

# SUPPORT VECTOR MACHINES

CS6140

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#### MAIN IDEA

Given:  $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n$ , where  $x_i \in \mathcal{X}$  and  $y_i \in \mathcal{Y}$ . Here,  $\mathcal{X} = \mathbb{R}, \ \mathcal{Y} = \{-1, +1\}.$ 



**Desiderata:** Avoid explicitly finding  $\phi : \mathbb{R} \to \mathbb{R}^2$ . Allow for  $\mathcal{X}$  to extend beyond  $\mathbb{R}^d$ . Sparse solution.

#### EQUATION OF THE PLANE



A plane is defined using:

- 1. a point  $\mathbf{x}_0$  lying in the plane
- 2. a vector  $\mathbf{w}$  normal to the plane

Let  $\mathbf{x}$  be on the plane defined by  $\mathbf{w}$  and  $\mathbf{x}_0$ :

$$\mathbf{w}^{T}(\mathbf{x} - \mathbf{x}_{0}) = 0$$
$$\mathbf{w}^{T}\mathbf{x} - \mathbf{w}^{T}\mathbf{x}_{0} = 0$$
$$\mathbf{w}^{T}\mathbf{x} + w_{0} = 0$$

## DISTANCE FROM POINT TO THE PLANE



 $\mathbf{x} =$ outside the plane



$$\mathbf{w}^T \mathbf{x} + w_0 = \underbrace{\mathbf{w}^T \mathbf{x}_\perp + w_0}_0 + r ||\mathbf{w}|$$

$$r = \frac{\mathbf{w}^T \mathbf{x} + w_0}{||\mathbf{w}||}$$

**EXAMPLE** 



$$\mathbf{x}, \mathbf{w} \in \mathbb{R}^2$$
  
 $\mathbf{w}^T \mathbf{x} + w_0 = 0$ 

where 
$$\mathbf{w} = (2, -1)$$
 and  $w_0 = 1$ .

$$r = \frac{\mathbf{w}^T \mathbf{x} + w_0}{||\mathbf{w}||} \qquad \qquad \mathbf{x} = (0,0) \implies r = \frac{1}{\sqrt{5}} \\ \mathbf{x} = (-1,1) \implies r = -\frac{2}{\sqrt{5}}$$

The vector  $\mathbf{w}$  defines what side of the plane is positive.

EXAMPLE



What if w = (-2, 1)?

 $\mathbf{x},\mathbf{w}\in\mathbb{R}^2$ 

$$\mathbf{w}^T \mathbf{x} + w_0 = 0$$
  
where  $\mathbf{w} = (-2, 1)$  and  $w_0 = -1$ .

$$r = \frac{\mathbf{w}^T \mathbf{x} + w_0}{||\mathbf{w}||} \qquad \qquad \mathbf{x} = (0,0) \implies r = -\frac{1}{\sqrt{5}}$$
$$\mathbf{x} = (-1,1) \implies r = \frac{2}{\sqrt{5}}$$

#### EXAMPLE



Distances are unchanged when  $\mathbf{w}$  and  $w_0$  are multiplied by a constant!

## **PROBLEM FORMULATION**

**Given:**  $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$ , where  $\mathbf{x}_i \in \mathbb{R}^d$  and  $y_i \in \{-1, +1\}$ . Data is linearly separable.

**Objective:** Find separating hyperplane such that the minimum distance from any data point to the hyperplane is maximized.



