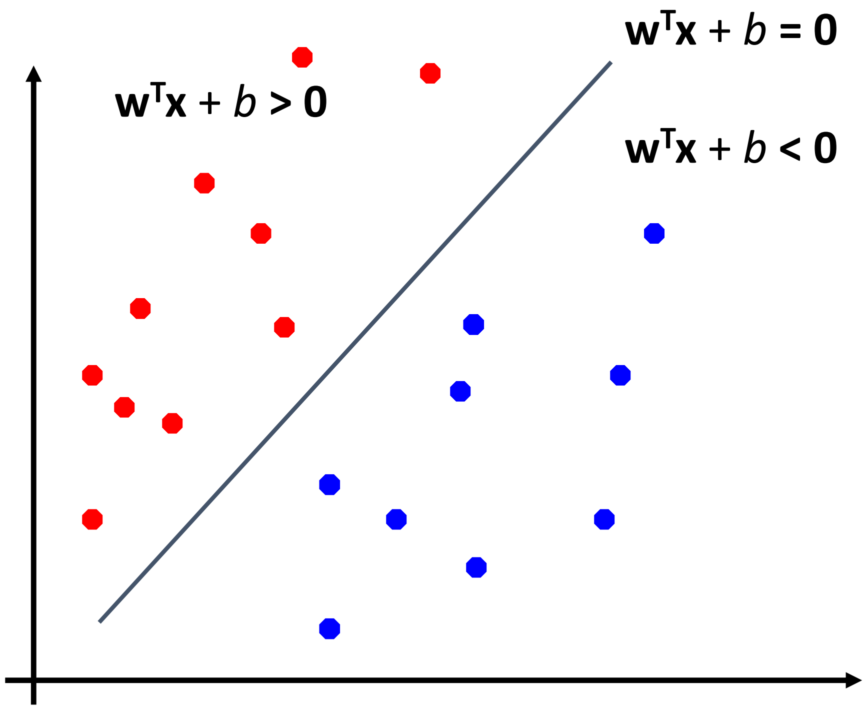
Support Vector Machines

Linear Separators

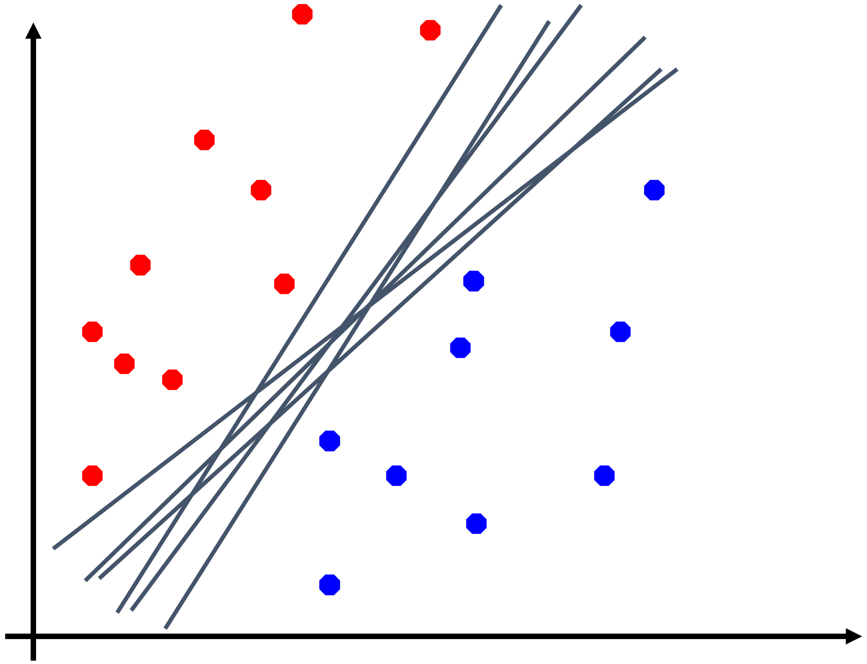
- Binary classification can be viewed as the task of separating classes in feature space:



$f(\mathbf{x}) = \text{sign}(\mathbf{w}^T\mathbf{x} + b)$

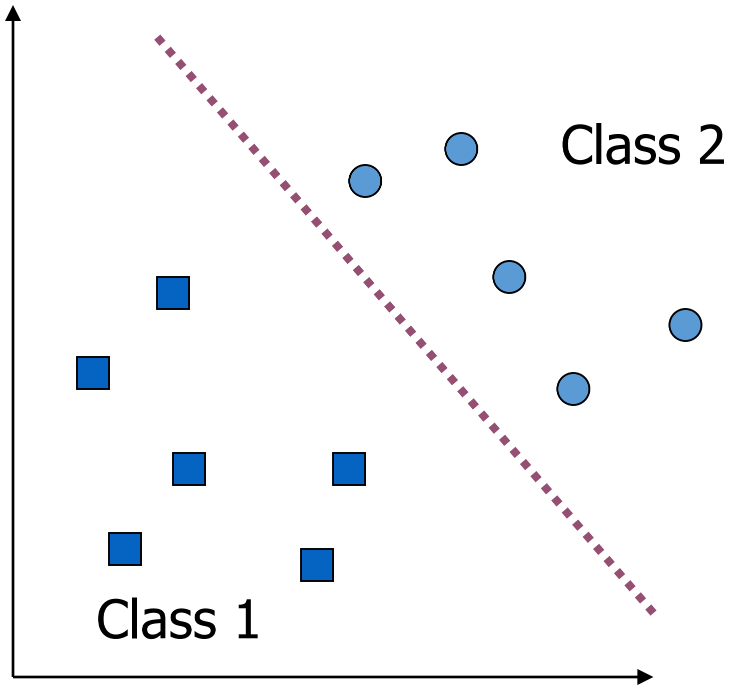
Linear Separators

- Which of the linear separators is optimal?

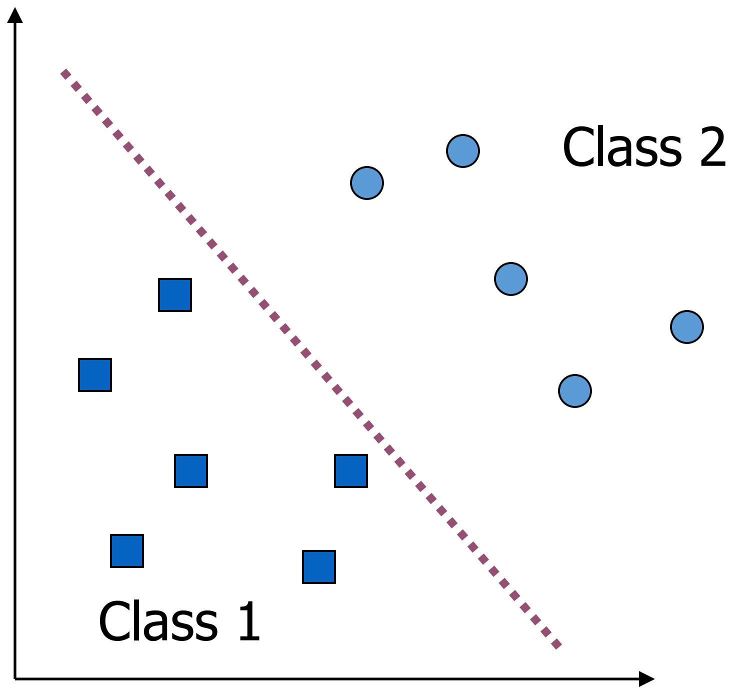


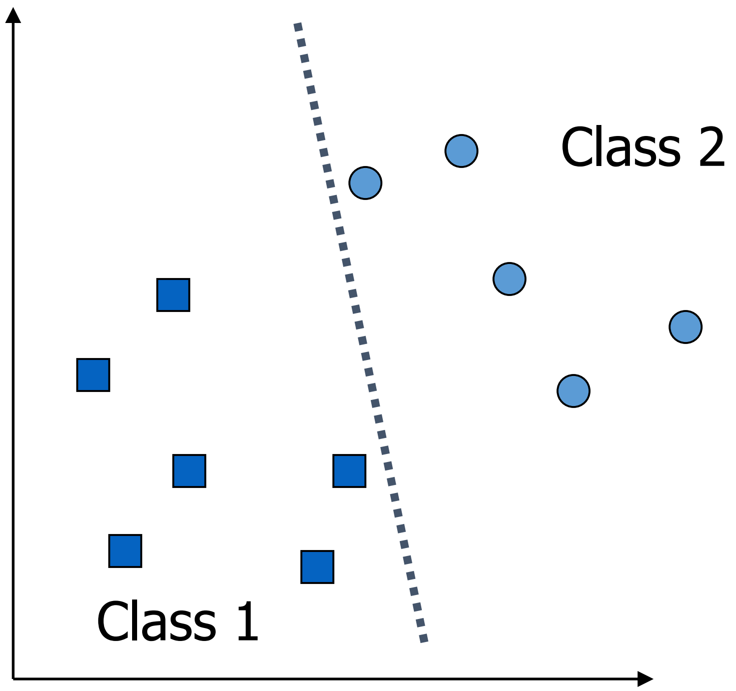
What is a good Decision Boundary?

- Many decision boundaries!
  - The Perceptron algorithm can be used to find such a boundary
- Are all decision boundaries equally good?

