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HANOI UNIVERSITY OF SCIENCE AND TECHNOLOGY

ONE LOVE. ONE FUTURE.

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Machine Learning

IT3190E

Lecture: Support vector machines

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Contents

Support Vector Machines (1)

- **Support Vector Machines (SVM)** (máy vectơ hỗ trợ) was proposed by Vapnik and his colleages in 1970s. Then it became famous and popular in 1990s.
- Originally, SVM is a method for linear classification. It finds a hyperplane (also called *linear classifier*) to separate the two classes of data.
- For *non-linear classification* for which no hyperplane separates well the data, *kernel functions* (hàm nhân) will be used.
  - Kernel functions play the role to transform the data into another space, in which the data is linearly separable.
- Sometimes, we call linear SVM when no kernel function is used. (in fact, linear SVM uses a linear kernel)

Support Vector Machines (2)

- SVM has a strong theory that supports its performance.
- It can work well with very high dimensional problems.
- It is now one of the most popular and strong methods.
- For text categorization, linear SVM performs very well.

1. SVM: the linearly separable case

- Problem representation:
  - Training data **D** = {($\mathbf{x}_1$, y_1), ($\mathbf{x}_2$, y_2), …, ($\mathbf{x}_r$, y_r)} with *r* instances.
  - Each $\mathbf{x}_i$ is a vector in an n-dimensional space, e.g., $\mathbf{x}_i = (x_{i1}, x_{i2}, \ldots, x_{in})^T$. Each dimension represents an attribute.
  - Bold characters denote vectors.
  - y_i is a class label in {-1; 1}. '1' is possitive class, '-1' is negative class.
- **Linear separability assumption:** there exists a hyperplane (of linear form) that well separates the two classes
(giả thuyết tồn tại một siêu phẳng mà phân tách 2 lớp được)

Linear SVM

- SVM finds a hyperplane of the form:

$$f(\mathbf{x}) = \langle \mathbf{w} \cdot \mathbf{x} \rangle + b$$

  - $\mathbf{w}$ is the weight vector; b is a real number (bias). [Eq.1]
  - $\langle \mathbf{w} \cdot \mathbf{x} \rangle$ and $\langle \mathbf{w}, \mathbf{x} \rangle$ denote the inner product of two vectors (tích vô hướng của hai véctơ)

- Such that for each x_i:

$$y_i = \begin{cases} 1 & if \quad \langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b \geq 0 \\ -1 & if \quad \langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b < 0 \end{cases}$$

[Eq.2]

Separating hyperplane

- The hyperplane (H_0) which separates the possitive from negative class is of the form:

$$\langle \mathbf{w} \cdot \mathbf{x} \rangle + b = 0$$

- It is also known as the *decision boundary*/surface.
- But there might be infinitely many separating hyperplanes. Which one should we choose?

[Liu, 2006]

Hyperplane with max margin

- SVM selects the hyperplane with **max margin**.
  (SVM tìm siêu phẳng tách mà có lề lớn nhất)
- It is proven that *the max-margin hyperplane has minimal errors among all possible hyperplanes.*

[Liu, 2006]

Marginal hyperplanes

- Assume that the two classes in our data can be separated clearly by a hyperplane.
- Denote $(\mathbf{x}^+,1)$ in possitive class and $(\mathbf{x}^-,-1)$ in negative class which are *closest* to the separating hyperplane H_0 $(\langle \mathbf{w} \cdot \mathbf{x} \rangle + b = 0)$
- We define two parallel *marginal hyperplanes* as follows:
  - H_+ crosses $\mathbf{x}^+$ and is parallel with H_0: $\langle \mathbf{w} \cdot \mathbf{x}^+ \rangle + b = 1$
  - H_- crosses $\mathbf{x}^-$ and is parallel with H_0: $\langle \mathbf{w} \cdot \mathbf{x}^- \rangle + b = -1$
  - No data point lies between these two marginal hyperplanes. And satisfying:

$$\begin{aligned} \langle \mathbf{w} \cdot \mathbf{x_i} \rangle + b &\geq 1, && \text{if } y_i = 1 \\ \langle \mathbf{w} \cdot \mathbf{x_i} \rangle + b &\leq -1, && \text{if } y_i = -1 \end{aligned} \qquad \text{[Eq.3]}$$

The margin (1)

- **Margin** (mức lề) is defined as the distance between the two marginal hyperplanes.
  - Denote d_+ the distance from H_0 to H_+.
  - Denote d_- the distance from H_0 to H_-.
  - $(d_+ + d_-)$ is the margin.
- Remember that the distance from a point $\mathbf{x_i}$ to the hyperplane H_0 ($\langle \mathbf{w} \cdot \mathbf{x} \rangle + b = 0$) is computed as:

$$\frac{|\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b|}{\|\mathbf{w}\|} \qquad \text{[Eq.4]}$$

  - Where:

$$\|\mathbf{w}\| = \sqrt{<\mathbf{w} \cdot \mathbf{w}>} = \sqrt{w_1^2 + w_1^2 + \ldots + w_1^2} \qquad \text{[Eq.5]}$$

The margin (2)

- So the distance d_+ from $\mathbf{x}^+$ to H_0 is

$$d_+ = \frac{|\langle \mathbf{w} \cdot \mathbf{x}^+ \rangle + b|}{\|\mathbf{w}\|} = \frac{|1|}{\|\mathbf{w}\|} = \frac{1}{\|\mathbf{w}\|} \qquad \text{[Eq.6]}$$

- Similarly, the distance d_- from $\mathbf{x}^-$ to H_0 is

$$d_- = \frac{|\langle \mathbf{w} \cdot \mathbf{x}^- \rangle + b|}{\|\mathbf{w}\|} = \frac{|-1|}{\|\mathbf{w}\|} = \frac{1}{\|\mathbf{w}\|} \qquad \text{[Eq.7]}$$

- As a result, the margin is:

$$margin = d_+ + d_- = \frac{2}{\|\mathbf{w}\|} \qquad \text{[Eq.8]}$$

SVM: learning with max margin (1)

- *SVM learns a classifier H_0 with a maximum margin*, i.e., the hyperplane that has the greatest margin among all possible hyperplanes.

