SUPPORT VECTOR MACHINES

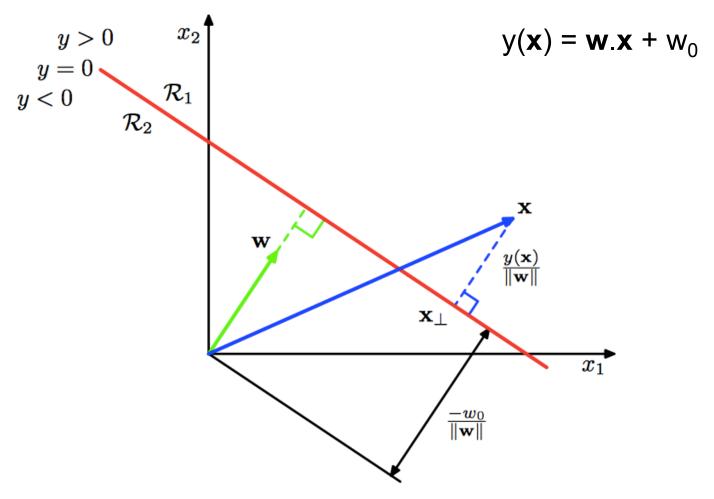
TRU CAO

HO CHI MINH CITY UNIVERSITY OF TECHNOLOGY AND JOHN VON NEUMANN INSTITUTE

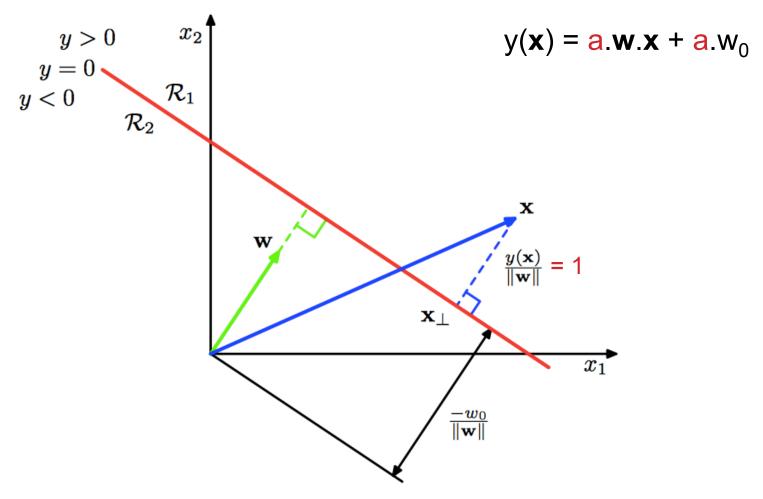
OUTLINE

- Review of analytical geometry
- Maximum margin classifiers
- Optimization using Langrage multipliers
- Kernel trick for non-linearly separable data
- Soft-margin SVMs