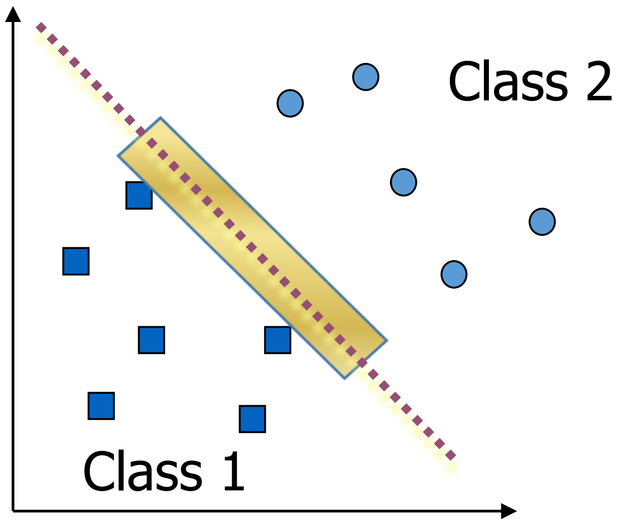


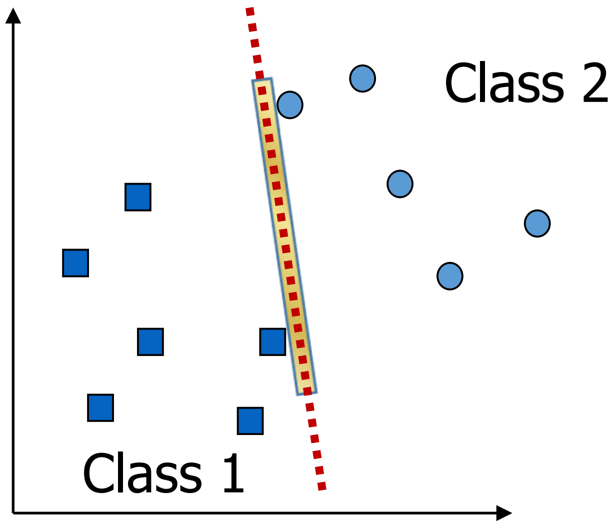
Examples of Bad Decision Boundaries

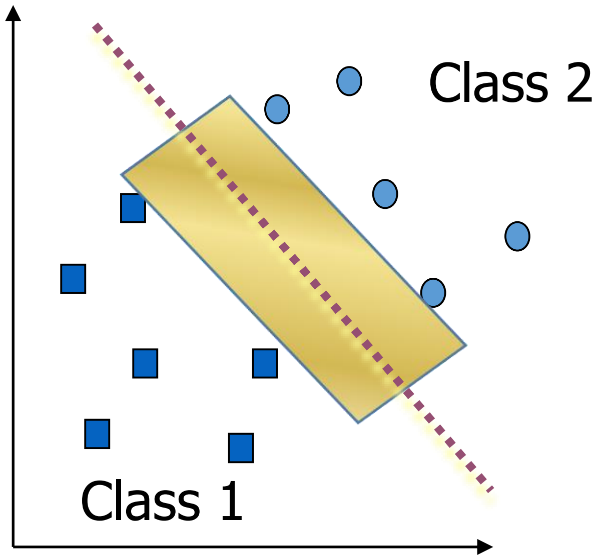




Better Linear Separation

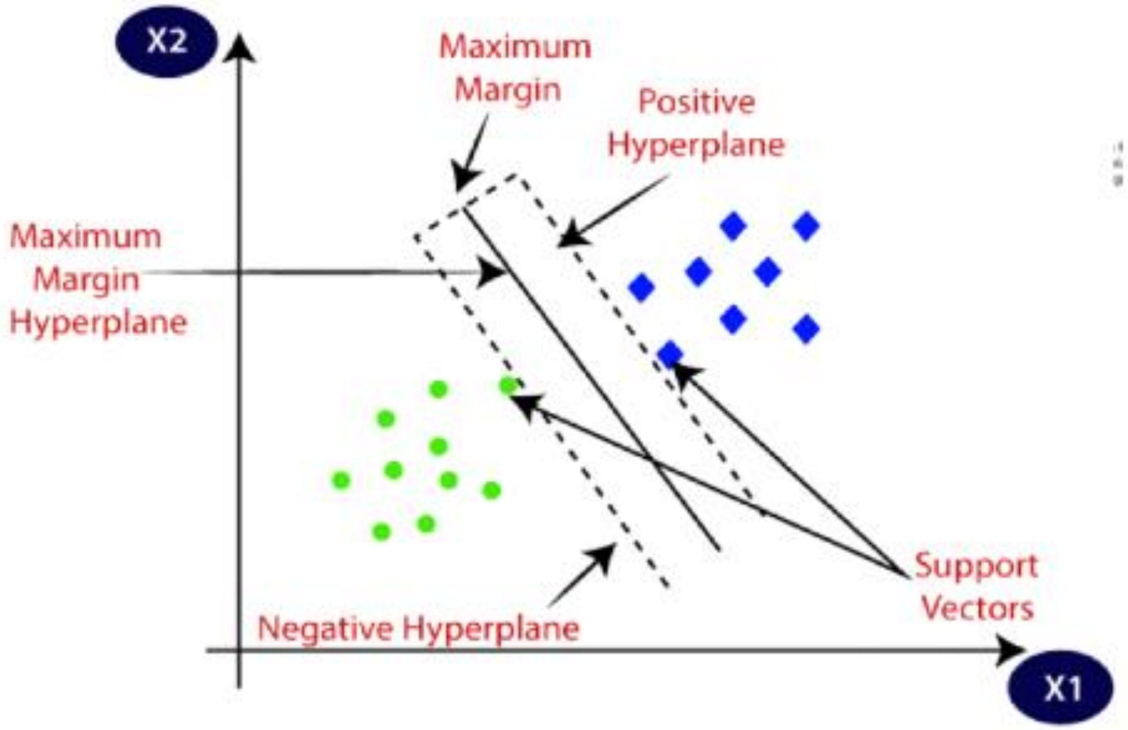




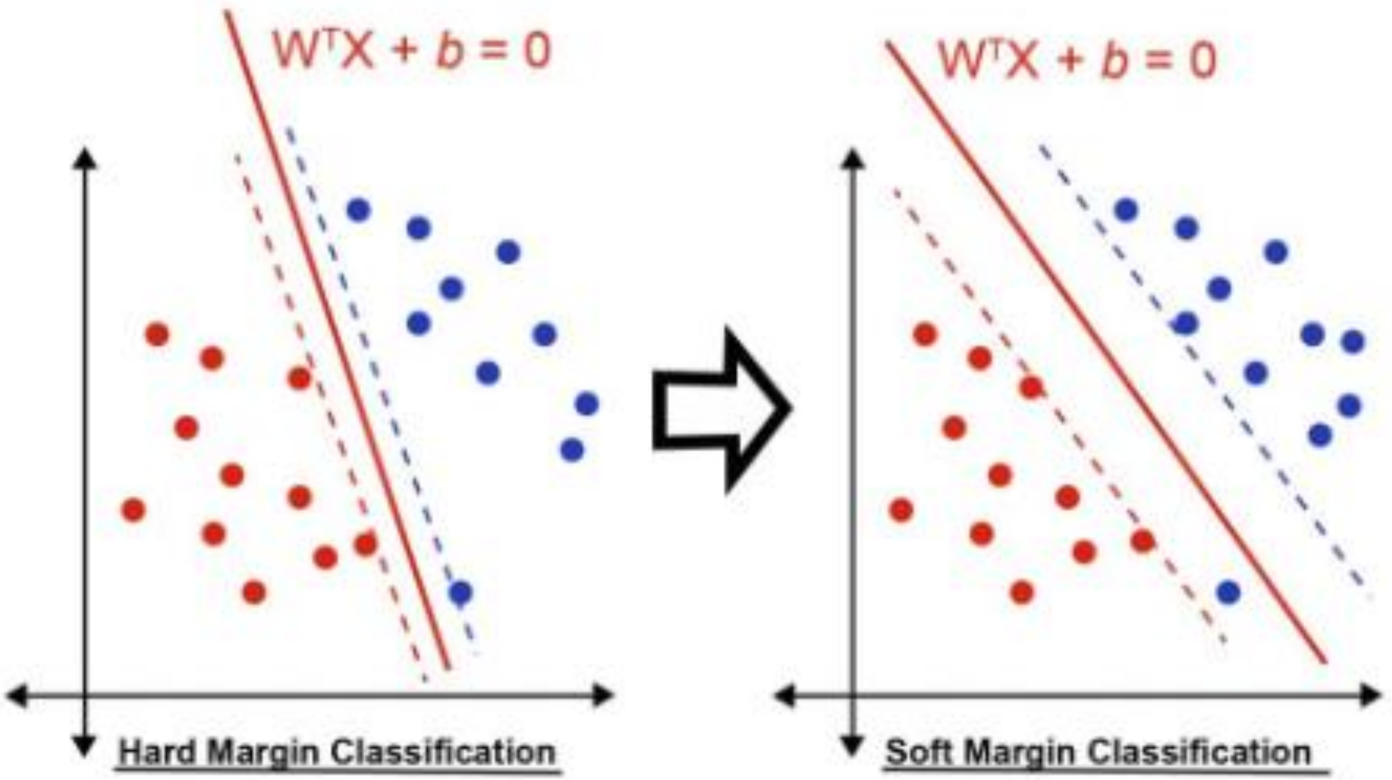


1. Why is bigger margin better?
2. Which **w** maximizes the margin?

SVM Feature



- Support Vectors
- Hyper plane
- Marginal Distance



$W^TX + b = 0$
Hard Margin Classification
$W^TX + b = 0$
Soft Margin Classification