\*Margin can also be defined as double of the minimum distance to the separating hyperplane  $% \left( {{{\bf{n}}_{\rm{m}}}} \right)$ 

# MAXIMIZING MARGIN



Idea: find  $(\mathbf{w}, w_0)$  to maximize minimum unsigned distance  $d_i = \frac{y_i(\mathbf{w}^T \mathbf{x}_i + w_0)}{||\mathbf{w}||}$ 

$$(\mathbf{w}^*, w_0^*) = \operatorname*{arg\,max}_{\mathbf{w}, w_0} \left\{ \frac{1}{||\mathbf{w}||} \min_i \left( y_i (\mathbf{w}^T \mathbf{x}_i + w_0) \right) \right\}$$

#### **REFORMULATING THE PROBLEM**

$$(\mathbf{w}^*, w_0^*) = \operatorname*{arg\,max}_{\mathbf{w}, w_0} \left\{ \frac{1}{||\mathbf{w}||} \min_i \left( y_i (\mathbf{w}^T \mathbf{x}_i + w_0) \right) \right\}$$

Scale  $\mathbf{w}$  and  $w_0$  such that  $\min_i \{y_i(\mathbf{w}^T \mathbf{x}_i + w_0)\} = 1$  $\mathbf{w} \leftarrow k \cdot \mathbf{w}$  $w_0 \leftarrow k \cdot w_0$ 

$$(\mathbf{w}^*, w_0^*) = \underset{\mathbf{w}}{\operatorname{arg\,min}} \{ ||\mathbf{w}|| \}$$
  
Subject to:  
$$y_i(\mathbf{w}^T \mathbf{x}_i + w_0) \ge 1 \quad \forall i \in \{1, 2, \dots, n\}$$

# FINAL PROBLEM FORMULATION



Subject to:

 $y_i(\mathbf{w}^T \mathbf{x}_i + w_0) \ge 1 \quad \forall i \in \{1, 2, \dots, n\} \quad \longleftarrow \text{ Linear constraints!}$ 

# HOW CAN WE SOLVE IT?

$$(\mathbf{w}^*, w_0^*) = \operatorname*{arg\,min}_{\mathbf{w}} \left\{ \frac{1}{2} \mathbf{w}^T \mathbf{w} \right\}$$

Subject to:

$$y_i(\mathbf{w}^T \mathbf{x}_i + w_0) \ge 1 \quad \forall i \in \{1, 2, \dots, n\}$$

Solution: use Lagrangians!

$$L(\mathbf{w}, w_0, \boldsymbol{\alpha}) = \frac{1}{2} \mathbf{w}^T \mathbf{w} - \sum_{i=1}^n \alpha_i \left( y_i \left( \mathbf{w}^T \mathbf{x}_i + w_0 \right) - 1 \right) \qquad \alpha_i \ge 0$$

## SOLVING IT

$$\frac{\partial}{\partial w_j} L(\mathbf{w}, w_0, \boldsymbol{\alpha}) = 0 \qquad \Longrightarrow \qquad w_j = \sum_{i=1}^n \alpha_i y_i x_{ij}$$
  
After *d* derivatives... 
$$\implies \qquad \mathbf{w} = \sum_{i=1}^n \alpha_i y_i \mathbf{x}_i$$

$$\frac{\partial}{\partial w_0} L(\mathbf{w}, w_0, \boldsymbol{\alpha}) = 0 \qquad \Longrightarrow \qquad \sum_{i=1}^n \alpha_i y_i = 0$$

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

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

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

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

Subject to:

$$\alpha_i \ge 0 \qquad \forall i \in \{1, 2, \dots, n\}$$

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

For the "duality" theorem see Fletcher. Practical methods of optimization. 1987.

#### SOLVING THE DUAL PROBLEM

Use quadratic programming to solve for  $\pmb{\alpha}$ 

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

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

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$$= \sum_{i=1}^n \alpha_i y_i \mathbf{x}_i^T \mathbf{x} + w_0$$
$$= \sum_{i=1}^n \alpha_i y_i k(\mathbf{x}_i, \mathbf{x}) + w_0$$

## ANALYSIS OF THE SOLUTION

Karush-Kuhn-Tucker (KKT) conditions:

$$\alpha_i \ge 0$$
  

$$y_i(\mathbf{w}^T \mathbf{x}_i + w_0) - 1 \ge 0 \qquad \forall i \in \{1, 2, \dots, n\}$$
  

$$\alpha_i \left( y_i \left( \mathbf{w}^T \mathbf{x}_i + w_0 \right) - 1 \right) = 0$$