REVIEW OF ANALYTICAL GEOMETRY



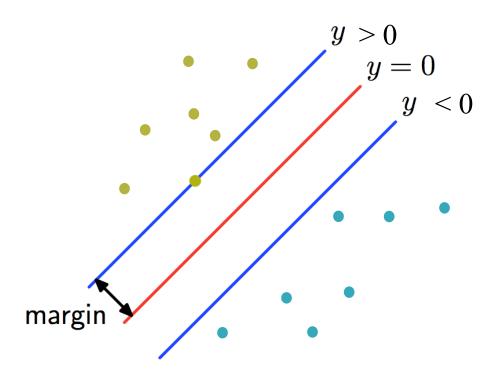
REVIEW OF ANALYTICAL GEOMETRY



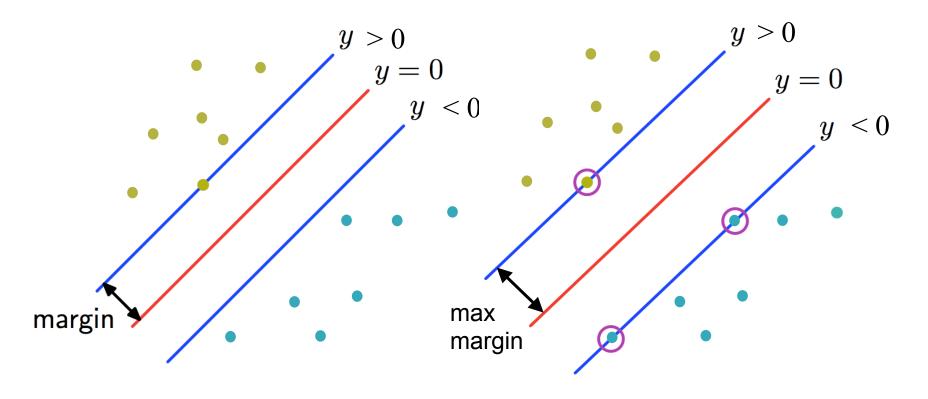
- Assume that the data are linearly separable.
- Decision boundary equation:

$$y(x) = w.x + b$$

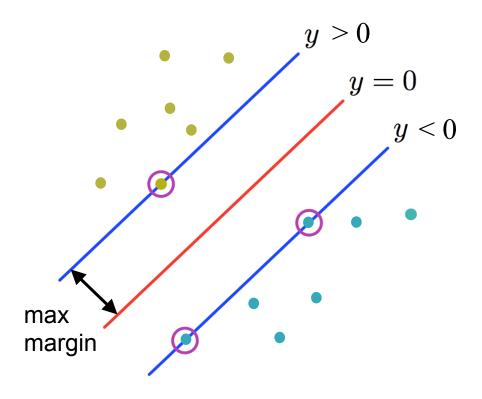
 Margin: the smallest distance between the decision boundary and any of the samples.



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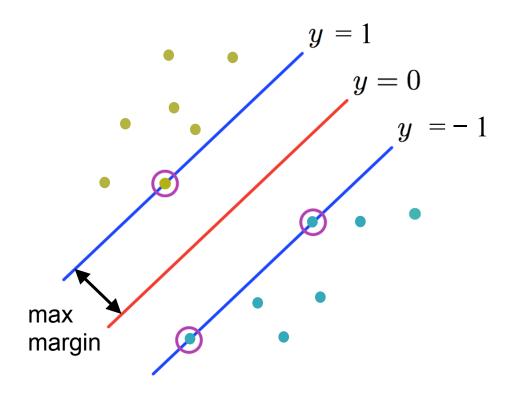


Support vectors: samples at the two margins.



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• Scaling the maximum margin to be 1:



 Signed distance between the decision boundary and a sample x_n:

$$\frac{y(\mathbf{x}_n)}{||\mathbf{w}||}$$

 Signed distance between the decision boundary and a sample x_n:

$$\frac{y(\mathbf{x}_n)}{||\mathbf{w}||}$$

 Absolute distance between the decision boundary and a sample x_n:

$$\frac{\mathsf{t}_{\mathsf{n}}.\mathsf{y}(\mathbf{x}_{\mathsf{n}})}{||\mathbf{w}||}$$

$$t_n = +1$$
 iff $y(\mathbf{x}_n) > 0$ and $t_n = -1$ iff $y(\mathbf{x}_n) < 0$

Maximum margin:

$$\operatorname{argmax}_{\mathbf{w},b} \left\{ \frac{1}{||\mathbf{w}||} \min_{n} (t_{n}.(\mathbf{w}.\mathbf{x}_{n} + b)) \right\}$$

with the constraint:

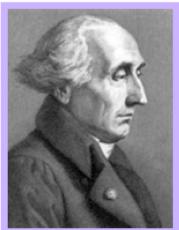
$$t_n.(\mathbf{w}.\mathbf{x}_n + \mathbf{b}) \ge 1$$