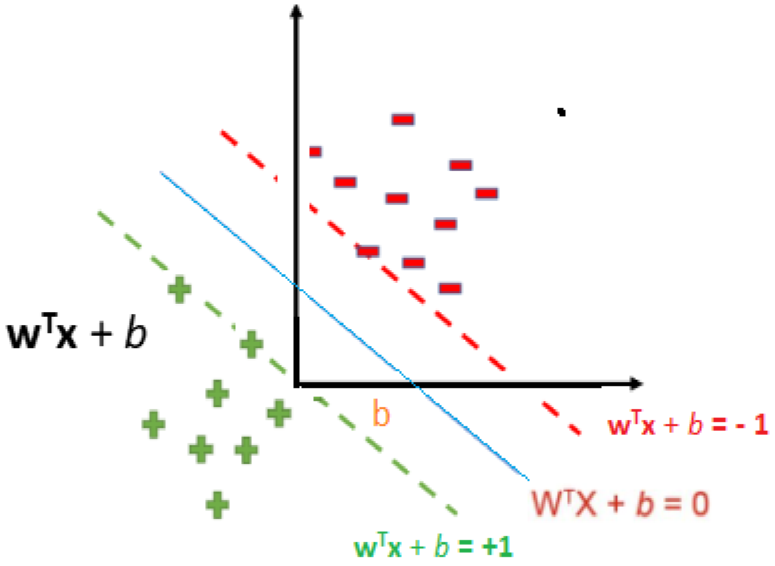
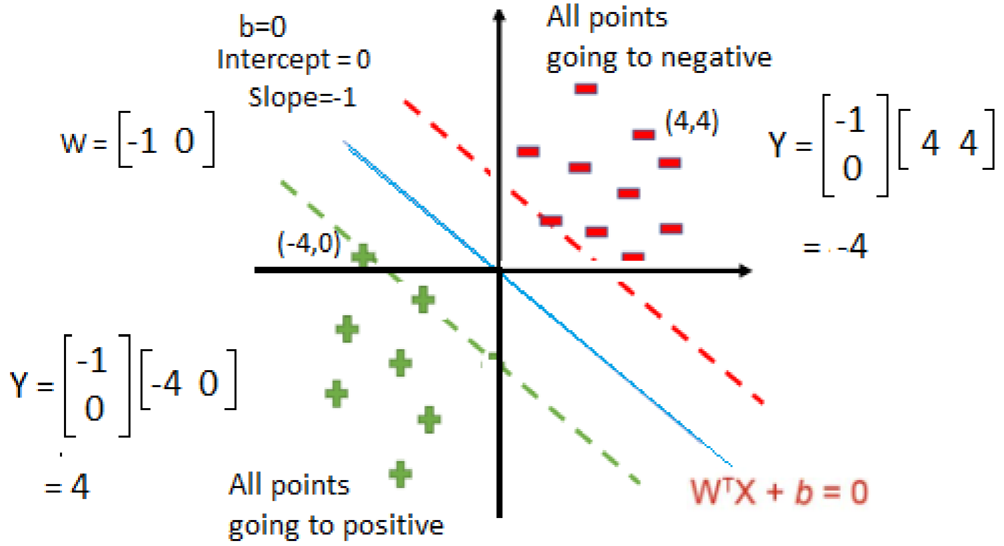


Figure 1



$$w^Tx_- + b = -1$$
$$w^Tx_+ + b = +1$$
$$\text{-------------------}$$
$$w^T(x_+ - x_-) = 2$$
$$\frac{w^T}{||w||}(x_+ - x_-) = \frac{2}{||w||}$$

remove W^T need to divided by Norm of W

Find out (W, b) to Max $\frac{2}{||W||}$

$$Y_i \begin{cases} 1 & w^Tx + b >= +1 \\ -1 & w^Tx + b <= -1 \end{cases} \qquad Y_i(w^Tx + b) >= 1$$

Finding the Decision Boundary

- The decision boundary should classify all points correctly $\Rightarrow$

$$y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1, \qquad \forall i$$

- The decision boundary can be found by solving the following constrained optimization problem

$$\text{Minimize } \frac{1}{2}||\mathbf{w}||^2$$
$$\text{subject to } y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1 \qquad \forall i$$

- This is a constrained optimization problem. Solving it requires to use Lagrange multipliers

Finding the Decision Boundary

$$\text{Minimize } \frac{1}{2}||\mathbf{w}||^2$$

$$\text{subject to } 1 - y_i(\mathbf{w}^T\mathbf{x}_i + b) \leq 0 \qquad \text{for } i = 1, \ldots, n$$

- The Lagrangian is

$$\mathcal{L} = \frac{1}{2}\mathbf{w}^T\mathbf{w} + \sum_{i=1}^{n} \alpha_i \left(1 - y_i(\mathbf{w}^T\mathbf{x}_i + b)\right)$$

- $\alpha_i \geq 0$
- Note that $||\mathbf{w}||^2 = \mathbf{w}^T\mathbf{w}$

Prerequisite

Optimization Problems using Subject to Constraint

$$MAX_{xy}\, Z \quad where \;\; [z = x^2 y] \qquad STC\; x^2 + y^2 = 1$$

Lagrange Multiplier

$$L(h,s,\lambda) = f(h,s) - \lambda(\mathrm{H}(\mathrm{h},\mathrm{s}))$$

more condtions

$$L(h,s,\lambda) = f(h,s) - \lambda 1(\mathrm{H1}(\mathrm{h},\mathrm{s})) - \lambda 2(\mathrm{H2}(\mathrm{h},\mathrm{s}))$$

Example

$$MAX_{hs}\; 200h^{2/3}s^{1/3}\; f(h,s)$$

$$20h + 170s = 20000\; H(h,s) \;\; [Equality\ condition]$$

$$L(h,s,\lambda) = 200h^{2/3}s^{1/3} - \lambda(20h + 170s - 20000)$$

$$\frac{\partial L}{\partial h} = 200\frac{2}{3}h^{-1/3}s^{1/3} - 20\lambda = 0$$

$$\frac{\partial L}{\partial s} = 200\frac{1}{3}h^{2/3}s^{-2/3} - 170\lambda = 0$$

$$\frac{\partial L}{\partial \lambda} = -20h - 170s + 20000 = 0$$

$$h = 666.66, s = 39.12, \lambda = 2.59$$

$$\max f(hs) = 51777$$

Prerequisite

Karush Kuhn Tucker

KKT Conditions

1. *Convert to Lagrange funtions, partially derive variables and equals to 0*
2. $\lambda_i h^i = 0$
3. $h^i \leq 0$
4. $\lambda_i \geq 0$

$$Max\ -x_1^{\,2} - x_2^{\,2} - x_3^{\,2} + 4x_1 + 6x_2$$

$$STC\ \ x_1 + x_2 \leq 2$$

$$2x_1 + 3x_2 \leq 12$$

$$x_1, x_2 \geq 0$$

Conditions 1:

$$\mathrm{L}(x_1, x_2, x_3, \lambda_1, \lambda_2) = \ -x_1^{\,2} - x_2^{\,2} - x_3^{\,2} + 4x_1 + 6x_2 - \lambda_1(x_1 + x_2 - 2) - \ \lambda_2(2x_1 + 3x_2 - 12)$$

$$\frac{\partial L}{\partial x_1} = 2x_1 + 4 - \ \lambda_1 - 2\lambda_2 = 0\ \ \ldots..(1a)$$

$$\frac{\partial L}{\partial x_2} = 2x_2 + 6 - \ \lambda_1 - 3\lambda_2 = 0\ \ \ldots\ldots(1b)$$

$$\frac{\partial L}{\partial x_3} = 2x_3 = 0\qquad i.e:\ x_3 = 0$$

Conditions 2:

$$\lambda_1(x_1 + x_2 - 2) = 0\ \ \ldots\ldots(2a)$$

$$\lambda_2(2x_1 + 3x_2 - 12) = 0\ \ \ldots\ldots(2b)$$

Conditions 3:

$$x_1 + x_2 - 2\ \leq 0\ \ \ldots\ldots(3a)$$

$$2x_1 + 3x_2 - 12\ \leq 0\ \ \ldots..(3b)$$

Conditions 4:

$$\lambda_1 \geq 0\,, \lambda_2 \geq 0$$

Prerequisite

Karush Kuhn Tucker

Case 1: $\lambda_1 = 0\,,\ \lambda_2 = 0$

Substitute 1a, 1b → $x_1 = 2\,,\ x_2 = 3$

Substitute $x_1\ x_2\ in\ 3a, 3b$ $\quad x_1 + x_2 - 2 \le 0$

$5 - 2 \le 0$

$3 \le 0$ X

$2x_1 + 3x_2 - 12 \le 0$

$1 \le 0$ X

Case 2: $\lambda_1 \neq 0\,,\ \lambda_2 \neq 0$

Means from condition 2

$x_1 + x_2 - 2 = 0, 2x_1 + 3x_2 - 12 = 0\ \ by\ solving\ \ x_2 = 8\,, x_1 = -6$

Substitute in 1a, 1b → Solve $\lambda_1\,,\ \lambda_2$

$\lambda_2 = -26$ X

Case 3: $\lambda_1 = 0\,,\ \lambda_2 \neq 0$

Substitute in 1a, 1b

$-2x_1 + 4 - 2\lambda_2 = 0$

$-2x_1 + 6 - 3\lambda_2 = 0$, solving $x_1 = \frac{2}{3}x_2$

$\lambda_2 \neq 0\ , so$

$2x_1 + 3x_2 - 12 = 0$

$\frac{4}{3}x_1 + 3x_2 - 12 = 0$

$x_1 = 2\,,\ x_2 = 3$

$x_1 + x_2 - 2 \le 0$

$5 - 2 \le 0$ X

$2x_1 + 3x_2 - 12 \le 0$

$4 + 9 - 12 \le 0$ X

Case 4: $\lambda_1 \neq 0\,,\ \lambda_2 = 0$

$\lambda_1 = 3\,,\ \lambda_2 = 0 \quad , \ x_1 = \frac{1}{2}\ , x_2 = {}^{3}/_{2}$ ✓

$x_1 + x_2 - 2 \le 0\quad (0 \le 0)\quad 2x_1 + 3x_2 - 12\ (-13 \le 0)$

Prerequisite

Primal and dual problem for understanding support vector machine:

$M_{in} f(w)$

STC $g_i(w) \leq 0 \quad i = 1 \ldots\ldots k$

$h_i(w) = 0 \quad i = 1 \ldots\ldots l$

Generalized Lagrange function:

L $(w, \alpha, \beta) = f(w) + \sum_{i=1}^{k} \alpha_i g_i(w) + \sum_{i=1}^{l} \beta_i h_i(w)$

Define: $\theta_p(w) = Max_{\alpha\,\beta, \alpha \leq 0}\, L(w, \alpha, \beta)$

$\theta_p(w) = Max_{\alpha\,\beta, \alpha \leq 0}\, f(w) + \sum_{i=1}^{k} \alpha_i g_i(w) + \sum_{i=1}^{l} \beta_i h_i(w)$