This means that for  $\forall i$ , either  $\alpha_i = 0$  or  $y_i \left( \mathbf{w}^T \mathbf{x}_i + w_0 \right) = 1$  $\implies \alpha_i = 0$  for all vectors that are not support vectors

$$f(\mathbf{x}) = \sum_{\mathbf{x}_i \in \mathcal{S}} \alpha_i y_i k(\mathbf{x}, \mathbf{x}_i) + w_0$$

Pick  $\mathbf{x}_s \in \mathcal{S}$  where  $y_s = 1 \longrightarrow w_0 = 1 - \sum_{\mathbf{x}_i \in \mathcal{S}} \alpha_i y_i k(\mathbf{x}_s, \mathbf{x}_i)$ , where  $\mathbf{x}_s \in \mathcal{S}$ 

## LAGRANGE MULTIPLIERS FOR SUPPORT VECTORS



## POPULAR KERNELS

Polynomial kernel

$$k(\mathbf{x}_i, \mathbf{x}_j) = (1 + \mathbf{x}_i^T \mathbf{x}_j)^p$$
, where  $p \ge 1$ 

Radial basis function (RBF) kernel

$$k(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\frac{1}{2\sigma^2} ||\mathbf{x}_i - \mathbf{x}_j||^2\right)$$
, where  $\sigma > 0$ 

Hyperbolic tangent function kernel

$$k(\mathbf{x}_i, \mathbf{x}_j) = \tanh\left(\beta_0 \mathbf{x}_i^T \mathbf{x}_j + \beta_1\right)$$
, though not all pairs  $(\beta_0, \beta_1)$  work

## A SUPPORT VECTOR MACHINE



A support vector machine is a neural network.

#### EXAMPLE: XOR

**Given:**  $\mathcal{D} = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^4$  for the XOR concept. **Goal:** train SVM with a quadratic kernel.

$$x_{2} = (-1, +1) + -x_{4} = (+1, +1)$$

$$x_{1} = (-1, -1) + x_{3} = (+1, -1)$$

$$egin{aligned} & m{x}_i = (x_{i1}, x_{i2}) \ & k(m{x}_i, m{x}_j) = (1 + \mathbf{x}_i^T \mathbf{x}_j)^2 \end{aligned}$$

Haykin. Neural networks. 1999.

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$$x_{1} = (-1, -1) + x_{3} = (+1, -1)$$

$$oldsymbol{x}_i = (x_{i1}, x_{i2})$$
  
 $k(oldsymbol{x}_i, oldsymbol{x}_j) = (1 + \mathbf{x}_i^T \mathbf{x}_j)^2$ 

 $k(\boldsymbol{x}_i, \boldsymbol{x}_j) = (1 + x_{i1}x_{j1} + x_{i2}x_{j2})^2$ 

Haykin. Neural networks. 1999.

#### EXAMPLE: XOR

$$k(\boldsymbol{x}_i, \boldsymbol{x}_j) = (1, \sqrt{2}x_{i1}, \sqrt{2}x_{i2}, x_{i1}^2, \sqrt{2}x_{i1}x_{i2}, x_{i2}^2)^T (1, \sqrt{2}x_{j1}, \sqrt{2}x_{j2}, x_{j1}^2, \sqrt{2}x_{j1}x_{j2}, x_{j2}^2)$$
  
=  $\varphi(\boldsymbol{x}_i)^T \varphi(\boldsymbol{x}_j)$ 

Kernel matrix **K** for the data set  $\mathcal{D}$ , where  $K_{ij} = k(\boldsymbol{x}_i, \boldsymbol{x}_j)$ 

e.g., 
$$K_{11} = k(\boldsymbol{x}_1, \boldsymbol{x}_1) = (1 + (-1) \cdot (-1) + (-1) \cdot (-1))^2 = 9$$
  
