Machine Learning

Session 7 Support Vector Machines

Optimal separating Hyperplanes

SVM: Primal and dual formulations

Example

The non separable case

Non Linear sym

Example



From

S. Theordiridis, K.Koutroumbas. Pattern Recognition Elsevier 2009, 3.7.{1,2} Slides of Ricardo Gutierrez-Osuna Bishop, 7, 7.1

Problem Statement

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

$$\{(\mathbf{x}^{(n)}, y^{(n)})\}, n = 1, ..., N$$

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

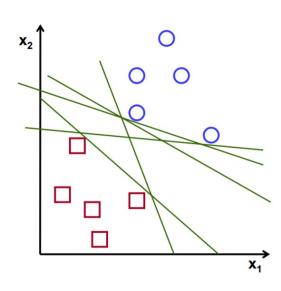
- Which hyperplane would you choose?
- The hyperplane is:

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

The discriminant function is

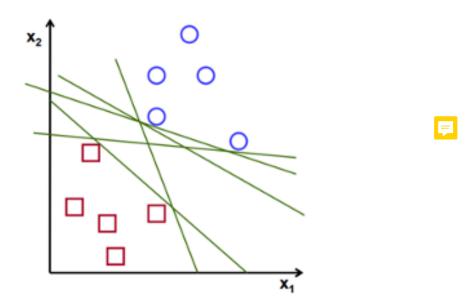
$$g(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b$$





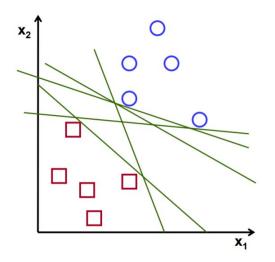
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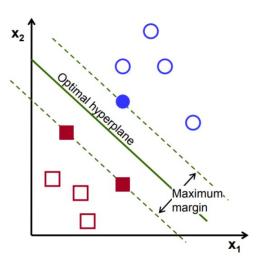
- Which hyperplane would you choose?
 - A hyperplane that passes too close to the training examples will be sensitive to noise and less likely to generalize well for unseen data
 - Instead, it seems reasonable to expect that a hyperplane that is farthest from all training examples will generalize better



Problem Statement

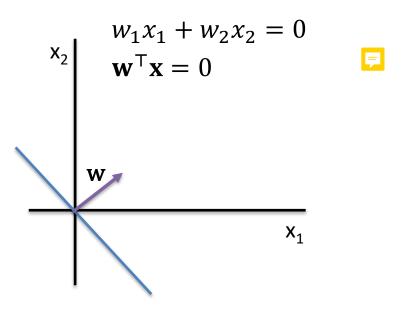
- Which hyperplane would you choose?
 - A hyperplane that passes too close to the training examples will be sensitive to noise and less likely to generalize well for unseen data
 - Instead, it seems reasonable to expect that a hyperplane that is farthest from all training examples will generalize better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

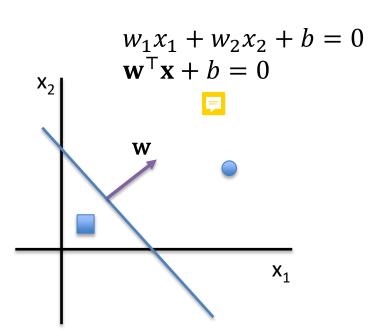




• Geometry: let's express the margin as a function of the weight vector and bias of the separating hyperplane

Remember:



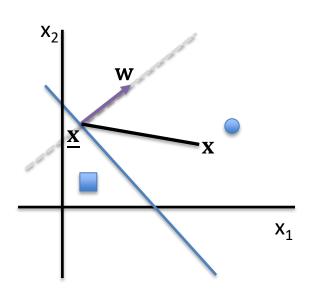


x are the points orthogonal to w

The discriminant is
$$g(\mathbf{x}) = \mathbf{w}^{\mathsf{T}}\mathbf{x} + b$$

 $g(\mathbf{o}) > 0$ class +1
 $g(\mathbf{o}) < 0$ class -1

- 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 x and a hyperplane (w, b) is



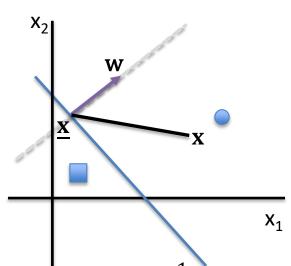
$$\frac{|\mathbf{w}^{\mathsf{T}}\mathbf{x} + b|}{||\mathbf{w}||}$$

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

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

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

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

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

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

- Geometry: let's express the margin as a function of the weight vector and bias of the separating hyperplane.
- Step 1: The distance point **x** and a hyperplane (\mathbf{w}, b) is $\frac{|\mathbf{w}^T \mathbf{x} + b|}{||\mathbf{w}||}$
- 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 $\mathbf{w}^{\mathsf{T}}\mathbf{x} + b = 1$. This is the **Canonical Hyperplane**