If $g_i(w) > 0$ $[violates\ condition]$ $\quad \theta_p(w) = \infty$

If $h_i(w) \neq 0$ $[violates\ condition]$ $\quad \theta_p(w) = \infty$

If $g_i(w), h_i(w)$ $[satisfies\ condition]$ $\quad \theta_p(w) = f(w)$

So, $\theta_p(w) = \begin{cases} f(w) \rightarrow satisfies \\ \infty \rightarrow violates \end{cases}$

Primal problem:

$p^* = min_w\, \theta_p(w)$

$p^* = min_w Max_{\alpha\,\beta, \alpha \leq 0}\, L(w, \alpha, \beta)$

Dual problem:

$d^* = Max_{\alpha\,\beta, \alpha \leq 0}\, min_w\, L(w, \alpha, \beta)$

$= Max_{\alpha\,\beta, \alpha \leq 0}\, \theta_d(\alpha, \beta)$

$d^* \leq p^*$ But under some conditions $d^* = p^*$

$\exists\ w^* \alpha^* \beta^*$

Where w^* solution to Primal,

$\alpha^* \beta^*$ Solution to Dual,

$d^* = p^*$,

$w^* \alpha^* \beta^*$ Satisfy KKT conditions,

1) Derivative w.r.t variable =0
2) $\alpha_i g_i(w) = 0$
3) $g_i(w) \leq 0$
4) $\alpha_i \geq 0$

Fact: $MaxMinf(x) \leq MinMaxf(x)$ $\quad Example:\ MaxMin\,Sin(x+y) \leq MinMaxSin(x+y)$

Gradient with respect to *w* and *b*

- Setting the gradient of $\mathcal{L}$ w.r.t. **w** and b to zero, we have

$$L = \frac{1}{2} w^T w + \sum_{i=1}^{n} \alpha_i \left(1 - y_i \left(w^T x_i + b\right)\right) =$$

$$= \frac{1}{2} \sum_{k=1}^{m} w^k w^k + \sum_{i=1}^{n} \alpha_i \left(1 - y_i \left(\sum_{k=1}^{m} w^k x_i{}^k + b\right)\right)$$

n: no of examples, m: dimension of the space

$$\begin{cases} \dfrac{\partial L}{\partial w^k} = 0, \forall k \\ \dfrac{\partial L}{\partial b} = 0 \end{cases}$$

$$\mathbf{w} + \sum_{i=1}^{n} \alpha_i (-y_i) \mathbf{x}_i = \mathbf{0} \quad \Rightarrow \quad \mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i$$

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

The Dual Problem

- If we substitute $\mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i$, we have $\mathcal{L}$

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

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

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

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

- This is a function of α_i only

The Dual Problem

- The new objective function is in terms of α_i only
- It is known as the dual problem: if we know **w**, we know all α_i; if we know all α_i, we know **w**
- The original problem is known as the primal problem
- The objective function of the dual problem needs to be maximized (comes out from the KKT theory)
- The dual problem is therefore:

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

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

Properties of α_i when we introduce the Lagrange multipliers

The result when we differentiate the original Lagrangian w.r.t. b

The Dual Problem

$$\text{max. } W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

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

- This is a quadratic programming (QP) problem
  - A global maximum of α_i can always be found

- **w** can be recovered by

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

QP Solver provides us α

Solution: $\boldsymbol{\alpha} = \alpha_1, \alpha_2, \ldots, \alpha_N$

- Note: **w** need not be formed explicitly

$$\mathbf{w} = \sum_{n=1}^{N} \alpha_n y_n \mathbf{x}_n$$

KKT Condition: For n = 1, 2, …, N

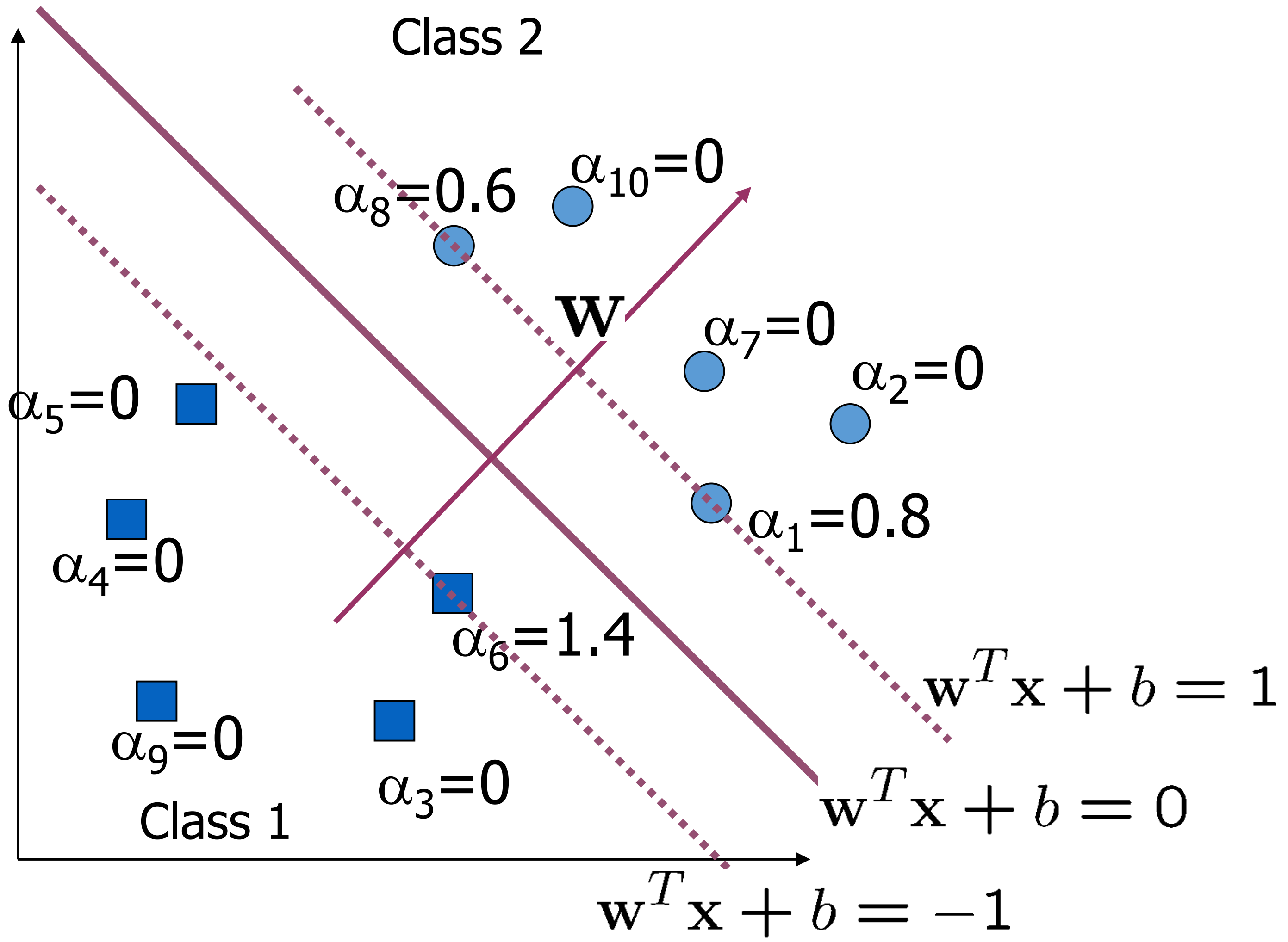
$$\alpha_i\left(1 - y_i\left(w^T x_i + b\right)\right) = 0$$

$\alpha_n > 0 \Rightarrow \mathbf{x_n}$ is **support vector**

Characteristics of the Solution

- For testing with a new data **z**
  - Compute $\mathbf{w}^T\mathbf{z} + b = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} (\mathbf{x}_{t_j}^T \mathbf{z}) + b$ and classify **z** as class 1 if the sum is positive, and class 2 otherwise
  - Note: **w** need not be formed explicitly

A Geometrical Interpretation



SVM Classifier to Find Hyperplane – Solved Example

X1	X2	Class
2	2	-1 √
4	5	+1
7	4	+1

- $N = 3$
- $\vec{x}_1 = (2, 2)$
- $\vec{x}_2 = (4, 5)$
- $\vec{x}_3 = (7, 4)$
- $y_1 = -1$
- $y_2 = +1$
- $y_3 = +1$

$$f(\vec{x}) = \vec{w} \cdot \vec{x} - b$$

- $\vec{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$
- subject to the conditions
- $\sum_{i=1}^{N} \alpha_i y_i = -\alpha_1 + \alpha_2 + \alpha_3 = 0$
- $\alpha_1 > 0, \alpha_2 > 0, \alpha_3 > 0$

SVM Classifier to Find Hyperplane – Solved Example – Step 1

$$\phi(\vec{\alpha}) = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{N} \alpha_i \alpha_j y_i y_j (\vec{x}_i \cdot \vec{x}_j)$$

$$= \sum_{i=1}^{3} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{3} \alpha_i \alpha_j y_i y_j (\vec{x}_i \cdot \vec{x}_j)$$

$$(\vec{x}_1 \cdot \vec{x}_1) = 08, \quad (\vec{x}_1 \cdot \vec{x}_2) = 18, \quad (\vec{x}_1 \cdot \vec{x}_3) = 22$$

$$(\vec{x}_2 \cdot \vec{x}_1) = 18, \quad (\vec{x}_2 \cdot \vec{x}_2) = 41, \quad (\vec{x}_2 \cdot \vec{x}_3) = 48,$$

$$(\vec{x}_3 \cdot \vec{x}_1) = 22, \quad (\vec{x}_3 \cdot \vec{x}_2) = 48, \quad (\vec{x}_3 \cdot \vec{x}_3) = 65$$

$$\phi(\vec{\alpha}) = (\alpha_1 + \alpha_2 + \alpha_3) - \frac{1}{2}[8\alpha_1^2 + 41\alpha_2^2 + 65\alpha_3^2 - 36\alpha_1\alpha_2 - 44\alpha_1\alpha_3 + 96\alpha_2\alpha_3]$$

$$\phi(\vec{\alpha}) = 2(\alpha_2 + \alpha_3) - \frac{1}{2}(13\alpha_2^2 + 32\alpha_2\alpha_3 + 29\alpha_3^2)$$

$$N = 3$$

$$\vec{x}_1 = (2, 2)$$

$$\vec{x}_2 = (4, 5)$$

$$\vec{x}_3 = (7, 4)$$

$$y_1 = -1$$

$$y_2 = +1$$

$$y_3 = +1$$

$$-\alpha_1 + \alpha_2 + \alpha_3 = 0$$

SVM Classifier to Find Hyperplane – Solved Example – Step 1

- Find values of α_1, α_2 and α_3 which maximizes

$$\phi(\vec{\alpha}) = 2(\alpha_2 + \alpha_3) - \frac{1}{2}(13\alpha_2^2 + 32\alpha_2\alpha_3 + 29\alpha_3^2)$$