 $x_{11}$   $x_{11}$   $x_{12}$   $x_{12}$   
 $K_{12} = k(\boldsymbol{x}_1, \boldsymbol{x}_2) = (1 + (-1) \cdot (-1) + (-1) \cdot 1)^2 = 1$   
 $x_{11}$   $x_{21}$   $x_{12}$   $x_{22}$ 

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



## EXAMPLE: SOLVING THE DUAL PROBLEM (MANUALLY)

$$L(\boldsymbol{w}, \boldsymbol{\alpha}) = \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 - \frac{1}{2}(9\alpha_1^2 - \alpha_1\alpha_2 - \alpha_1\alpha_3 + \alpha_1\alpha_4)$$
$$-\alpha_1\alpha_2 + 9\alpha_2^2 + \alpha_2\alpha_3 - \alpha_2\alpha_4$$
$$-\alpha_1\alpha_3 + \alpha_2\alpha_3 + 9\alpha_3^2 - \alpha_3\alpha_4$$
$$+\alpha_1\alpha_4 - \alpha_2\alpha_4 - \alpha_3\alpha_4 + 9\alpha_4^2)$$

$$\frac{\partial L(\boldsymbol{w},\boldsymbol{\alpha})}{\partial \alpha_i} = 0$$

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

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

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

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

 $\Rightarrow \qquad \alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = \frac{1}{8}$ 

All examples are support vectors!

# EXAMPLE: SOLUTION TO THE DUAL PROBLEM

$$\begin{split} \boldsymbol{w} &= \sum_{i=1}^{4} \alpha_{i} y_{i} \varphi(\boldsymbol{x}_{i}) \\ &= \frac{1}{8} (-\varphi(\boldsymbol{x}_{1}) + \varphi(\boldsymbol{x}_{2}) + \varphi(\boldsymbol{x}_{3}) - \varphi(\boldsymbol{x}_{4})) \\ &= \frac{1}{8} (0, 0, 0, 0, -4\sqrt{2}, 0) \\ &= (0, 0, 0, 0, -\frac{1}{\sqrt{2}}, 0) \end{split}$$

$$w_0 = 1 - \sum_{\boldsymbol{x}_i \in \mathcal{S}} \alpha_i y_i k(\boldsymbol{x}_s, \boldsymbol{x}_i) = 0$$

for any  $\boldsymbol{x}_s \in \mathcal{S}$  where  $y_s = +1$ 

# EXAMPLE: VISUALIZING PREDICTION SCORES

New prediction:

$$f(\boldsymbol{x}) = \sum_{\boldsymbol{x}_s \in \mathcal{S}} \alpha_s y_s k(\boldsymbol{x}_s, \boldsymbol{x}) + w_0$$

 $\mathcal{S} = \mathrm{support} \ \mathrm{vectors}$ 



## (HARD MARGIN) SUPPORT VECTOR MACHINES



## NON-SEPARABLE CASE (SOFT MARGIN)

Introduce "slack" variables  $\xi_i \ge 0$ , one for each data point  $x_i$ .



#### NON-SEPARABLE CASE

 $\xi_i = 0$ :  $\mathbf{x}_i$  is on or inside the correct halfspace.  $\xi_i = |y_i - \mathbf{w}^T \mathbf{x}_i - w_0|$ : for all other  $\mathbf{x}_i$ . Examples with  $\xi_i > 1$  are misclassified.