• To be optimized:

$$\operatorname{argmin}_{\mathbf{w},b} \frac{1}{2} ||\mathbf{w}||^2$$

with the constraint:

$$t_n.(\mathbf{w}.\mathbf{x}_n + \mathbf{b}) \ge 1$$



Joseph-Louis Lagrange

Although widely considered to be a French mathematician, Lagrange was born in Turin in Italy. By the age of nineteen, he had already made important contributions mathematics and had been appointed as Pro-

fessor at the Royal Artillery School in Turin. For many

years, Euler worked hard to persuade Lagrange to move to Berlin, which he eventually did in 1766 where he succeeded Euler as Director of Mathematics at the Berlin Academy. Later he moved to Paris, narrowly escaping with his life during the French revolution thanks to the personal intervention of Lavoisier (the French chemist who discovered oxygen) who himself was later executed at the guillotine. Lagrange made key contributions to the calculus of variations and the foundations of dynamics.

Problem:

$$argmax_{x} f(x)$$

with the constraint:

$$g(\mathbf{x}) = 0$$

Solution is the stationary point of the Lagrange function:

$$L(\mathbf{x}, \boldsymbol{\lambda}) = f(\mathbf{x}) + \boldsymbol{\lambda}.g(\mathbf{x})$$

such that:

$$\partial L(\mathbf{x}, \boldsymbol{\lambda})/\partial x_n = \partial f(\mathbf{x})/\partial x_n + \boldsymbol{\lambda}.\partial g(\mathbf{x})/\partial x_n = 0$$

and

$$\partial L(\mathbf{x}, \boldsymbol{\lambda})/\partial \boldsymbol{\lambda} = g(\mathbf{x}) = 0$$

Example:

$$f(\mathbf{x}) = 1 - u^2 - v^2$$

with the constraint:

$$g(x) = u + v - 1 = 0$$

Lagrange function:

$$L(\mathbf{x}, \lambda) = f(\mathbf{x}) + \lambda \cdot g(\mathbf{x}) = (1 - u^2 - v^2) + \lambda \cdot (u + v - 1)$$

$$\frac{\partial L(\mathbf{x}, \lambda)}{\partial u} = \frac{\partial f(\mathbf{x})}{\partial u} + \lambda \cdot \frac{\partial g(\mathbf{x})}{\partial u} = -2u + \lambda = 0$$

$$\frac{\partial L(\mathbf{x}, \lambda)}{\partial v} = \frac{\partial f(\mathbf{x})}{\partial v} + \lambda \cdot \frac{\partial g(\mathbf{x})}{\partial v} = -2v + \lambda = 0$$

$$\frac{\partial L(\mathbf{x}, \lambda)}{\partial \lambda} = g(\mathbf{x}) = u + v - 1 = 0$$

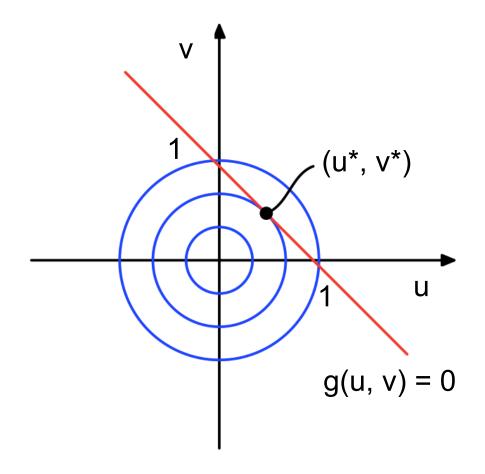
Solution: u = 1/2 and v = 1/2

Example:

$$f(\mathbf{x}) = 1 - u^2 - v^2$$

with the constraint:

$$g(x) = u + v - 1 = 0$$



Problem:

$$\operatorname{argmax}_{\mathbf{x}} f(\mathbf{x})$$

with the inequality constraint:

$$g(\mathbf{x}) \ge 0$$

Solution is the stationary point of the Lagrange function:

$$L(\mathbf{x}, \boldsymbol{\lambda}) = f(\mathbf{x}) + \boldsymbol{\lambda}.g(\mathbf{x})$$

such that:

$$\partial L(\mathbf{x}, \boldsymbol{\lambda})/\partial x_n = \partial f(\mathbf{x})/\partial x_n + \boldsymbol{\lambda}.\partial g(\mathbf{x})/\partial x_n = 0$$

and

$$g(\mathbf{x}) \ge 0$$
$$\lambda \ge 0$$
$$\lambda . g(\mathbf{x}) = 0$$

To be optimized:

$$\operatorname{argmin}_{\mathbf{w},b} \frac{1}{2} ||\mathbf{w}||^2$$

with the constraint:

$$t_n.(\mathbf{w}.\mathbf{x}_n + \mathbf{b}) \ge 1$$

• Lagrange function for maximum margin classifier:

$$L(\mathbf{w}, b, \mathbf{a}) = \frac{1}{2} ||\mathbf{w}||^2 - \sum_{n=1..N} \mathbf{a}_n \cdot (\mathbf{t}_n \cdot (\mathbf{w} \cdot \mathbf{x}_n + b) - 1)$$

$$t_{n}.(\mathbf{w}.\mathbf{x}_{n} + \mathbf{b}) - 1 \ge 0$$
$$\mathbf{a}_{n} \ge 0$$

$$a_n \cdot (t_n \cdot (\mathbf{w} \cdot \mathbf{x}_n + \mathbf{b}) - 1) = 0$$

Lagrange function for maximum margin classifier:

$$L(\mathbf{w}, b, \mathbf{a}) = \frac{1}{2} ||\mathbf{w}||^2 - \sum_{n=1..N} \mathbf{a}_n \cdot (t_n \cdot (\mathbf{w} \cdot \mathbf{x}_n + b) - 1)$$

• Solution for w: $\partial L(\mathbf{w}, \mathbf{b}, \mathbf{a})/\partial \mathbf{w} = 0$

$$\mathbf{w} = \sum_{n=1..N} \mathbf{a}_n . t_n . \mathbf{x}_n$$

$$\partial L(\mathbf{w}, \mathbf{b}, \mathbf{a})/\partial \mathbf{b} = \sum_{n=1}^{\infty} \mathbf{a}_n \cdot \mathbf{t}_n = 0$$

Lagrange function for maximum margin classifier:

$$L(\mathbf{w}, b, \mathbf{a}) = \frac{1}{2} ||\mathbf{w}||^2 - \sum_{n=1..N} \mathbf{a}_n \cdot (t_n \cdot (\mathbf{w} \cdot \mathbf{x}_n + b) - 1)$$

Solution for a: dual representation to be minimized

$$L^*(\mathbf{a}) = \sum_{n=1..N} \mathbf{a}_n - \frac{1}{2} \sum_{n=1..N} \sum_{n=1..M} \mathbf{a}_n \cdot \mathbf{a}_n \cdot \mathbf{t}_n \cdot \mathbf{t}_m \cdot \mathbf{x}_n \cdot \mathbf{x}_m$$

with the constraints:

$$\mathbf{a}_{n} \ge 0$$

$$\sum_{n=1..N} \mathbf{a}_{n} \cdot \mathbf{t}_{n} = 0$$

Lagrange function for maximum margin classifier:

$$L(\mathbf{w}, b, \mathbf{a}) = \frac{1}{2} ||\mathbf{w}||^2 - \sum_{n=1..N} \mathbf{a}_n \cdot (t_n \cdot (\mathbf{w} \cdot \mathbf{x}_n + b) - 1)$$

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Why optimization via dual representation?