- This learning principle can be formulated as the following quadratic optimization problem:
  - *Find **w** and b that maximize*

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

  - *and satisfy the below conditions for any training data **x_i**:*

$$\begin{cases} \langle \mathbf{w} \cdot \mathbf{x_i} \rangle + b \geq 1, \text{if } \mathrm{y_i} = 1 \\ \langle \mathbf{w} \cdot \mathbf{x_i} \rangle + b \leq -1, \text{if } \mathrm{y_i} = \text{-}1 \end{cases}$$

SVM: learning with max margin (2)

- Learning SVM is equivalent to the following minimization problem:
  - Minimize

$$\frac{\langle \mathbf{w} \cdot \mathbf{w} \rangle}{2} \qquad \text{[Eq.9]}$$

  - Conditioned on

$$\begin{cases} \langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b \geq 1, & \text{if } y_i = 1 \\ \langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b \leq -1, & \text{if } y_i = -1 \end{cases}$$

- Note, it can be reformulated as:
  - Minimize

$$\frac{\langle \mathbf{w} \cdot \mathbf{w} \rangle}{2} \qquad \text{[Eq.10]}$$

(P)

  - Conditioned on

$$y_i(\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b) \geq 1, \quad \forall i = 1..r$$

- This is a *constrained optimization problem*.

Constrained optimization (1)

- Consider the problem:

Minimize *f(**x**)* conditioned on *g(**x**)* = 0

- *Necessary condition:* a solution $\mathbf{x}_0$ will satisfy

$$\begin{cases} \left.\dfrac{\partial}{\partial \mathbf{x}}\big(f(\mathbf{x}) + \alpha g(\mathbf{x})\big)\right|_{\mathbf{x}=\mathbf{x}_0} = 0 \\ g(\mathbf{x}) = 0 \end{cases};$$

  - Where α is a *Lagrange multiplier*.

- In the cases of many constraints ($g_i(x)=0$ for i=1…r), a solution $\mathbf{x}_0$ will satisfy:

$$\begin{cases} \left.\dfrac{\partial}{\partial \mathbf{x}}\left(f(\mathbf{x}) + \sum_{i=1}^{r} \alpha_i g_i(\mathbf{x})\right)\right|_{\mathbf{x}=\mathbf{x}_0} = 0 \\ g_i(\mathbf{x}) = 0 \end{cases};$$

Constrained optimization (2)

- Consider the problem with inequality constraints:

Minimize $f(\boldsymbol{x})$ conditioned on $g_i(\boldsymbol{x}) \le 0$

- *Necessary condition:* a solution $\mathbf{x}_0$ will satisfy

$$\begin{cases} \dfrac{\partial}{\partial \mathbf{x}}\left(f(\mathbf{x}) + \sum_{i=1}^{r} \alpha_i g_i(\mathbf{x}) \right)\Bigg|_{\mathbf{x}=\mathbf{x}_0} = 0 ; \\ g_i(\mathbf{x}) \le 0 \end{cases}$$

  - Where $\alpha_i \ge 0$ is a Lagrange multiplier.
- $L = f(\mathbf{x}) + \sum_{i=1}^{r} \alpha_i g_i(\mathbf{x})$ is known as the Lagrange function.
  - $\mathbf{x}$ is called *primal variable* (biến gốc)
  - α is called *dual variable* (biến đối ngẫu)

SVM: learning with max margin (3)

- The Lagrange function for problem [Eq. 10] is

$$L(\mathbf{w}, b, \alpha) = \frac{1}{2}\langle \mathbf{w} \cdot \mathbf{w} \rangle - \sum_{i=1}^{r} \alpha_i [y_i(\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b) - 1] \quad \text{[Eq.11a]}$$

  - Where each $\alpha_i \geq 0$ is a Lagrange multiplier.

- Solving [Eq. 10] is equivalent to the following minimax problem:

$$\arg\min_{\mathbf{w},b} \max_{\alpha \geq 0} L(\mathbf{w}, b, \alpha) \quad \text{[Eq.11b]}$$

$$= \arg\min_{\mathbf{w},b} \max_{\alpha \geq 0} \left(\frac{1}{2}\langle \mathbf{w} \cdot \mathbf{w} \rangle - \sum_{i=1}^{r} \alpha_i [y_i(\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b) - 1] \right)$$

SVM: learning with max margin (4)

- The *primal problem* [Eq. 10] can be derived by solving:

$$\max_{\alpha \geq 0} L(\mathbf{w}, b, \alpha) = \max_{\alpha \geq 0} \left(\frac{1}{2} \langle \mathbf{w} \cdot \mathbf{w} \rangle - \sum_{i=1}^{r} \alpha_i [y_i (\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b) - 1] \right)$$

- Its *dual problem* (đối ngẫu) can be derived by solving:

$$\min_{\mathbf{w}, b} L(\mathbf{w}, b, \alpha) = \min_{\mathbf{w}, b} \left(\frac{1}{2} \langle \mathbf{w} \cdot \mathbf{w} \rangle - \sum_{i=1}^{r} \alpha_i [y_i (\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b) - 1] \right)$$

- It is known that the optimal solution to [Eq. 10] will satisfy some conditions which is called the **Karush-Kuhn-Tucker** (KKT) conditions.