New constraints:

$$y_i(\mathbf{w}^T \mathbf{x}_i + w_0) \ge 1 \qquad \longrightarrow \qquad y_i(\mathbf{w}^T \mathbf{x}_i + w_0) \ge 1 - \xi_i$$

We now minimize:

such that  $y_i(\mathbf{w}^T \mathbf{x}_i + w_0) \ge 1 - \xi_i, \, \xi_i \ge 0$ 

#### **OPTIMIZATION STEPS**

$$L(\mathbf{w}, w_0, \boldsymbol{\alpha}, \boldsymbol{\xi}, \boldsymbol{\mu}) = \frac{1}{2} \mathbf{w}^T \mathbf{w} + C \cdot \sum_{i=1}^n \xi_i - \sum_{i=1}^n \alpha_i (y_i(\mathbf{w}^T \mathbf{x}_i + w_0) - 1 + \xi_i) - \sum_{i=1}^n \mu_i \xi_i$$

where  $\alpha_i \geq 0$ ,  $\mu_i \geq 0$  are Langrange multipliers

KKT conditions are now:

$$\alpha_i \ge 0, \ \mu_i \ge 0, \ \xi_i \ge 0$$
$$y_i(\mathbf{w}^T \mathbf{x}_i + w_0) - 1 + \xi_i \ge 0$$
$$\alpha_i(y_i(\mathbf{w}^T \mathbf{x}_i + w_0) - 1 + \xi_i) = 0$$
$$\mu_i \xi_i = 0$$

$$L^{\text{dual}}(\mathbf{w}, w_0, \boldsymbol{\alpha}) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j k(\mathbf{x}_i, \mathbf{x}_j)$$
 Same as before

Subject to:

$\alpha_i \ge 0,  \mu_i \ge 0$		More constraints
$0 \le \alpha_i \le C$	$\forall i \in \{1, 2, \dots, n\}$	
$\sum_{i=1}^{n} \alpha_i y_i = 0$		

Note:  $\alpha_i > 0 \rightarrow \text{support vector}$ 

 $\begin{array}{ll} \alpha_i < C & \to & \mu_i > 0, \xi_i = 0 \quad \text{points on the margin} \\ \alpha_i = C & \to & \xi_i \leq 1 \text{ (inside margin) or } \xi_i > 1 \text{ (misclassified)} \end{array}$ 

# A DIFFERENT VIEW ON MINIMIZATION

Objective function to minimize:



# A DIFFERENT VIEW ON MINIMIZATION

Support vector machine:

$$\sum_{i=1}^{n} \underbrace{(1 - y_i(\mathbf{w}^T \mathbf{x}_i + w_0))^+}_{\xi_i} + \lambda ||\mathbf{w}||^2 \qquad \lambda = \frac{1}{2C} \qquad \text{Hinge loss}$$

Logistic regression, regularized:

$$y_i \in \{-1, +1\}$$
 for  $\forall i \qquad \Rightarrow \quad s_i = \frac{1}{1 + e^{-y_i(w_0 + \mathbf{w}^T \mathbf{x}_i)}}$ 

Negative log-likelihood becomes:

$$\sum_{i=1}^{n} \log \left( 1 + e^{-y_i(w_0 + \mathbf{w}^T \mathbf{x}_i)} \right) + \lambda ||\mathbf{w}||^2$$

\*Logistic regression loss is visualized when multiplied by  $\frac{1}{\log 2}$ 



# QUADRATIC PROGRAMMING (QP)

$$\mathbf{x}^* = \operatorname*{arg\,min}_{\mathbf{x}} \left\{ \frac{1}{2} \mathbf{x}^T \mathbf{G} \mathbf{x} + \mathbf{x}^T \mathbf{c} \right\}$$

Subject to:

$$\mathbf{a}_i^T \mathbf{x} = \mathbf{b}_i$$
  
 $\mathbf{a}_j^T \mathbf{x} \ge \mathbf{b}_j$ 

Always solvable or shown to be infeasible in finite computation

If  ${\bf G}$  is positive semi-definite we have a convex QP

If  ${\bf G}$  is not positive semi-definite we have a multiple minima and stationary points

If  ${\bf G}$  is positive definite, the optimal solution is also unique

 $\rm QP$  falls under the group of problems called linear constraint programming (QP, LP)