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

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

$$\left(\frac{1}{3}, \frac{1}{3}\right) \left(\frac{2}{2}\right) - \frac{1}{3} = \frac{3}{3}$$
 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: $m = \frac{2}{||\mathbf{w}||}$

Geometry

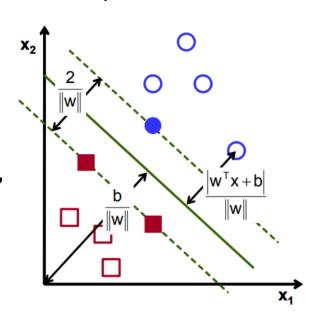
 We choose the solution for which the discriminant function becomes one for the training examples closest to the boundary

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

This is known as the canonical hyperplane

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

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



We estimate w in such a way that the margin becomes largest.

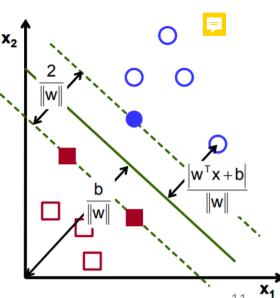
Equivalently: minimize $||\mathbf{w}||$ such that it classifies well all the points

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

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

$$y^{(n)}(\mathbf{w}^{\mathsf{T}}\mathbf{x}^{(n)} + b) \ge 1$$
, $n = 1 \dots N$

Once found **w**, the **canonical** hyperplane is calculated and this discriminant function is our classifier



The Optimization Problem

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

minimize
$$J(\mathbf{w}) = \frac{1}{2} ||\mathbf{w}||^2$$
 subject to $y^{(n)}(\mathbf{w}^{\mathsf{T}}\mathbf{x}^{(n)} + b) \ge 1$, $\forall n = 1, ..., N$

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

minimize
$$f(\mathbf{z})$$
 $\mathbf{z} \in \Omega$
subject to $g_n(\mathbf{z}) \le 0$ $n \in 1, ..., N$
 $h_m(\mathbf{z}) = 0$ $m \in 1, ..., M$

- 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 α^* , $\boldsymbol{\beta}^*$ such that

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

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

$$\alpha_n^* g_n(\mathbf{z}^*) = 0$$

$$g_n(\mathbf{z}^*) \leq 0$$

$$n \in 1, ..., N$$

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

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

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

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

Kuhn-Tucker Theorem

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for active constraints $\rightarrow \alpha_n^* \ge 0$ 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, $lpha_n^*=0$

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

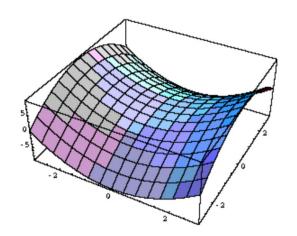
$$L_p(\mathbf{w}, b, \mathbf{\alpha}) = \frac{1}{2} ||\mathbf{w}||^2 - \sum_{n=1}^N \alpha_n (y^{(n)} (\mathbf{w}^\mathsf{T} \mathbf{x}^{(n)} + b) - 1)$$

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 α_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

• 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:

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

• Expansion of L_p yields $||\mathbf{w}||^2 = \mathbf{w}^t \cdot \mathbf{w}$

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

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

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

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

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

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

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

- 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 $\frac{\partial J}{\partial b}=0$

Merging these expressions together we obtain

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

Subject to the simpler constraints $\alpha_n \ge 0$ and $\sum_{n=1}^N \alpha_n y^{(n)} = 0$ [the 1st term is the previous 3rd term and the 2nd one comes from $(1/2 - 1)\mathbf{w}^{\mathsf{T}}\mathbf{w}$]

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

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 - The **primal problem scales with dimensionality** D (w has one coefficient for each dimension), whereas **the dual problem scales with** N, the amount of training data (there is one Lagrange multiplier α_n per example)
 - Moreover, the training data appears only as dot products $\mathbf{x}_n^\mathsf{T}\mathbf{x}_m$

Support Vectors

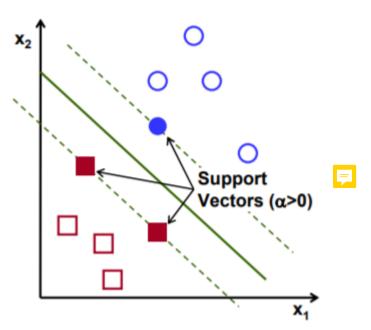
 The KTT complementary condition states that, for every point in the training set, the following equality must hold