SVM: Karush-Kuhn-Tucker

$$\frac{\partial L}{\partial \mathbf{w}} = \mathbf{w} - \sum_{i=1}^{r} \alpha_i y_i \mathbf{x_i} = 0$$ [Eq.12]

$$\frac{\partial L}{\partial b} = -\sum_{i=1}^{r} \alpha_i y_i = 0$$ [Eq.13]

$$y_i(\langle \mathbf{w} \cdot \mathbf{x_i} \rangle + b) - 1 \geq 0, \ \forall \mathbf{x_i} \ (i = 1..r)$$ [Eq.14]

$$\alpha_i \geq 0$$ [Eq.15]

$$\alpha_i(y_i(\langle \mathbf{w} \cdot \mathbf{x_i} \rangle + b) - 1) = 0$$ [Eq.16]

- The last equation [Eq. 16] comes from a nice result from the duality theory.
  - Note: any $\alpha_i > 0$ will imply that the associated point $\mathbf{x_i}$ lies in a boundary hyperplane (H_+ or H_-).
  - Such a boundary point is named as a ***support vector***.
  - A non-support vector will correspond to $\alpha_i = 0$.

SVM: learning with max margin (5)

- In general, the KKT conditions do not guarantee the optimality of the solution.
- Fortunately, due to the convexity of the primal problem [Eq.10], the *KKT conditions are both necessary and sufficient to assure the global optimality of the solution. It means a vector satisfying all KKT conditions provides the globally optimal classifier.*
  - Convex optimization is 'easy' in the sense that we always can find a good solution with a provable guarantee.
  - There are many algorithms in the literature, but most are iterative.
- In fact, problem [Eq.10] is pretty hard to derive an efficient algorithm. Therefore, its **dual problem** is more preferable.

SVM: the dual form (1)

- Remember that the dual counterpart of [Eq.10] is

$$\min_{\mathbf{w},b} L(\mathbf{w},b,\alpha) = \min_{\mathbf{w},b}\left(\frac{1}{2}\langle\mathbf{w}\cdot\mathbf{w}\rangle - \sum_{i=1}^{r}\alpha_i[y_i(\langle\mathbf{w}\cdot\mathbf{x}_i\rangle + b) - 1]\right)$$

- By taking the gradient of L(**w**,b,α) in variables (**w**,b) and zeroing it, we can find the following dual function:

$$L_D(\alpha) = \sum_{i=1}^{r}\alpha_i - \frac{1}{2}\sum_{i,j=1}^{r}\alpha_i\alpha_j y_i y_j\langle\mathbf{x}_i\cdot\mathbf{x}_j\rangle \quad \text{[Eq.17]}$$

SVM: the dual form (2)

- Solving problem [Eq.10] is equivalent to solving its dual problem below:
  - Maximize $L_D(\boldsymbol{\alpha}) = \sum_{i=1}^{r} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{r} \alpha_i \alpha_j y_i y_j \langle \mathbf{x_i} \cdot \mathbf{x_j} \rangle$ [Eq.18]
  - Such that $\begin{cases} \sum_{i=1}^{r} \alpha_i y_i = 0 \\ \alpha_i \geq 0, \forall i = 1..r \end{cases}$ **(D)**
- The constraints in **(D)** is much simpler than those of the primal problem. Therefore deriving an efficient method to solve this problem might be easier.
  - However, existing algorithms for this problem are iterative and complicated. Therefore, we will not discuss any algorithm in detail !

SVM: the optimal classifier

- Once the dual problem is solved for $\boldsymbol{\alpha}$, we can recover the optimal solution to problem [Eq.10] by using the KKT.
- Let SV be the set of all support vectors
  - SV is a subset of the training data.
  - $\alpha_i > 0$ suggests that $\mathbf{x_i}$ is a support vector.
- We can compute **w*** by using [Eq.12]. So:

$$\mathbf{w}^* = \sum_{i=1}^{r} \alpha_i y_i \mathbf{x}_i = \sum_{\mathbf{x_i} \in SV} \alpha_i y_i \mathbf{x}_i; \qquad \text{(due to } \alpha_j = 0 \text{ for any } \mathbf{x_j} \text{ not in SV)}$$

- To find b*, we take an index k such that $\alpha_k > 0$:
  - It means $y_k(\langle \mathbf{w}^* \cdot \mathbf{x}_k \rangle + b^*) - 1 = 0$ due to [Eq.16].
  - Hence,
  - $b^* = y_k - \langle \mathbf{w}^* \cdot \mathbf{x}_k \rangle$

SVM: classifying new instances

- The decision boundary is

$$f(\mathbf{x}) = \langle \mathbf{w}^* \cdot \mathbf{x} \rangle + b^* = \sum_{\mathbf{x_i} \in SV} \alpha_i y_i \langle \mathbf{x_i} \cdot \mathbf{x} \rangle + b^* = 0 \qquad \text{[Eq.19]}$$

- For a new instance **z**, we compute:

$$sign(\langle \mathbf{w}^* \cdot \mathbf{z} \rangle + b^*) = sign\left(\sum_{\mathbf{x_i} \in SV} \alpha_i y_i \langle \mathbf{x_i} \cdot \mathbf{z} \rangle + b^* \right) \qquad \text{[Eq.20]}$$

  - If the result is 1, **z** will be assigned to the possitive class; otherwise **z** will be assigned to the negative class.