- For $\phi(\vec{\alpha})$ to be maximum we must have

$$\frac{\partial \phi}{\partial \alpha_2} = 0, \quad \frac{\partial \phi}{\partial \alpha_3} = 0$$

- That is,

$$2 - 13\alpha_2 - 16\alpha_3 = 0, \quad 2 - 16\alpha_2 - 29\alpha_3 = 0$$

- Solving these, we get

$$\alpha_2 = \frac{26}{121}, \quad \alpha_3 = -\frac{6}{121} \quad \alpha_1 = \frac{20}{121}$$

$N = 3$

$\vec{x}_1 = (2, 2)$

$\vec{x}_2 = (4, 5)$

$\vec{x}_3 = (7, 4)$

$y_1 = -1$

$y_2 = +1$

$y_3 = +1$

$-\alpha_1 + \alpha_2 + \alpha_3 = 0$

SVM Classifier to Find Hyperplane – Solved Example – Step 2

$$\vec{w} = \sum_{i=1}^{N} \alpha_i y_i \vec{x}_i$$

$$= \frac{20}{121}(-1)(2,2) + \frac{26}{121}(+1)(4,5) - \frac{6}{121}(+1)(7,4)$$

$$= \left(\frac{2}{11}, \frac{6}{11}\right)$$

$$\alpha_1 = \frac{20}{121}$$

$$\alpha_2 = \frac{26}{121}$$

$$\alpha_3 = -\frac{6}{121}$$

$$N = 3$$

$$\vec{x}_1 = (2,2)$$

$$\vec{x}_2 = (4,5)$$

$$\vec{x}_3 = (7,4)$$

$$y_1 = -1$$

$$y_2 = +1$$

$$y_3 = +1$$

$$-\alpha_1 + \alpha_2 + \alpha_3 = 0$$

SVM Classifier to Find Hyperplane – Solved Example – Step 3

$$b = \frac{1}{2}\left(\min_{i:y_i=+1}(\vec{w}\cdot\vec{x}_i) + \max_{i:y_i=-1}(\vec{w}\cdot\vec{x}_i)\right)$$

$$= \frac{1}{2}\left(\min\{(\vec{w}\cdot\vec{x}_2),(\vec{w}\cdot\vec{x}_3)\} + \max\{(\vec{w}\cdot\vec{x}_1)\}\right)$$

$$= \frac{1}{2}\left(\min\{\tfrac{38}{11},\tfrac{38}{11}\} + \max\{\tfrac{16}{11}\}\right)$$

$$= \frac{1}{2}\left(\frac{38}{11} + \frac{16}{11}\right)$$

$$= \frac{27}{11}$$

$$\alpha_1 = \frac{20}{121}$$

$$\alpha_2 = \frac{26}{121}$$

$$\alpha_3 = -\frac{6}{121}$$

$$\vec{w} = \left(\frac{2}{11}, \frac{6}{11}\right)$$

$$N = 3$$

$$\vec{x}_1 = (2,2)$$

$$\vec{x}_2 = (4,5)$$

$$\vec{x}_3 = (7,4)$$

$$y_1 = -1$$

$$y_2 = +1$$

$$y_3 = +1$$

$$-\alpha_1 + \alpha_2 + \alpha_3 = 0$$

SVM Classifier to Find Hyperplane – Solved Example – Step 4

- The SVM classifier function is given by

$$f(\vec{x}) = \vec{w} \cdot \vec{x} - b$$

- Where,

- $\vec{x} = (x_1, x_2)$

$$= \frac{2}{11}x_1 + \frac{6}{11}x_2 - \frac{27}{11}$$

- The equation of the maximal margin hyperplane is

$$f(\vec{x}) = 0 \qquad f(\vec{x}) = \frac{2}{11}x_1 + \frac{6}{11}x_2 - \frac{27}{11}$$