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

- Therefore, for each example, either $\alpha_n=0$ or $y^{(n)}\big(\mathbf{w}^{\mathsf{T}}\mathbf{x}^{(n)}+b-1\big)=0$ 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 $y^{(n)}(\mathbf{w}^{\mathsf{T}}\mathbf{x}^{(n)} + b 1)$ becomes zero)

These points are known as **Support Vectors**

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



Support Vectors

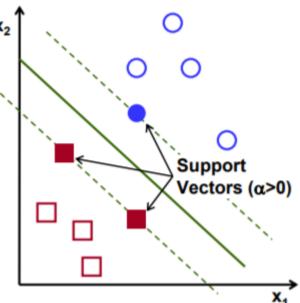
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- Therefore, for each example, either $\alpha_n=0$ or $y^{(n)}\big(\mathbf{w}^{\mathsf{T}}\mathbf{x}^{(n)}+b-1\big)=0$ must hold
- Note that only the support vectors contribute x₂
 to defining the optimal hyperplane

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

- 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: $\{(x^{(1)} = 1, y^{(1)} = +1), (x^{(2)} = -1, y^{(2)} = -1)\}$ We want the maxim margin hyperplane that separate both classes.
- Plot the situation

- **Example**: $\{(x^{(1)} = 1, y^{(1)} = +1), (x^{(2)} = -1, y^{(2)} = -1)\}$ We want the maxim margin hyperplane that separate both classes.
- Plot the situation $x^{(2)} = -1$ 0 $x^{(1)} = 1$
- Model of the classifier for this case: g(x) = wx + b
- w will be the solution to: $\min_{\mathbf{w}} \frac{1}{2} ||\mathbf{w}||^2 \to \min_{\mathbf{w}} \frac{w^2}{2}$ subject to: $y^{(n)} (\mathbf{w}^\mathsf{T} \mathbf{x}^{(n)} + b) \ge 1 \text{ for } n = 1 \text{ and } n = 2$ $+1(w \cdot 1 + b) \ge 1 \to w + b 1 \ge 0$ $-1(w \cdot (-1) + b) \ge 1 \to w b 1 \ge 0$
- Primal

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

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

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

- **Example**: $\{(x^{(1)} = 1, y^{(1)} = +1), (x^{(2)} = -1, y^{(2)} = -1)\}$ We want the maxim margin hyperplane that separate both classes
- Plot the situation

$$x^{(2)} = -1$$
 0 $x^{(1)} = 1$

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

$$\begin{split} L_p(w,b,\alpha_1,\alpha_2) &= \frac{w^2}{2} - \alpha_1(w+b-1) - \alpha_2(w-b-1) \\ L_D(\alpha_1,\alpha_2) &= \frac{2\alpha_1}{2} - \alpha_1(2\alpha_1+b-1) - \alpha_1(2\alpha_1-b-1) = 2\alpha_1^2 - 4\alpha_1 + 2\alpha_1 = -2\alpha_1^2 + 2\alpha_1 \\ \frac{\partial L_D(\alpha_1,\alpha_2)}{\partial \alpha_1} &= -4\alpha_1 + 2 = 0 \to \alpha_1 = \frac{1}{2} \end{split}$$

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

• 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**: $\{(x^{(1)} = 1, y^{(1)} = +1), (x^{(2)} = -1, y^{(2)} = -1)\}$ We want the maxim margin hyperplane that separate both classes
- Plot the situation

$$x^{(2)} = -1$$
 0 $x^{(1)} = 1$

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:

$$\mathbf{w} = \sum_{n=1}^{N} \alpha_n y^{(n)} x^{(n)} = (+1)\alpha_1 (+1) + (-1)\alpha_2 (-1) = \alpha_1 + \alpha_2$$
$$\sum_{n=1}^{N} \alpha_n y^{(n)} = 0 \implies \alpha_1 - \alpha_2 = 0$$

The dual (in matrix notation):

$$L_{D}(\boldsymbol{\alpha}) = \sum_{n=1}^{N} \alpha_{n} - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_{n} \alpha_{m} y^{(n)} y^{(m)} \mathbf{x}^{(m)^{\mathsf{T}}} \mathbf{x}^{(n)} =$$

$$= (\alpha_{1} ... \alpha_{N}) \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} - \frac{1}{2} (\alpha_{1} ... \alpha_{N}) \begin{pmatrix} y^{(1)} \mathbf{x}^{(1)^{\mathsf{T}}} \mathbf{x}^{(1)} y^{(1)} & \dots & y^{(1)} \mathbf{x}^{(1)^{\mathsf{T}}} \mathbf{x}^{(N)} y^{(N)} \\ \vdots & \dots & \vdots \\ y^{(N)} \mathbf{x}^{(N)^{\mathsf{T}}} \mathbf{x}^{(1)} y^{(1)} & \dots & y^{(N)} \mathbf{x}^{(N)^{\mathsf{T}}} \mathbf{x}^{(N)} y^{(N)} \end{pmatrix} \begin{pmatrix} \alpha_{1} \\ \vdots \\ \alpha_{N} \end{pmatrix} =$$

$$= (\alpha_{1} ... \alpha_{N}) \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} - \frac{1}{2} (\alpha_{1} ... \alpha_{N}) \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} \alpha_{1} \\ \alpha_{2} \end{pmatrix}$$

