \sum_{n=1}^N \alpha_n \mathbf{y}^{(n)} \mathbf{x}^{(n)}$  the vector is a linear combination of only Support Vectors
  - $\sum_{n=1}^N \alpha_n \mathbf{y}^{(n)} = 0$
- Formulate the Dual

$$\cdot \quad L_D(\boldsymbol{\alpha}) = (\alpha_1 \dots \alpha_N) \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} - \frac{1}{2} (\alpha_1 \dots \alpha_N) \begin{pmatrix} \mathbf{y}^{(1)} \mathbf{x}^{(1)\top} \mathbf{x}^{(1)} \mathbf{y}^{(1)} & \dots & \mathbf{y}^{(1)} \mathbf{x}^{(1)\top} \mathbf{x}^{(N)} \mathbf{y}^{(N)} \\ \vdots & \dots & \vdots \\ \mathbf{y}^{(N)} \mathbf{x}^{(N)\top} \mathbf{x}^{(1)} \mathbf{y}^{(1)} & \dots & \mathbf{y}^{(N)} \mathbf{x}^{(N)\top} \mathbf{x}^{(N)} \mathbf{y}^{(N)} \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_N \end{pmatrix}$$

$$\text{Obtain: } \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} = \begin{pmatrix} \mathbf{y}^{(1)} \mathbf{x}^{(1)\top} \mathbf{x}^{(1)} \mathbf{y}^{(1)} & \dots & \mathbf{y}^{(1)} \mathbf{x}^{(1)\top} \mathbf{x}^{(N)} \mathbf{y}^{(N)} \\ \vdots & \dots & \vdots \\ \mathbf{y}^{(N)} \mathbf{x}^{(N)\top} \mathbf{x}^{(1)} \mathbf{y}^{(1)} & \dots & \mathbf{y}^{(N)} \mathbf{x}^{(N)\top} \mathbf{x}^{(N)} \mathbf{y}^{(N)} \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_N \end{pmatrix}$$

Find  $\alpha_1 \dots \alpha_N$

The  $\alpha_i \neq 0$  are the Support Vectors

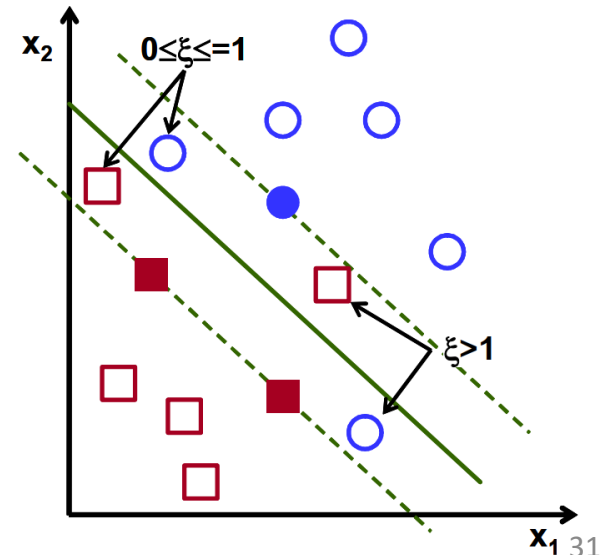
Impose that in the model the supports give +1 or -1, and calculate  $b$

# The non-separable case

- So far, we focused on **linearly separable** problems
  - SVMs can be modified to handle datasets that are *non*-linearly separable
- **Solution**
  - The solution for the non-separable case is to *introduce slack variables* that relax the constraints of the canonical hyperplane equation

$$y^{(n)}(\mathbf{w}^\top \mathbf{x}^{(n)} + b) \geq 1 - \xi_n \quad \forall n = 1, \dots, N$$

- For  $0 \leq \xi_n \leq 1$ , the data points fall on the **right side** of the hyperplane, but within the region of maximum margin
- For  $\xi_n > 1$ , the data points fall on the **wrong side** of the hyperplane



# The non-separable case

- We minimize the following objective

$$\begin{aligned} \text{minimize} \quad & J(\mathbf{w}, \boldsymbol{\xi}) = \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{n=1}^N \xi_n \\ \text{subject to} \quad & y^{(n)}(\mathbf{w}^\top \mathbf{x}^{(n)} + b) \geq 1 - \xi_n, \\ & \xi_n \geq 0, \quad \forall n = 1, \dots, N \end{aligned}$$