$$\alpha_1 = \frac{20}{121}$$

$$\alpha_2 = \frac{26}{121}$$

$$\alpha_3 = -\frac{6}{121}$$

$$\vec{w} = \left(\frac{2}{11}, \frac{6}{11}\right)$$

$$b = \frac{27}{11}$$

$$N = 3$$

$$\vec{x}_1 = (2, 2)$$

$$\vec{x}_2 = (4, 5)$$

$$\vec{x}_3 = (7, 4)$$

$$y_1 = -1$$

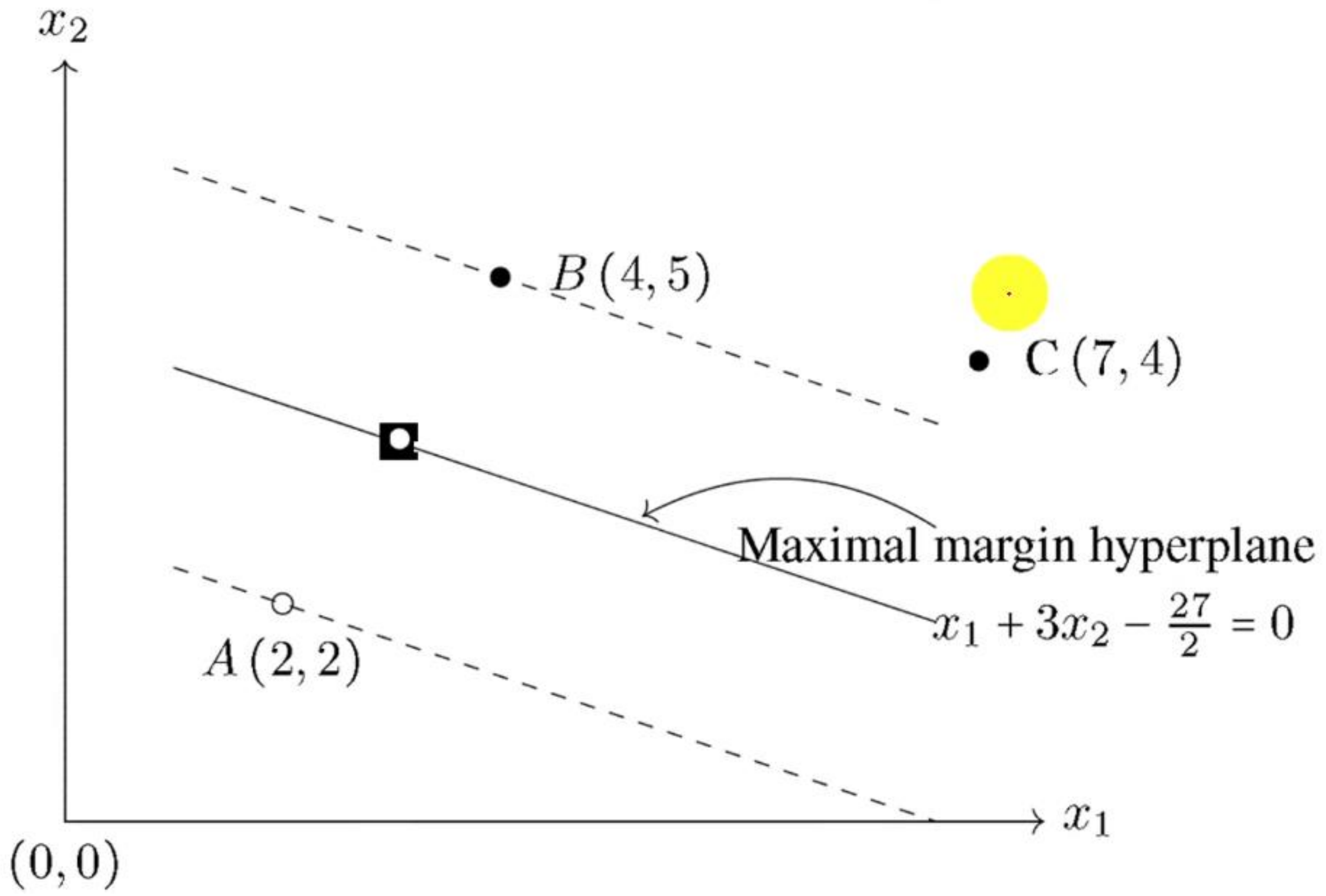
$$y_2 = +1$$

$$y_3 = +1$$

$$-\alpha_1 + \alpha_2 + \alpha_3 = 0$$

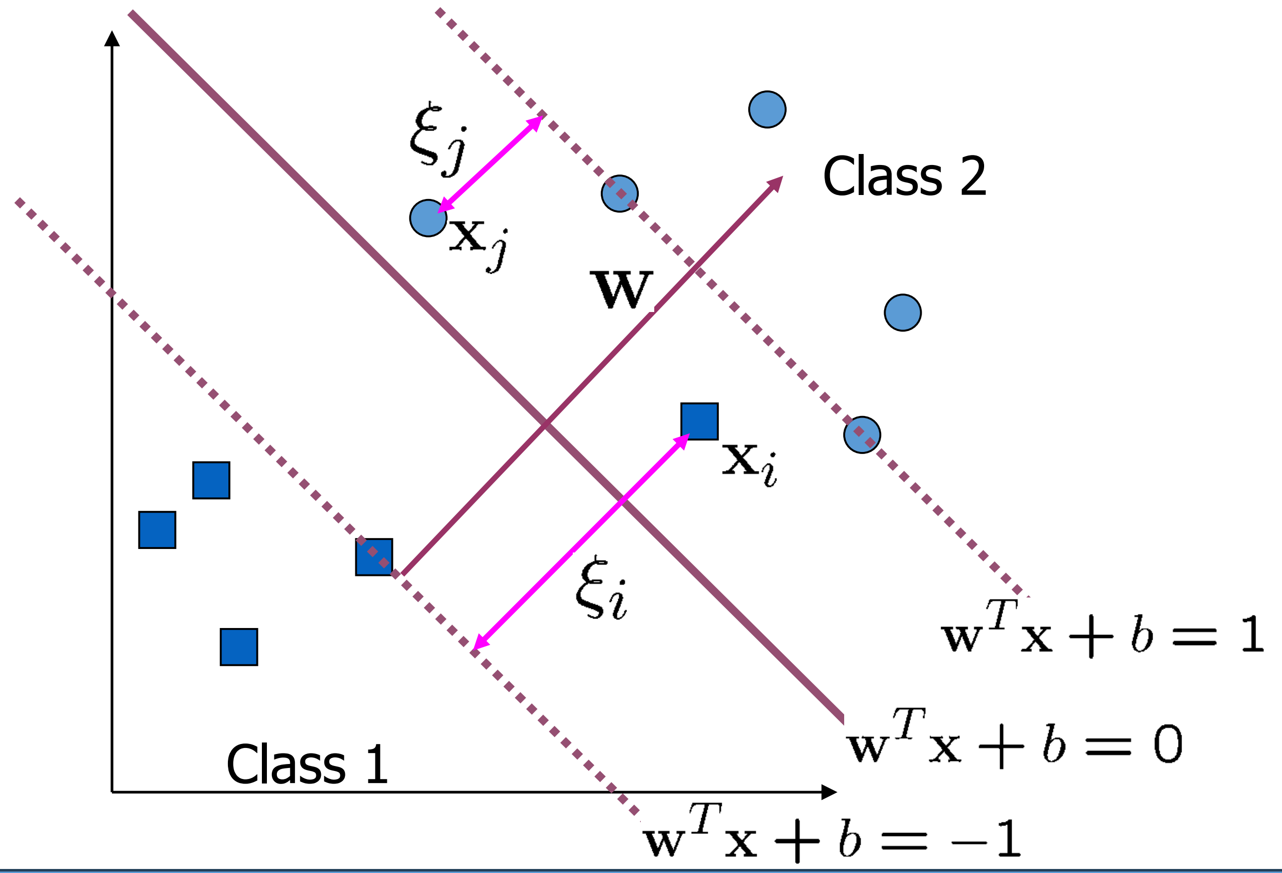
SVM Classifier to Find Hyperplane – Solved Example – Step 5

$$x_1 + 3x_2 - \frac{27}{2} = 0$$



Non-linearly Separable Problems

- We allow "error" ξ_i in classification; it is based on the output of the discriminant function $\mathbf{w}^T\mathbf{x}$+b
- ξ_i approximates the number of misclassified samples



Soft Margin Hyperplane

- The new conditions become

$$\begin{cases} \mathbf{w}^T\mathbf{x}_i + b \geq 1 - \xi_i & y_i = 1 \\ \mathbf{w}^T\mathbf{x}_i + b \leq -1 + \xi_i & y_i = -1 \\ \xi_i \geq 0 & \forall i \end{cases}$$

  - ξ_i are "slack variables" in optimization
  - Note that ξ_i=0 if there is no error for $\mathbf{x}_i$
  - ξ_i is an upper bound of the number of errors
- We want to minimize

$$\frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}\xi_i$$

$$\text{subject to } y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1 - \xi_i, \quad \xi_i \geq 0$$

- *C* : tradeoff parameter between error and margin

The Optimization Problem

$$L = \frac{1}{2} w^T w + C \sum_{i=1}^{n} \xi_i + \sum_{i=1}^{n} \alpha_i \left(1 - \xi_i - y_i \left(w^T x_i + b\right)\right) - \sum_{i=1}^{n} \mu_i \xi_i$$

With α and μ Lagrange multipliers, POSITIVE

$$\frac{\partial L}{\partial w_j} = w_j - \sum_{i=1}^{n} \alpha_i y_i x_{ij} = 0$$

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

$$\frac{\partial L}{\partial \xi_j} = C - \alpha_j - \mu_j = 0$$

$$\frac{\partial L}{\partial b} = \sum_{i=1}^{n} y_i \alpha_i = 0$$

The Dual Problem

$$L = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j \vec{x}_i^{\,T}\vec{x}_j + C\sum_{i=1}^{n}\xi_i +$$

$$+\sum_{i=1}^{n}\alpha_i\left(1-\xi_i - y_i\left(\sum_{j=1}^{n}\alpha_j y_j x_j^{\,T} x_i + b\right)\right) - \sum_{i=1}^{n}\mu_i\xi_i$$

With $\sum_{i=1}^{n} y_i\alpha_i = 0$ $\qquad C = \alpha_j + \mu_j$

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

The Optimization Problem

- The dual of this new constrained optimization problem is

$$\text{max. } W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

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

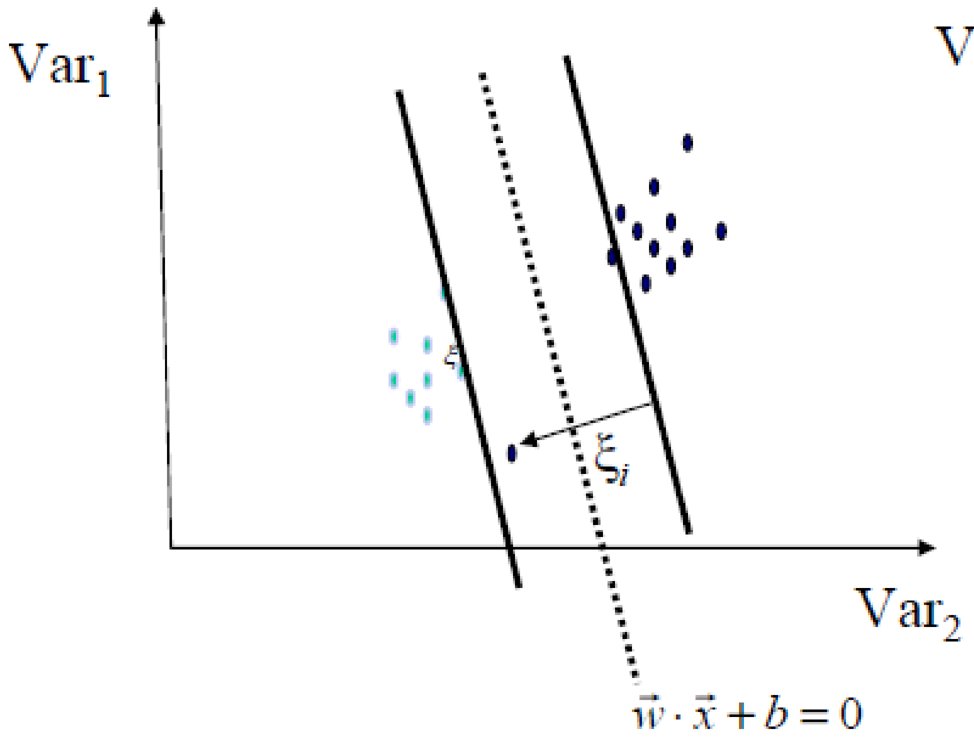
- New constrains derive from $C = \alpha_j + \mu_j$ since μ and α are positive.
- **w** is recovered as $\mathbf{w} = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \mathbf{x}_{t_j}$
- This is very similar to the optimization problem in the linear separable case, except that there is an upper bound *C* on α_i now
- Once again, a QP solver can be used to find α_i

$$\frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}\xi_i$$

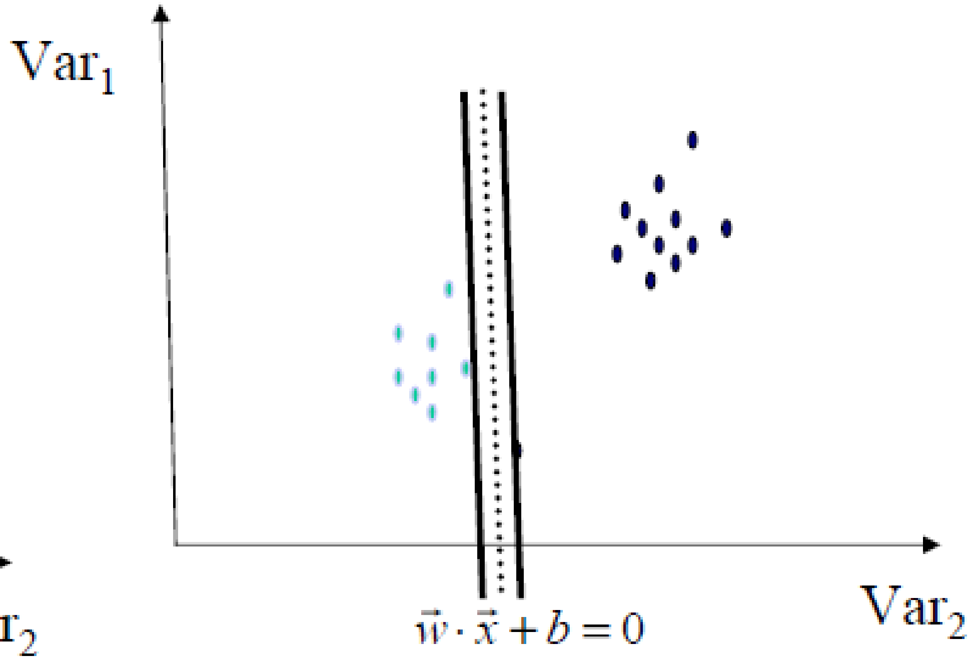
- The algorithm try to keep ξ null, maximising the margin
- The algorithm does not minimise the number of error. Instead, it minimises the sum of distances fron the hyperplane