Lagrange function for maximum margin classifier:

$$L(\mathbf{w}, b, \mathbf{a}) = \frac{1}{2} ||\mathbf{w}||^2 - \sum_{n=1..N} \mathbf{a}_n \cdot (t_n \cdot (\mathbf{w} \cdot \mathbf{x}_n + b) - 1)$$

Solution for a: dual representation to be minimized

$$L^*(\mathbf{a}) = \sum_{n=1..N} \mathbf{a}_n - \frac{1}{2} \sum_{n=1..N} \sum_{n=1..M} \mathbf{a}_n \cdot \mathbf{a}_n \cdot \mathbf{t}_n \cdot \mathbf{t}_m \cdot \mathbf{x}_n \cdot \mathbf{x}_m$$

Why optimization via dual representation?

• Sparsity: $a_n = 0$ if x_n is not a support vector.

Lagrange function for maximum margin classifier:

$$L(\mathbf{w}, b, \mathbf{a}) = \frac{1}{2} ||\mathbf{w}||^2 - \sum_{n=1..N} \mathbf{a}_n \cdot (t_n \cdot (\mathbf{w} \cdot \mathbf{x}_n + b) - 1)$$

$$a_n \cdot (t_n \cdot (\mathbf{w} \cdot \mathbf{x}_n + \mathbf{b}) - 1) = 0$$

Solution for b:

$$b = \frac{1}{|S|} \sum_{n \in S} (t_n - \sum_{m \in S} a_m \cdot t_m \cdot \mathbf{x}_m \cdot \mathbf{x}_n)$$

where S is the set of support vectors $(a_n \neq 0)$.

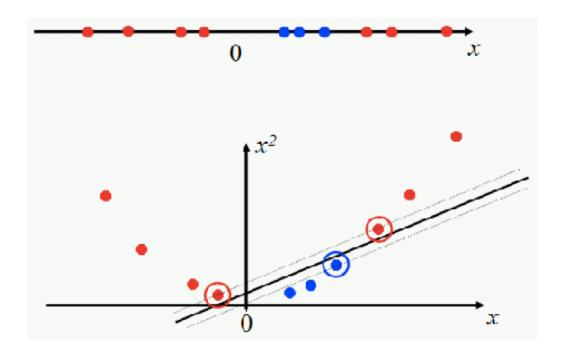
Classification:

$$y(x) = w.x + b = \sum_{n=1..N} a_n.t_n.x_n.x + b$$

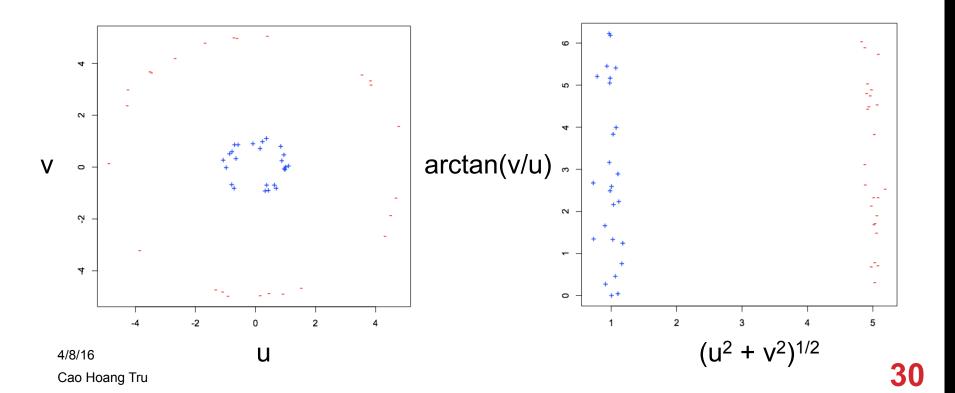
$$y(\mathbf{x}) > 0 \Rightarrow +1$$

$$y(\mathbf{x}) \leq \Rightarrow -1$$

- Mapping the data points into a high dimensional feature space.
- Example 1:
 - Original space: (x)
 - New space: (x, x²)