## Interpretation of $C$

- Represents a trade-off between misclassification and capacity
- **Large  $C$**  favors solutions with **few classification errors**
- **Small  $C$**  favors **low-complexity** solutions
- $C$  can be viewed as a **regularization parameter**
- Typically determined through **cross-validation**



# The non-separable case

## Solution

- We can derive the *dual problem* as

$$L_D(\boldsymbol{\alpha}) = \sum_{n=1}^N \alpha_n - \frac{1}{2} \sum_{n=1}^N \sum_{m=1}^N \alpha_n \alpha_m y^{(n)} y^{(m)} \mathbf{x}^{(m)\top} \mathbf{x}^{(n)}$$

subject to

$$\begin{aligned} 0 &\leq \alpha_n \leq C \\ \sum_{n=1}^N \alpha_n y^{(n)} &= 0 \end{aligned}$$

- **Remarks**

- Neither the slack variables nor associated Lagrange multipliers appear in the formulation
- The problem is the same as the linearly separable case, with the difference in the constraints  $0 \leq \alpha_n$  that become  $0 \leq \alpha_n \leq C$

# The non-separable case

## Solution

- We can derive the *dual problem* as

$$L_D(\boldsymbol{\alpha}) = \sum_{n=1}^N \alpha_n - \frac{1}{2} \sum_{n=1}^N \sum_{m=1}^N \alpha_n \alpha_m y^{(n)} y^{(m)} \mathbf{x}^{(m)\top} \mathbf{x}^{(n)}$$

subject to

$$\begin{aligned} 0 &\leq \alpha_n \leq C \\ \sum_{n=1}^N \alpha_n y^{(n)} &= 0 \end{aligned}$$

- Remarks**

- The optimum solution for the weights remains the same

$$\mathbf{w} = \sum_{n=1}^N \alpha_n y^{(n)} \mathbf{x}^{(n)}$$

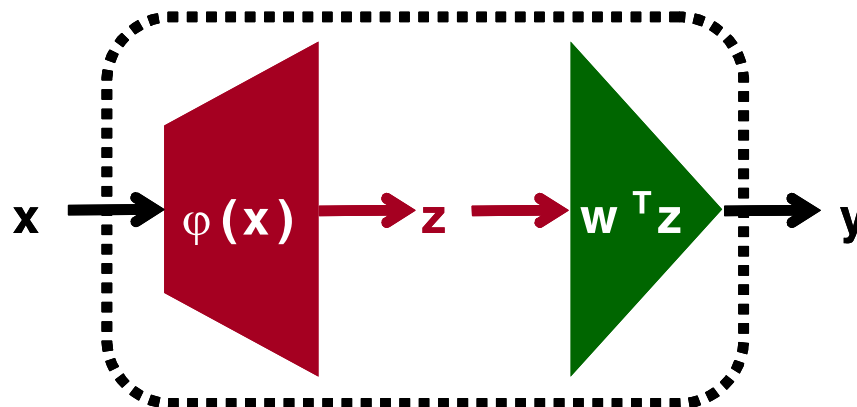
- The bias can be found with a training point for which  $0 < \alpha_n < C$  ( $\xi_n = 0$ )