- When C increases the number of errors tend to lower. At the limit of C tending to infinite, the solution tend to that given by the hard margin formulation, with 0 errors

Soft margin is more robust



Soft Margin SVM



Hard Margin SVM

Extension to Non-linear Decision Boundary

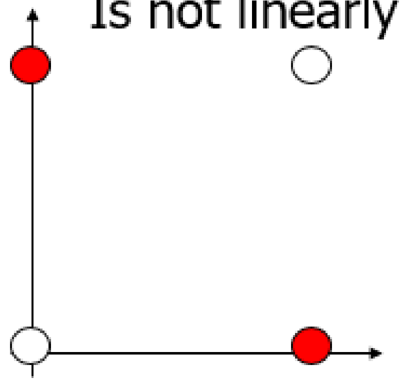
- So far, we have only considered large-margin classifier with a linear decision boundary
- How to generalize it to become nonlinear?
- Key idea: transform $\mathbf{x}_i$ to a higher dimensional space to “make life easier”
  - Input space: the space the point $\mathbf{x}_i$ are located
  - Feature space: the space of $\phi(\mathbf{x}_i)$ after transformation
- Why transform?
  - Linear operation in the feature space is equivalent to non-linear operation in input space
  - Classification can become easier with a proper transformation. In the XOR problem, for example, adding a new feature of x_1x_2 make the problem linearly separable

XOR

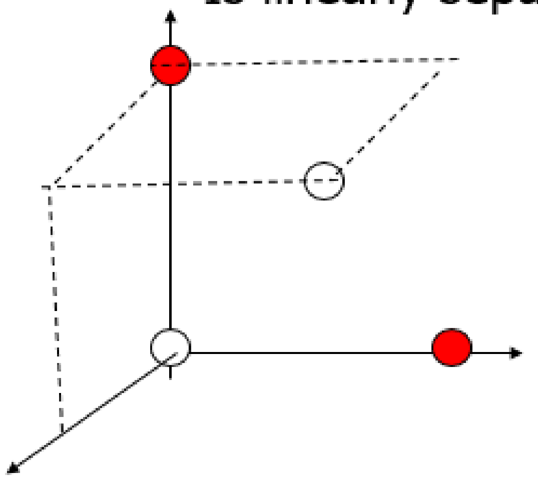
X	Y	
0	0	0
0	1	1
1	0	1
1	1	0

X	Y	XY	
0	0	0	0
0	1	0	1
1	0	0	1
1	1	1	0

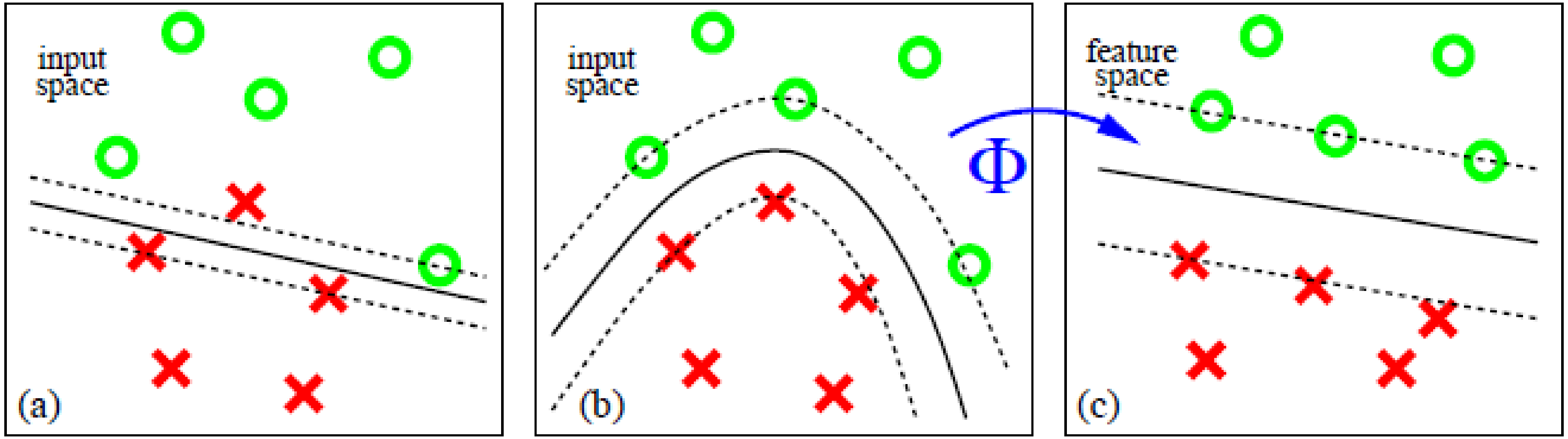
Is not linearly separable



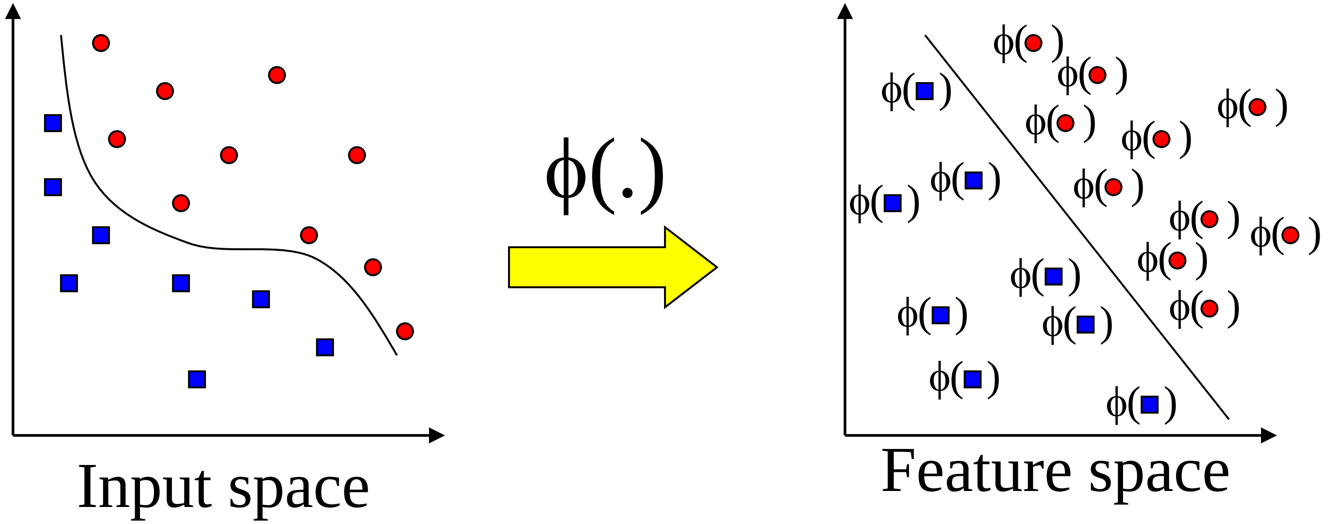
Is linearly separable



Find a feature space



Transforming the Data



Note: feature space is of higher dimension than the input space in practice

- Computation in the feature space can be costly because it is high dimensional
  - The feature space is typically infinite-dimensional!
- The kernel trick comes to rescue

The Kernel Trick

- Recall the SVM (

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

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

- The data points only appear as inner product
- As long as we can calculate the inner product in the feature space, we do not need the mapping explicitly
- Many common geometric operations (angles, distances) can be expressed by inner products
- Define the kernel function *K* by $K(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$

An Example for ϕ(.) and K(.,.)

- Suppose ϕ(.) is given as follows

$$\phi(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}) = (1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, x_2^2, \sqrt{2}x_1x_2)$$

- An inner product in the feature space is

$$\langle \phi(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}), \phi(\begin{bmatrix} y_1 \\ y_2 \end{bmatrix}) \rangle = (1 + x_1y_1 + x_2y_2)^2$$

- So, if we define the kernel function as follows, there is no need to carry out ϕ(.) explicitly

$$K(\mathbf{x}, \mathbf{y}) = (1 + x_1y_1 + x_2y_2)^2$$

- This use of kernel function to avoid carrying out ϕ(.) explicitly is known as the kernel trick

Kernels

- Given a mapping: $\mathbf{x} \to \boldsymbol{\varphi}(\mathbf{x})$

a kernel is represented as the inner product

$$K(\mathbf{x},\mathbf{y}) \to \sum_i \varphi_i(\mathbf{x})\varphi_i(\mathbf{y})$$

A kernel must satisfy the Mercer's condition:

$$\forall g(\mathbf{x}) \text{ such that } \int g^2(\mathbf{x})d\mathbf{x} \geq 0 \Rightarrow \int K(\mathbf{x},\mathbf{y})g(\mathbf{x})g(\mathbf{y})d\mathbf{x}d\mathbf{y} \geq 0$$

Modification Due to Kernel Function

- Change all inner products to kernel functions
- For training,

Original

$$\text{max. } W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

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

With kernel function

$$\text{max. } W(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$$

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

Modification Due to Kernel Function

- For testing, the new data **z** is classified as class 1 if *f* ≥0, and as class 2 if *f* <0

Original

$$\mathbf{w} = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \mathbf{x}_{t_j}$$

$$f = \mathbf{w}^T \mathbf{z} + b = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \mathbf{x}_{t_j}^T \mathbf{z} + b$$