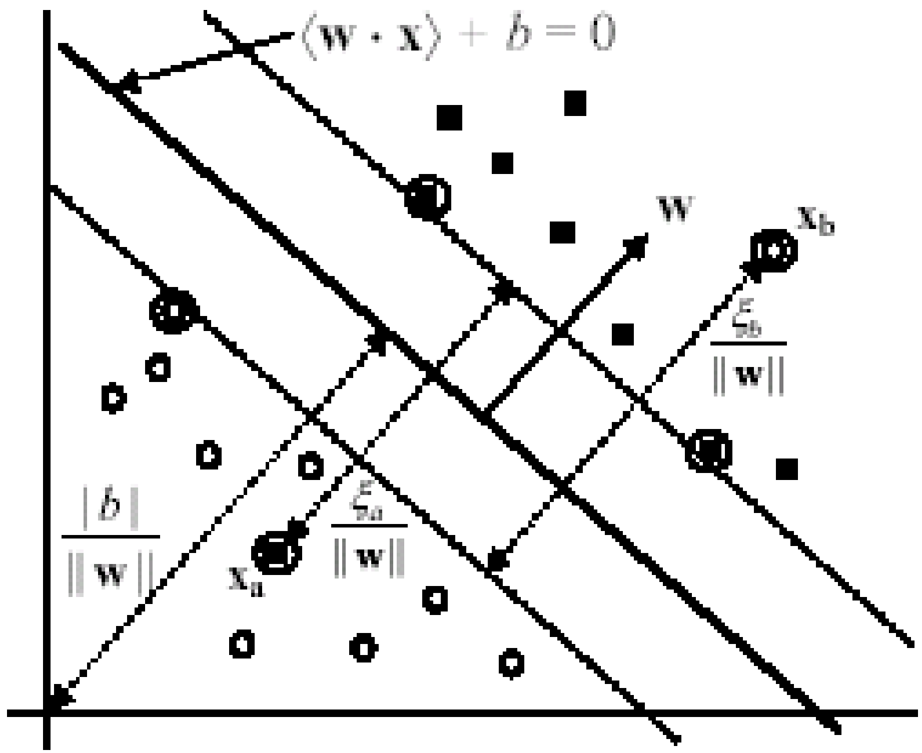
- Note that this classification principle
  - Just depends on the support vectors.
  - Just needs to compute some dot products.

2. Soft-margin SVM

- *What if the two classes are not linearly separable?* *(Trường hợp 2 lớp không thể phân tách tuyến tính thì sao?)*
  - Linear separability is ideal in practice.
  - Data are often noisy or erronous, making two classes overlapping (nhiễu/lỗi có thể làm 2 lớp giao nhau)
- In the case of linear separability:
  - *Minimize* $\frac{\langle \mathbf{w} \cdot \mathbf{w} \rangle}{2}$
  - *Conditioned on* $y_i(\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b) \geq 1, \quad \forall i = 1..r$
- In the cases of **noises** or **overlapping**, those constraints may never meet simutaneously.
  - It means we cannot solve for **w*** and b*.

Example of inseparability

- Noisy points $\mathbf{x}_a$ and $\mathbf{x}_b$ are mis-labeled.



Relaxing the constraints

- To work with noises/errors, we need to relax the constraints about margin by using some slack variables ξ_i (≥ 0):
  (Ta sẽ mở rộng ràng buộc về lề bằng cách thêm biến bù)

$$\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b \geq 1 - \xi_i \qquad \text{if } y_i = 1$$

$$\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b \leq -1 + \xi_i \qquad \text{if } y_i = -1$$

  - For a noisy/erronous point $\mathbf{x}_i$, we have: $\xi_i > 1$
  - Otherwise $\xi_i = 0$.

- Therefore, we have the following conditions for the cases of nonlinear separability:

$$y_i(\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b) \geq 1 - \xi_i \qquad \text{for all } i = 1 \ldots r$$

$$\xi_i \geq 0 \qquad \text{for all } i = 1 \ldots r$$

Penalty on noises/errors

- We should enclose some information on noises/errors into the objective function when learning
(ta nên đính thêm thông tin về nhiễu/lỗi vào hàm mục tiêu)
  - Otherwise, the resulting classifier easily overfits the data.
- A penalty term will be used so that learning is to minimize

$$\frac{\langle \boldsymbol{W}, \boldsymbol{W} \rangle}{2} + C \sum_{i=1}^{r} \xi_i^k$$

  - Where C (>0) is the penalty constant (hằng số phạt).
  - The greater C, the heavier the penalty on noises/errors.
- $k = 1$ is often used in practice, due to simplicity for solving the optimization problem.