$$\alpha_n [y^{(n)} (\mathbf{w}^\top \mathbf{x}^{(n)} + b) - 1 + \xi_n] = 0$$

# Non-linear SVMs

## Cover's theorem on the separability of patterns

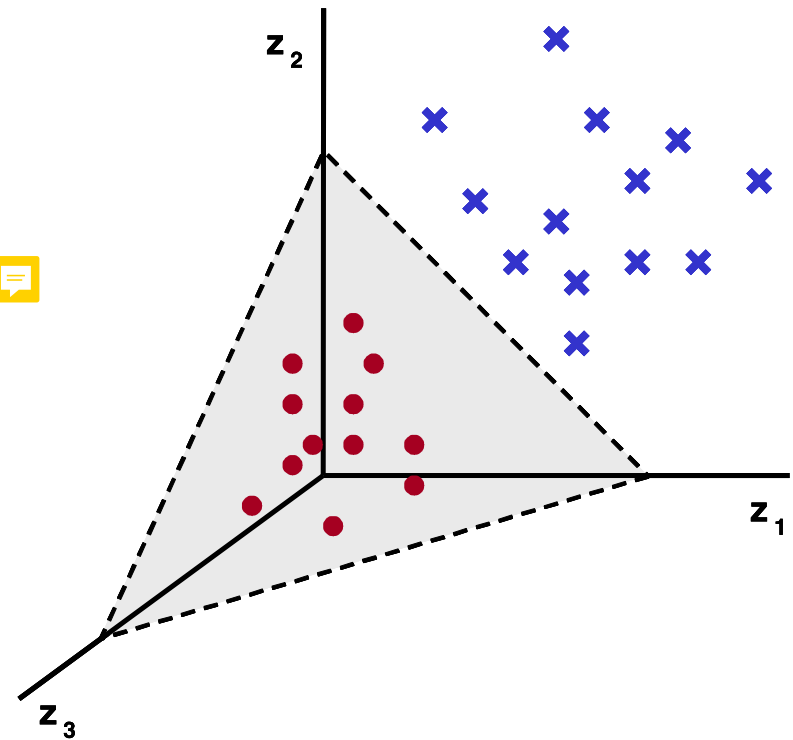
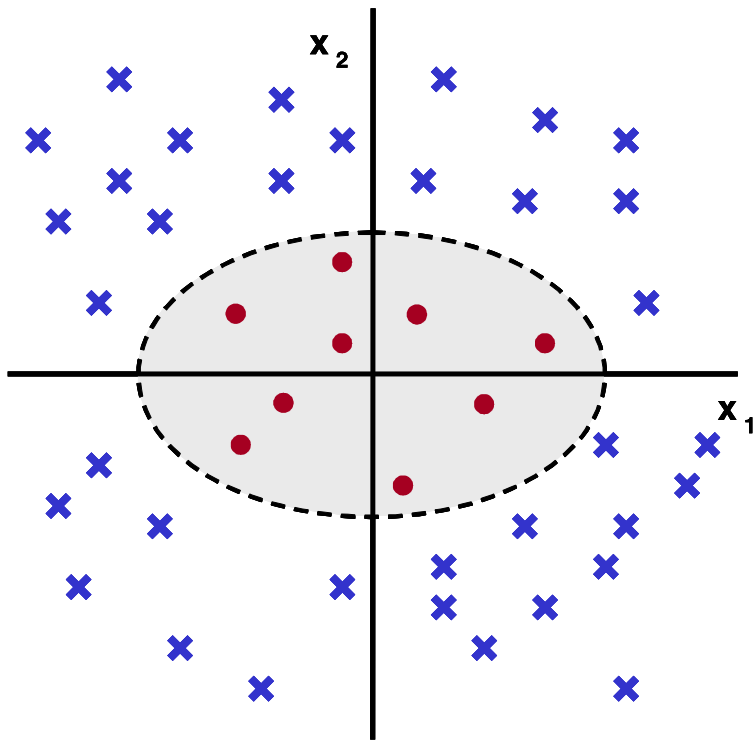
- “A complex pattern-classification problem cast in a high-dimensional space non-linearly is more likely to be linearly separable than in a low-dimensional space”
- The power of SVMs resides in the fact that they represent a robust and efficient implementation of Cover's theorem
- SVMs operate in two stages
  - Perform a non-linear mapping of the feature vector  $x$  onto a high-dimensional space that is hidden from the inputs or the outputs
  - Construct an optimal separating hyperplane in the high-dim space



# Nonlinear SVMs

$$\varphi : \mathbb{R}^2 \rightarrow \mathbb{R}^3$$

$$(x_1, x_2) \mapsto (z_1, z_2, z_3) = (x_1^2, \sqrt{2}x_1x_2, x_2^2)$$





[Schölkopf, 2002 @; <http://kernel-machines.org/>]

# Nonlinear SVMs

- Naïve application of this concept by simply projecting to a high-dimensional non-linear manifold has two major problems:
  1. **Statistical**: operation on high-dimensional spaces is ill-conditioned due to the *curse of dimensionality* and the subsequent risk of overfitting
  2. **Computational**: working in high-dimensions requires higher computational power, which poses limits on the size of the problems that can be tackled

# Nonlinear SVMs

- SVMs bypass these two problems in a robust and efficient way
  1. Generalization capabilities in the high-dimensional manifold are ensured by enforcing a **largest margin classifier** 
    - SVMs optimize the **the margin** (dual is independent of  $D$ )
  2. High-dimensional projection is **implicit**
    - The SVM solution depends only on the dot product  $\mathbf{x}^{(n)\top} \mathbf{x}^{(m)}$  between training examples
    - Operations in high-dimensional space  $\Phi(\mathbf{x})$  do not have to be performed **explicitly** if we find a function 
$$K(\mathbf{x}^{(n)}, \mathbf{x}^{(m)}) = \Phi(\mathbf{x}^{(n)})^\top \Phi(\mathbf{x}^{(m)})$$
    - $K(\mathbf{x}^{(n)}, \mathbf{x}^{(m)})$  is called a **kernel function**