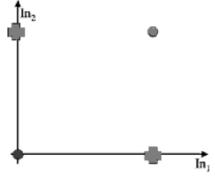


- Example 2:
 - Original space: (u, v)
 - New space: $((u^2 + v^2)^{1/2}, arctan(v/u))$

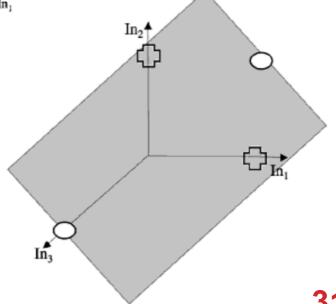


Example 3: XOR function

In_1	In_2	t
0	0	0
0	1	1
1	0	1
1	1	0



\ln_1	In_2	\ln_3	Output
0	0	1	1
0	1	0	0
1	0	0	0
1	1	0	1



Classification in the new space:

$$y(\mathbf{x}) = \mathbf{w}.\mathbf{\Phi}(\mathbf{x}) + \mathbf{b} = \sum_{n=1..N} a_n \cdot t_n \cdot \mathbf{\Phi}(\mathbf{x}_n) \cdot \mathbf{\Phi}(\mathbf{x}) + \mathbf{b}$$

Classification in the new space:

$$y(\mathbf{x}) = \mathbf{w}.\mathbf{\Phi}(\mathbf{x}) + \mathbf{b} = \sum_{n=1..N} a_n t_n \mathbf{\Phi}(\mathbf{x}_n).\mathbf{\Phi}(\mathbf{x}) + \mathbf{b}$$

• Computational complexity of $\Phi(\mathbf{x}_n).\Phi(\mathbf{x})$ is high due to the high dimension of $\Phi(.)$.

Classification in the new space:

$$y(\mathbf{x}) = \mathbf{w}.\mathbf{\Phi}(\mathbf{x}) + \mathbf{b} = \sum_{n=1..N} a_n t_n \mathbf{\Phi}(\mathbf{x}_n).\mathbf{\Phi}(\mathbf{x}) + \mathbf{b}$$

• Computational complexity of $\Phi(\mathbf{x}_n)^T \cdot \Phi(\mathbf{x})$ is high due to the high dimension of $\Phi(.)$.

Kernel trick:

$$\Phi(\mathbf{x}_n).\Phi(\mathbf{x}_m) = K(\mathbf{x}_n, \mathbf{x}_m)$$

A typical kernel function:

$$K(\mathbf{u}, \mathbf{v}) = (1 + \mathbf{u}.\mathbf{v})^{2}$$

$$\Phi((u_{1}, u_{2}, ..., u_{d})) = (1, \sqrt{2}u_{1}, \sqrt{2}u_{2}, ..., \sqrt{2}u_{d}, \frac{\sqrt{2}u_{1}.u_{2}, \sqrt{2}u_{1}.u_{3}, ..., \sqrt{2}u_{d-1}.u_{d}, \frac{u_{1}^{2}, u_{2}^{2}, ..., u_{d}^{2})}$$

$$\Phi(\mathbf{u}).\Phi(\mathbf{v}) = 1 + 2\sum_{i=1..d} u_i.v_i + 2\sum_{i=1..d} \sum_{i=1..d} u_i.v_i.u_j.v_j + \sum_{i=1..d} u_i^2 v_i^2$$

$$\Phi(\mathbf{u}).\Phi(\mathbf{v}) = K(\mathbf{u}, \mathbf{v})$$

• Is $\Phi(\mathbf{x})$ guaranteed to be linearly separable?

Soft-margin SVM is introduced.

HOMEWORK

- Reading Appendix E about Lagrange multipliers in Bishop (2006), Pattern Recognition and Machine Learning.
- Verify all computations and equations in the lecture slides.