The new optimization problem

- *Minimize* $$\frac{\langle \mathbf{w} \cdot \mathbf{w} \rangle}{2} + C\sum_{i=1}^{r} \xi_i$$ [Eq.21]
  - *Conditioned on* $$\begin{cases} y_i(\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b) \geq 1 - \xi_i, & \forall i = 1..r \\ \xi_i \geq 0, & \forall i = 1..r \end{cases}$$
- This problem is called **Soft-margin SVM**.
- It is equivalent to minimize the following function

$$\left[\frac{1}{r}\sum_{i=1}^{r} \max(0, 1 - y_i(\langle \boldsymbol{w} \cdot \boldsymbol{x}_i \rangle + b))\right] + \lambda \|\boldsymbol{w}\|_2^2$$

  - $\max(0, 1 - y_i(\langle \boldsymbol{w} \cdot \boldsymbol{x}_i \rangle + b))$ is called *Hinge loss*
  - Some popular losses: squared error, cross entropy, hinge
  - $\lambda > 0$ is a constant

The new optimization problem

- Its Lagrange function is

$$L = \frac{1}{2}\langle \mathbf{w} \cdot \mathbf{w} \rangle + C\sum_{i=1}^{r}\xi_i - \sum_{i=1}^{r}\alpha_i[y_i(\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b) - 1 + \xi_i] - \sum_{i=1}^{r}\mu_i\xi_i$$

[Eq.22]

  - Where α_i (≥ 0) and μ_i (≥ 0) are Lagrange multipliers.

Karush-Kuhn-Tucker conditions (1)

$$\frac{\partial L_P}{\partial \mathbf{w}} = \mathbf{w} - \sum_{i=1}^{r} \alpha_i y_i \mathbf{x_i} = 0$$ [Eq.23]

$$\frac{\partial L_P}{\partial b} = -\sum_{i=1}^{r} \alpha_i y_i = 0$$ [Eq.24]

$$\frac{\partial L_P}{\partial \xi_i} = C - \alpha_i - \mu_i = 0, \quad \forall i = 1..r$$ [Eq.25]

Karush-Kuhn-Tucker conditions (2)

$$y_i(\langle \mathbf{w} \cdot \mathbf{x_i} \rangle + b) - 1 + \xi_i \geq 0, \quad \forall i = 1..r$$ [Eq.26]

$$\xi_i \geq 0$$ [Eq.27]

$$\alpha_i \geq 0$$ [Eq.28]

$$\mu_i \geq 0$$ [Eq.29]

$$\alpha_i(y_i(\langle \mathbf{w} \cdot \mathbf{x_i} \rangle + b) - 1 + \xi_i) = 0$$ [Eq.30]

$$\mu_i \xi_i = 0$$ [Eq.31]

The dual problem

- *Maximize* $$L_D(\boldsymbol{\alpha}) = \sum_{i=1}^{r} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{r} \alpha_i \alpha_j y_i y_j \langle \mathbf{x_i} \cdot \mathbf{x_j} \rangle$$
  - *Such that* $$\begin{cases} \sum_{i=1}^{r} \alpha_i y_i = 0 \\ 0 \le \alpha_i \le C, \quad \forall i = 1..r \end{cases}$$ [Eq.32]

- Note that neither ξ nor μ_i appears in the dual problem.
- This problem is almost similar with that [Eq.18] in the case of linearly separable classification.
- The only difference is the constraint: $\alpha_i \le C$

Soft-margin SVM: the optimal classifier

- Once the dual problem is solved for α, we can recover the optimal solution to problem [Eq.21].
- Let SV be the set of all *support/noisy vectors*
  - SV is a subset of the training data.
  - $\alpha_i > 0$ suggests that $\mathbf{x}_i$ is a support/noisy vector.
- We can compute **w*** by using [Eq.12]. So:

$$\mathbf{w}^* = \sum_{i=1}^{r} \alpha_i y_i \mathbf{x}_i = \sum_{\mathbf{x}_i \in SV} \alpha_i y_i \mathbf{x}_i; \qquad \text{(due to } \alpha_j = 0 \text{ for any } \mathbf{x}_j \text{ not in SV)}$$

- To find b*, we take an index k such that $C > \alpha_k > 0$:
  - It means $\xi_k = 0$ due to [Eq.25] and [Eq.31];
  - And $y_k(\langle \mathbf{w}^* \cdot \mathbf{x}_k \rangle + b^*) - 1 = 0$ due to [Eq.30].
  - Hence, $b^* = y_k - \langle \mathbf{w}^* \cdot \mathbf{x}_k \rangle$

Some notes

- From [Eq.25-31] we conclude that

$$\boxed{\begin{array}{llll} \text{If} \quad \alpha_i = 0 & \text{then} & y_i(\langle \mathbf{w} \cdot \mathbf{x_i} \rangle + b) \geq 1, & \text{and} \ \xi_i = 0 \\ \text{If} \quad 0 < \alpha_i < C & \text{then} & y_i(\langle \mathbf{w} \cdot \mathbf{x_i} \rangle + b) = 1, & \text{and} \ \xi_i = 0 \\ \text{If} \quad \alpha_i = C & \text{then} & y_i(\langle \mathbf{w} \cdot \mathbf{x_i} \rangle + b) < 1, & \text{and} \ \xi_i > 0 \end{array}}$$

- The classifier can be expressed as a *linear combination* of few training points.
  - Most training points lie outside the margin area: $\alpha_i = 0$
  - The support vectors lie in the marginal hyperplanes: $0 < \alpha_i < C$
  - The noisy/erronous points will associate with $\alpha_i = C$
- Hence the optimal classifier is a very sparse *combination* of the training data.

Soft-margin SVM: classifying new instances

- The decision boundary is

$$f(\mathbf{x}) = \langle \mathbf{w}^* \cdot \mathbf{x} \rangle + b^* = \sum_{\mathbf{x_i} \in SV} \alpha_i y_i \langle \mathbf{x_i} \cdot \mathbf{x} \rangle + b^* = 0 \qquad \text{[Eq.19]}$$

- For a new instance **z**, we compute:

$$sign(\langle \mathbf{w}^* \cdot \mathbf{z} \rangle + b^*) = sign\left(\sum_{\mathbf{x_i} \in SV} \alpha_i y_i \langle \mathbf{x_i} \cdot \mathbf{z} \rangle + b^* \right) \qquad \text{[Eq.20]}$$

  - If the result is 1, **z** will be assigned to the possitive class; otherwise **z** will be assigned to the negative class.