With kernel function

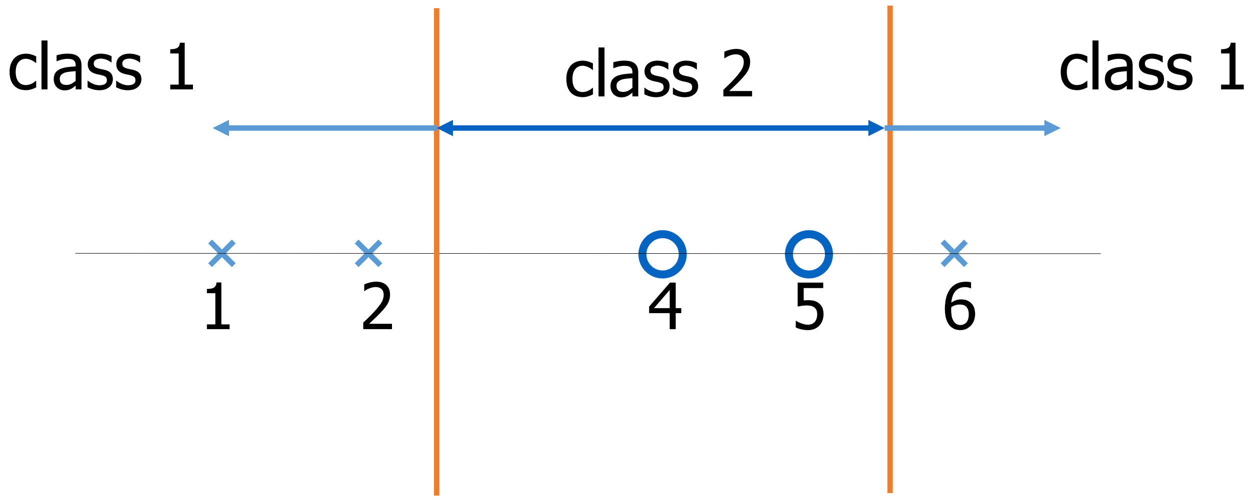
$$\mathbf{w} = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \phi(\mathbf{x}_{t_j})$$

$$f = \langle \mathbf{w}, \phi(\mathbf{z}) \rangle + b = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} K(\mathbf{x}_{t_j}, \mathbf{z}) + b$$

Example

- Suppose we have 5 1D data points
  - $x_1=1$, $x_2=2$, $x_3=4$, $x_4=5$, $x_5=6$, with 1, 2, 6 as class 1 and 4, 5 as class 2 $\Rightarrow$ $y_1=1$, $y_2=1$, $y_3=-1$, $y_4=-1$, $y_5=1$

Example



Example

- We use the polynomial kernel of degree 2
  - $K(x,y) = (xy+1)^2$
  - C is set to 100   first find α_i (i=1, …, 5) by

$$\text{max.} \quad \sum_{i=1}^{5} \alpha_i - \frac{1}{2} \sum_{i=1}^{5} \sum_{j=1}^{5} \alpha_i \alpha_j y_i y_j (x_i x_j + 1)^2$$

$$\text{subject to } 100 \geq \alpha_i \geq 0, \sum_{i=1}^{5} \alpha_i y_i = 0$$

Example

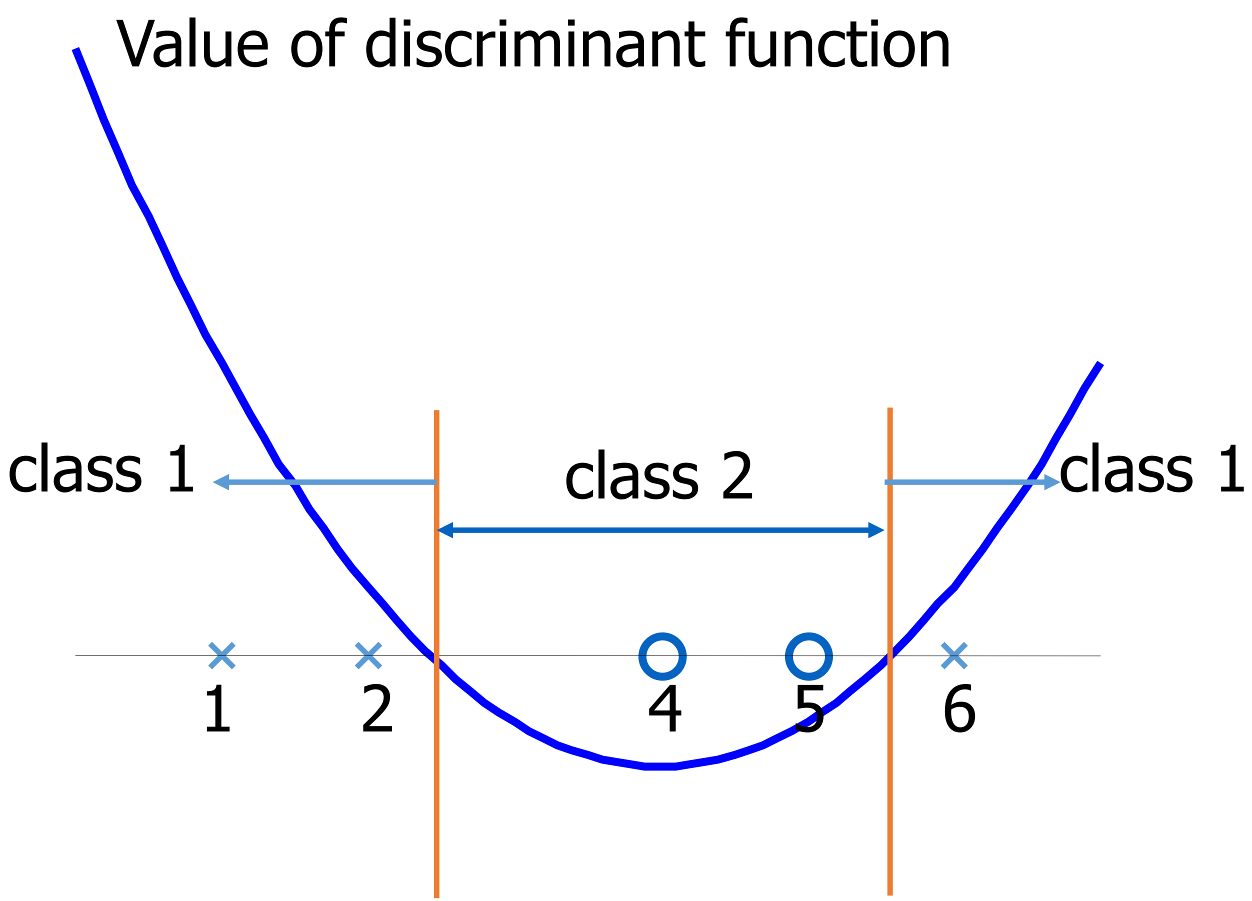
- By using a QP solver, we get
  - α_1=0, α_2=2.5, α_3=0, α_4=7.333, α_5=4.833
  - Note that the constraints are indeed satisfied
  - The support vectors are {x_2=2, x_4=5, x_5=6}
- The discriminant function is

$$
\begin{aligned}
&f(z)\\
&= 2.5(1)(2z+1)^2 + 7.333(-1)(5z+1)^2 + \overset{\alpha_5}{4.833}(\overset{y_5}{1})\overset{K(z,x_5)}{(6z+1)^2} + b\\
&= 0.6667z^2 - 5.333z + b
\end{aligned}
$$

- *b* is recovered by solving f(2)=1 or by f(5)=-1 or by f(6)=1,
- All three give b=9

$$\Rightarrow \quad f(z) = 0.6667z^2 - 5.333z + 9$$

Example



Value of discriminant function
class 1
class 2
class 1
1
2
4
5
6

Kernel Functions

- In practical use of SVM, the user specifies the kernel function; the transformation $\phi(.)$ is not explicitly stated
- Given a kernel function $K(\mathbf{x}_i, \mathbf{x}_j)$, the transformation $\phi(.)$ is given by its eigenfunctions (a concept in functional analysis)
  - Eigenfunctions can be difficult to construct explicitly
  - This is why people only specify the kernel function without worrying about the exact transformation
- Another view: kernel function, being an inner product, is really a similarity measure between the objects

A kernel is associated to a transformation

- Given a kernel, in principle it should be recovered the transformation in the feature space that originates it.

- $K(x,y) = (xy+1)^2 = x^2y^2+2xy+1$

It corresponds the transformation

$$x \rightarrow \begin{pmatrix} x^2 \\ \sqrt{2}x \\ 1 \end{pmatrix}$$

Examples of Kernel Functions

- Polynomial kernel up to degree *d*

$$K(\mathbf{u}, \mathbf{v}) = (\mathbf{u} \cdot \mathbf{v})^d$$

- Polynomial kernel up to degree *d*

$$K(\mathbf{x}, \mathbf{y}) = (\mathbf{x}^T\mathbf{y} + 1)^d$$

- Radial basis function kernel with width σ

$$K(\mathbf{x}, \mathbf{y}) = \exp(-||\mathbf{x} - \mathbf{y}||^2/(2\sigma^2))$$

  - The feature space is infinite-dimensional
- Sigmoid with parameter κ and θ

$$K(\mathbf{x}, \mathbf{y}) = \tanh(\kappa\mathbf{x}^T\mathbf{y} + \theta)$$

  - It does not satisfy the Mercer condition on all κ and θ

Summary: Steps for Classification

- Prepare the pattern matrix
- Select the kernel function to use
- Select the parameter of the kernel function and the value of *C*
  - You can use the values suggested by the SVM software, or you can set apart a validation set to determine the values of the parameter
- Execute the training algorithm and obtain the α_i
- Unseen data can be classified using the α_i and the support vectors

Strengths and Weaknesses of SVM

- Strengths
  - Training is relatively easy
    - No local optimal, unlike in neural networks
  - It scales relatively well to high dimensional data
  - Tradeoff between classifier complexity and error can be controlled explicitly
  - Non-traditional data like strings and trees can be used as input to SVM, instead of feature vectors
- Weaknesses
  - Need to choose a “good” kernel function.

Conclusion

- SVM is a useful alternative to neural networks
- Two key concepts of SVM: maximize the margin and the kernel trick
- Many SVM implementations are available on the web for you to try on your data set!

Thank You!

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