- **Example**: $\{(x^{(1)} = 1, y^{(1)} = +1), (x^{(2)} = -1, y^{(2)} = -1)\}$ We want the maxim margin hyperplane that separate both classes
- Plot the situation

$$x^{(2)} = -1$$
 0 $x^{(1)} = 1$

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

$$\begin{split} \mathsf{L}_{\mathsf{D}}(\alpha_1,\,\alpha_2\,) = & (\alpha_1,\,\alpha_2) \begin{pmatrix} 1 \\ 1 \end{pmatrix} \cdot \frac{1}{2} = & (\alpha_1,\,\alpha_2) \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} \\ & \frac{\partial L_D}{\partial \alpha} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} - \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \implies 1 = \alpha_1 + \alpha_2 \end{split}$$

From the primal we know:

•
$$\mathbf{w} = \alpha_1 + \alpha_2$$

•
$$\alpha_1 - \alpha_2 = 0$$

Then:
$$\alpha_1 = \alpha_2$$
 1=2 α_1 and $\alpha_1 = \alpha_1 = 1/2$ w=1

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

Using

$$\frac{\partial \mathbf{a}^{\mathsf{T}} \mathbf{x}}{\partial \mathbf{x}} = \mathbf{a}$$

and for **A** symmetric matrix

$$\frac{\partial \mathbf{x}^{\mathsf{T}} \mathbf{A} \, \mathbf{x}}{\partial \mathbf{x}} = 2\mathbf{A} \mathbf{x}$$

Example (recap)

From the set learning points

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

$$L_{D}(\boldsymbol{\alpha}) = (\alpha_{1} ... \alpha_{N}) \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} - \frac{1}{2} (\alpha_{1} ... \alpha_{N}) \begin{pmatrix} y^{(1)} \mathbf{x}^{(1)^{\mathsf{T}}} \mathbf{x}^{(1)} y^{(1)} & \dots & y^{(1)} \mathbf{x}^{(1)^{\mathsf{T}}} \mathbf{x}^{(N)} y^{(N)} \\ \vdots & \dots & \vdots \\ y^{(N)} \mathbf{x}^{(N)^{\mathsf{T}}} \mathbf{x}^{(1)} y^{(1)} & \dots & y^{(N)} \mathbf{x}^{(N)^{\mathsf{T}}} \mathbf{x}^{(N)} y^{(N)} \end{pmatrix} \begin{pmatrix} \alpha_{1} \\ \vdots \\ \alpha_{N} \end{pmatrix}$$

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

Find $\alpha_1 ... \alpha_N$

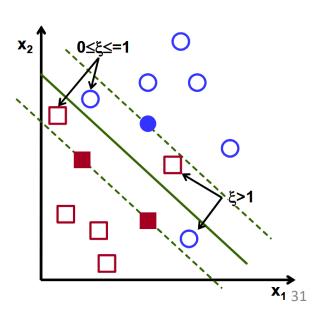
The $\alpha_i \neq 0$ are the Support Vectors

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

- 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

$$y^{(n)}(\mathbf{w}^{\mathsf{T}}\mathbf{x}^{(n)} + b) \ge 1 - \xi_n \quad \forall n = 1, ..., N$$

- For $0 \le \xi_n \le 1$, 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



We minimize the following objective

minimize
$$J(\mathbf{w}, \boldsymbol{\xi}) = \frac{1}{2} ||\mathbf{w}||^2 + C \sum_{n=1}^{N} \xi_n$$
subject to
$$y^{(n)} (\mathbf{w}^{\mathsf{T}} \mathbf{x}^{(n)} + b) \ge 1 - \xi_n,$$
$$\xi_n \ge 0, \quad \forall n = 1, ..., N$$

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

Solution

• We can derive the *dual problem* as

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

subject to

$$\sum_{n=1}^{N} \alpha_n y^{(n)} = 0$$

- 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 $0 \le \alpha_n$ that become $0 \le \alpha_n \le C$

Solution

• We can derive the *dual problem* as

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

subject to

$$0 \le \alpha_n \le C$$

$$\sum_{n=1}^{N} \alpha_n y^{(n)} = 0$$

- 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 $0 < \alpha_n < C$ $(\xi_n = 0)$

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