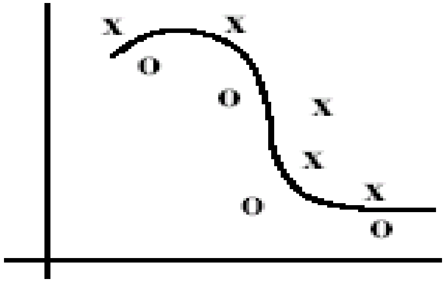
- *Note: it is important to choose a good value of C, since it significantly affects performance of SVM.*
  - We often use a validation set to choose a value for C.

Linear SVM: summary

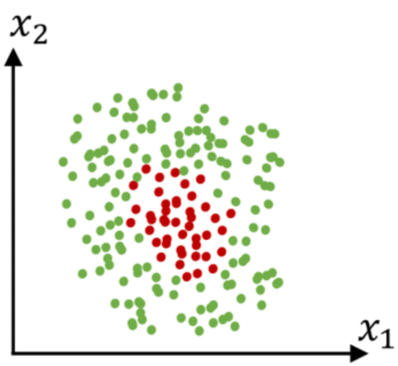
- Classification is based on a separating hyperplane.
- Such a hyperplane is represented as a combination of some support vectors.
- The determination of support vectors reduces to solve a quadratic programming problem.
- In the dual problem and the separating hyperplane, dot products can be used in place of the original training data.
  - This is the door for us to learn a nonlinear classifier.

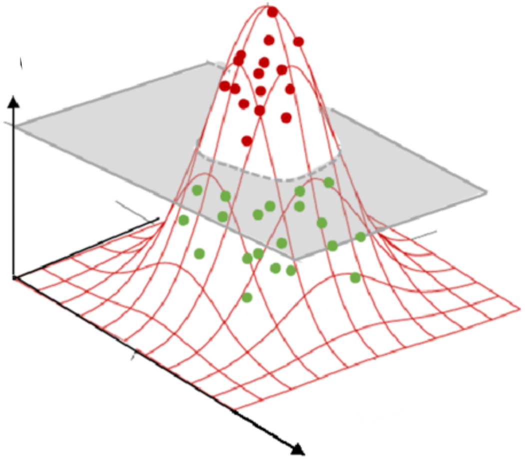
3. Non-linear SVM

- Consider the case in which our data are not linearly separable
  - This may often happen in practice



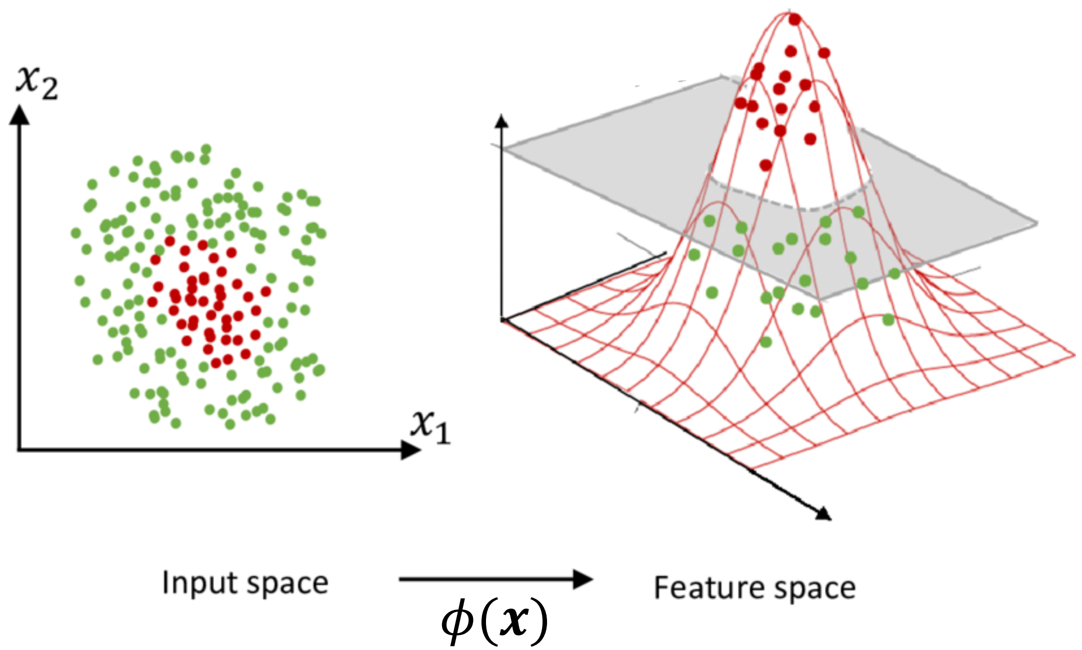
- How about using a non-linear function?
- **Idea of Non-linear SVM:**
  - **Step 1:** transform the input into another space, which often has *higher dimensions*, so that the projection of data is linearly separable
  - **Step 2:** use linear SVM in the new space





Non-linear SVM

- **Input space:** initial representation of data
- **Feature space:** the new space after the transformation