# Implicit mappings: an example

- Consider a problem in **two dimensions**
- Assume we choose kernel function  $K(\mathbf{x}^{(n)}, \mathbf{x}^{(m)}) = (\mathbf{x}^{(n)\top} \mathbf{x}^{(m)})^2$
- Our goal is to find a non-linear projection  $\phi(\cdot)$  such that
$$(\mathbf{x}^{(n)\top} \mathbf{x}^{(m)})^2 = \boldsymbol{\Phi}(\mathbf{x}^{(n)})^\top \boldsymbol{\Phi}(\mathbf{x}^{(m)})$$

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$$(\mathbf{x}^{(n)\top} \mathbf{x}^{(m)})^2 = \boldsymbol{\Phi}(\mathbf{x}^{(n)})^\top \boldsymbol{\Phi}(\mathbf{x}^{(m)})$$

- Performing the expansion of  $K(\mathbf{x}^{(n)}, \mathbf{x}^{(m)})$

$$\begin{aligned} K(\mathbf{x}^{(n)}, \mathbf{x}^{(m)}) &= (\mathbf{x}^{(n)\top} \mathbf{x}^{(m)})^2 = \left( (x_1^{(n)}, x_2^{(n)})^\top (x_1^{(m)}, x_2^{(m)}) \right)^2 = (x_1^{(n)} x_1^{(m)} + x_2^{(n)} x_2^{(m)})^2 \\ &= (x_1^{(n)2}, \sqrt{2} x_1^{(n)} x_2^{(n)}, x_2^{(n)2})^\top (x_1^{(m)2}, \sqrt{2} x_1^{(m)} x_2^{(m)}, x_2^{(m)2}) \quad \text{3 dimensions!} \end{aligned}$$



# Implicit mappings: an example

- Consider a problem in **two dimensions**
- Assume we choose kernel function  $K(\mathbf{x}^{(n)}, \mathbf{x}^{(m)}) = (\mathbf{x}^{(n)\top} \mathbf{x}^{(m)})^2$
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So in using the kernel  $K(\mathbf{x}^{(n)}, \mathbf{x}^{(m)}) = (\mathbf{x}^{(n)\top} \mathbf{x}^{(m)})^2$  we are implicitly operating on a higher-dimensional non-linear manifold defined by

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

The inner product can be computed in 2 dimensions by means of the kernel  $(\mathbf{x}^{(n)\top} \mathbf{x}^{(m)})^2$  without ever having to project onto 3 dimensions!

# Kernel Methods

Let's now see how to put together all these concepts:

- Assume that original feature vector lives in a space  $\mathbb{R}^D$
- Our interest is projecting onto a higher dimensional space  $\boldsymbol{\phi}(\mathbf{x}) \in \mathbb{R}^M (M > D)$ , where classes have a better chance of being linearly separable

- The separating hyperplane in  $M$  will be defined by

$$\sum_{j=1}^M w_j \phi_j(\mathbf{x}) + b = 0$$



- To eliminate the bias term  $b$ , as always, we consider a constant feature  $\phi_0(\mathbf{x}) = 1$
- The resulting hyperplane becomes  $\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}) = 0$
- From our previous results, the optimal (maximum margin) hyperplane in the implicit space is given by  $\mathbf{w} = \sum_{n=1}^N \alpha_n y^{(n)} \boldsymbol{\phi}(\mathbf{x}^{(n)})$

# Kernel Methods

Merging this optimal weight vector with the hyperplane equation:

$$\begin{aligned}\mathbf{w}^\top \boldsymbol{\phi}(\mathbf{x}) &= 0 \\ \left( \sum_{n=1}^N \alpha_n y^{(n)} \boldsymbol{\phi}(\mathbf{x}^{(n)}) \right)^\top \boldsymbol{\phi}(\mathbf{x}) &= 0 \\ \sum_{n=1}^N \alpha_n y^{(n)} \boldsymbol{\phi}(\mathbf{x}^{(n)})^\top \boldsymbol{\phi}(\mathbf{x}) &= 0\end{aligned}$$