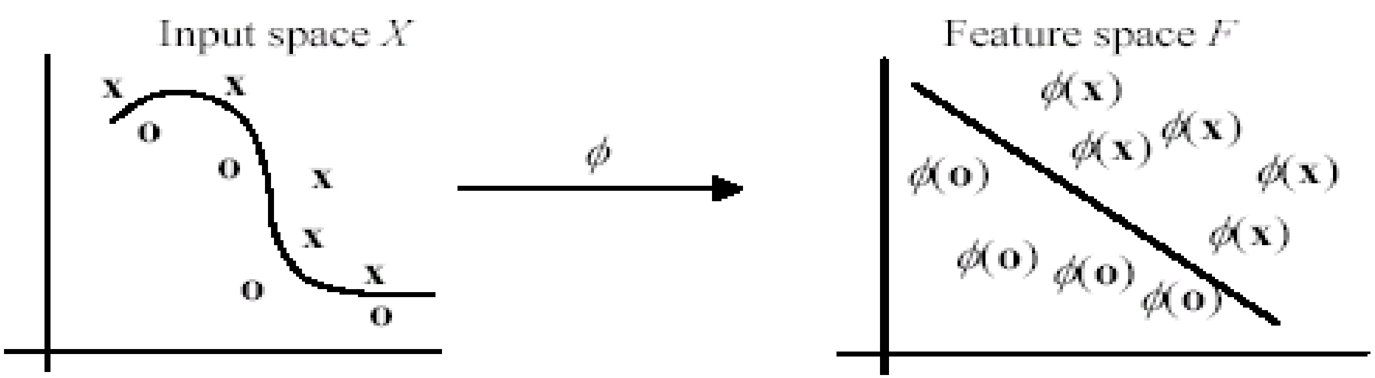
Non-linear SVM: transformation

- Our idea is to map the input **x** to a new representation, using a non-linear mapping

$$\phi:\ X \longrightarrow F$$
$$\boldsymbol{x} \longmapsto \phi(\boldsymbol{x})$$

- In the feature space, the original training data $\{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \ldots, (\boldsymbol{x}_r, y_r)\}$ are represented by

$$\{(\phi(\mathbf{x}_1), y_1), (\phi(\mathbf{x}_2), y_2), \ldots, (\phi(\mathbf{x}_r), y_r)\}$$



Non-linear SVM: transformation

- Consider the input space to be 2-dimensional, and we choose the following map

$$\phi: \ X \longrightarrow F$$
$$(x_1, x_2) \longmapsto (x_1^2, x_2^2, \sqrt{2}x_1x_2)$$

- So instance **x** = (2, 3) will have the representation in the feature space as

$$\phi(\mathbf{x}) = (4, 9, 8.49)$$

Non-linear SVM: learning & prediction

- **Training problem:**

Minimize
$$L_P = \frac{\langle \mathbf{w} \cdot \mathbf{w} \rangle}{2} + C\sum_{i=1}^{r} \xi_i \quad \text{[Eq.34]}$$

Such that
$$\begin{cases} y_i\left(\langle \mathbf{w} \cdot \phi(\mathbf{x_i})\rangle + b\right) \geq 1 - \xi_i, & \forall i = 1..r \\ \xi_i \geq 0, & \forall i = 1..r \end{cases}$$

- **The dual problem:**

Maximize
$$L_D = \sum_{i=1}^{r} \alpha_i - \frac{1}{2}\sum_{i,j=1}^{r} \alpha_i \alpha_j y_i y_j \langle \phi(\mathbf{x_i}) \cdot \phi(\mathbf{x_j})\rangle \quad \text{[Eq.35]}$$

Such that
$$\begin{cases} \sum_{i=1}^{r} \alpha_i y_i = 0 \\ 0 \leq \alpha_i \leq C, & \forall i = 1..r \end{cases}$$

- **Classifier:**

$$f(\mathbf{z}) = \langle \boldsymbol{w}^*, \phi(\mathbf{z})\rangle + b^* = \sum_{\boldsymbol{x}_i \in SV} \alpha_i y_i \langle \phi(\boldsymbol{x}_i), \phi(\mathbf{z})\rangle + b^* \quad \text{[Eq.36]}$$

Non-linear SVM: difficulties

- How to find the mapping?
  - An intractable problem
- The curse of dimensionality
  - As the dimensionality increases, the volume of the space increases so fast that the available data become sparse.
  - This sparsity is problematic.
  - Increasing the dimensionality will require significantly more training data.

Dữ liệu dù thu thập được lớn đến đâu thì cũng là **quá nhỏ** so với không gian của chúng

Non-linear SVM: Kernel functions

- An explicit form of a tranformation is not necessary
- **The dual problem:**

Maximize
$$L_D = \sum_{i=1}^{r} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{r} \alpha_i \alpha_j y_i y_j \langle \phi(\mathbf{x_i}) \cdot \phi(\mathbf{x_j}) \rangle$$

Such that
$$\begin{cases} \sum_{i=1}^{r} \alpha_i y_i = 0 \\ 0 \le \alpha_i \le C, \quad \forall i = 1..r \end{cases}$$

- **Classifier:** $f(\boldsymbol{z}) = \langle \boldsymbol{w}^*, \phi(\boldsymbol{z}) \rangle + b^* = \sum_{\boldsymbol{x}_i \in SV} \alpha_i y_i \langle \phi(\boldsymbol{x}_i), \phi(\boldsymbol{z}) \rangle + b^*$
- Both require only the inner product $\langle \phi(\mathbf{x}), \phi(\mathbf{z}) \rangle$
- **Kernel trick:** Nonlinear SVM can be used by replacing those inner products by evaluations of some ***kernel function***

$$K(\mathbf{x},\mathbf{z}) = \langle \phi(\mathbf{x}), \phi(\mathbf{z}) \rangle \qquad \text{[Eq.37]}$$