And, since  $\boldsymbol{\phi}(\mathbf{x}^{(n)})^\top \boldsymbol{\phi}(\mathbf{x}^{(m)}) = K(\mathbf{x}^{(n)}, \mathbf{x}^{(m)})$  the optimal hyperplane becomes

$$\sum_{n=1}^N \alpha_n y^{(n)} K(\mathbf{x}^{(n)}, \mathbf{x}) = 0$$

Therefore, classification of an unknown example  $\mathbf{x}$  is performed by computing the weighted sum of the kernel with respect to the support vectors  $\mathbf{x}^{(n)}$  (remember that only the support vectors have non-zero dual variables  $\alpha_n$ )

# Kernel Methods

How do we compute dual variables  $\alpha_n$  in the implicit space?

- Very simple: we use the same optimization problem as before and replace the dot product  $\Phi^\top(\mathbf{x}^{(n)})\Phi(\mathbf{x}^{(m)})$  with the kernel  $K(\mathbf{x}^{(n)}, \mathbf{x}^{(m)})$
- The Lagrangian dual problem for the non-linear SVM is simply

$$L_D(\boldsymbol{\alpha}) = \sum_{n=1}^N \alpha_n - \frac{1}{2} \sum_{n=1}^N \sum_{m=1}^N \alpha_n \alpha_m y^{(n)} y^{(m)} K(\mathbf{x}^{(n)}, \mathbf{x}^{(m)})$$

Subject to the constraints

$$\begin{cases} \sum_{n=1}^N \alpha_n y^{(n)} = 0 \\ 0 \leq \alpha_n \leq C \quad n = 1, \dots, N \end{cases}$$

# Kernel Methods

## Illustration : the XOR problem

- **Dataset :**

Class +1  $\mathbf{x}^{(1)} = (+1, +1), \mathbf{x}^{(4)} = (-1, -1)$

Class -1  $\mathbf{x}^{(2)} = (-1, +1), \mathbf{x}^{(3)} = (+1, -1)$

- Kernel function

Polynomial of 2<sup>nd</sup> order:  $K(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^\top \mathbf{x}' + 1)^2$

- **Solution**

- The implicit mapping can be shown to be five dimensional

$$\Phi(\mathbf{x}) = [1 \quad \sqrt{2}x_1 \quad \sqrt{2}x_2 \quad \sqrt{2}x_1x_2 \quad x_1^2 \quad x_2^2]^\top$$

- To achieve linear separability, we use  $C = \infty$
- The objective function for the dual problem becomes

$$L_D(\boldsymbol{\alpha}) = \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 - \frac{1}{2} \sum_{n=1}^4 \sum_{m=1}^4 \alpha_n \alpha_m y^{(n)} y^{(m)} K_{n,m}$$

Subject to the constraints  $\sum_{n=1}^N \alpha_n y^{(n)} = 0$  and  $0 \leq \alpha_n \leq C, n = 1, \dots, N$

- where the inner product is represented as a  $4 \times 4$  K matrix

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

- Optimizing with respect to the Lagrange multipliers leads to the following system of equations

$$\begin{aligned} 9\alpha_1 - \alpha_2 - \alpha_3 + \alpha_4 &= 1 \\ -\alpha_1 + 9\alpha_2 + \alpha_3 - \alpha_4 &= 1 \\ -\alpha_1 + \alpha_2 + 9\alpha_3 - \alpha_4 &= 1 \\ \alpha_1 - \alpha_2 - \alpha_3 + 9\alpha_4 &= 1 \end{aligned}$$

- whose solution is  $\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = 0.125$
- Thus, all data points are support vectors in this case

- For this simple problem, it is worthwhile to write the decision surface in terms of the polynomial expansion

$$\mathbf{w} = \sum_{n=1}^4 \alpha_n y^{(n)} \boldsymbol{\phi}(\mathbf{x}^{(n)}) = \begin{bmatrix} 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 \end{bmatrix}^T$$

- Resulting in the intuitive non-linear discriminant function

$$g(\mathbf{x}) = \sum_{i=1}^6 w_i \phi_i(\mathbf{x}) = x_1 x_2$$

- Which has zero empirical error in the XOR dataset

## Decision function defined by the SVM

- Notice that the decision boundaries are non-linear in the original space  $R^2$ , but linear in the implicit space  $R^6$