Kernel functions: example

- Polynomial

$$K(\boldsymbol{x}, \boldsymbol{z}) = \langle \boldsymbol{x}, \boldsymbol{z} \rangle^d$$

- Consider the polynomial with degree d=2. For any vectors **x**=(x_1,x_2) and **z**=(z_1,z_2)

$$\begin{aligned} \langle \boldsymbol{x}, \boldsymbol{z} \rangle^2 &= (x_1 z_1 + x_2 z_2)^2 \\ &= x_1^2 z_1^2 + 2 x_1 z_1 x_2 z_2 + x_2^2 z_2^2 \\ &= \left\langle \left(x_1^2, x_2^2, \sqrt{2} x_1 x_2\right), \left(z_1^2, z_2^2, \sqrt{2} z_1 z_2\right) \right\rangle \\ &= \langle \phi(\boldsymbol{x}), \phi(\boldsymbol{z}) \rangle = K(\boldsymbol{x}, \boldsymbol{z}) \end{aligned}$$

  - Where $\phi(\boldsymbol{x}) = \left(x_1^2, x_2^2, \sqrt{2} x_1 x_2\right)$.

- Therefore the polynomial is the product of two vectors $\phi(\boldsymbol{x})$ and $\phi(\boldsymbol{z})$.

Kernel functions: popular choices

- Polynomial

$$K(\mathbf{x},\mathbf{z}) = \left(\langle \mathbf{x} \cdot \mathbf{z} \rangle + \theta\right)^d; \quad \text{trong đó}: \ \theta \in R, d \in N$$

- Gaussian radial basis function (RBF)

$$K(\mathbf{x},\mathbf{z}) = e^{-\frac{\|\mathbf{x}-\mathbf{z}\|^2}{2\sigma}}; \quad \text{trong đó}: \ \sigma > 0$$

- Sigmoid

$$K(\mathbf{x},\mathbf{z}) = \tanh(\beta\langle \mathbf{x} \cdot \mathbf{z} \rangle - \lambda) = \frac{1}{1+e^{-(\beta\langle \mathbf{x} \cdot \mathbf{z} \rangle - \lambda)}}; \quad \text{trong đó}: \ \beta, \lambda \in R$$

- What conditions ensure a kernel function?

  Mercer's theorem

SVM: summary

- SVM works with real-value attributes
  - Any nominal attribute need to be transformed into a real one
- The learning formulation of SVM focuses on 2 classes
  - How about a classification problem with > 2 classes?
  - One-vs-the-rest, one-vs-one: a multiclass problem can be solved by reducing to many different problems with 2 classes
- The decision function is simple, but may be hard to interpret
  - It is more serious if we use some kernel functions

SVM: some packages

- LibSVM:
  - http://www.csie.ntu.edu.tw/~cjlin/libsvm/
- Linear SVM for large datasets:
  - http://www.csie.ntu.edu.tw/~cjlin/liblinear/
  - http://www.cs.cornell.edu/people/tj/svm_light/svm_perf.html
- Scikit-learn in python:
  - http://scikit-learn.org/stable/modules/svm.html
- SVM*light*:
  - http://www.cs.cornell.edu/people/tj/svm_light/index.html

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- C. J. C. Burges. A Tutorial on Support Vector Machines for Pattern Recognition. Data Mining and Knowledge Discovery, 2(2): 121-167, 1998.
- Cortes, Corinna, and Vladimir Vapnik. "Support-vector networks." *Machine learning* 20.3 (1995): 273-297.

Exercises

- **Question 1: Hyperplane Definition** What is the equation of a hyperplane in D-dimensional space?
- A) w^T x = 1
- B) w^T x + b = 0
- C) ||w|| = 1
- D) y = sign(w^T x)

Exercises

- **Question 2: Distance from a Point to Hyperplane** The distance of a point x_n from a hyperplane w^T x + b = 0 is given by:
- A) w^T x_n + b
- B) (w^T x_n + b) / ||w||^2
- C) |w^T x_n + b| / ||w||
- D) ||w|| × (w^T x_n + b)

Exercises

- **Question 3: Prediction Rule** For hyperplane-based binary classification, the prediction rule is:
- A) y* = w^T x* + b
- B) y* = sign(w^T x* + b)
- C) y* = ||w^T x* + b||
- D) y* = max(0, w^T x* + b)

Exercises

- **Question 4: 0-1 Loss Properties** The 0-1 loss function for classification is:
- A) Convex and differentiable
- B) Non-convex and differentiable
- C) Convex and non-differentiable
- D) Non-convex, non-differentiable, and NP-Hard to optimize

Exercises

- **Question 5: Perceptron Loss Function** The Perceptron loss function is:
- A) max{0, -yw^T x}
- B) max{0, 1 - yw^T x}
- C) log(1 + exp(-yw^T x))
- D) (y - ŷ)^2

Exercises

- **Question 6: Hinge Loss** The Hinge loss function used in SVMs is:
- A) max{0, -yw^T x}
- B) max{0, 1 - yw^T x}
- C) log(1 + exp(-yw^T x))
- D) |y - ŷ|

Exercises

- **Question 7: Perceptron Learning Characteristics** When using SGD with Perceptron loss (with k=0), the weight update occurs:
- A) After every iteration
- B) Only when the model makes a mistake
- C) When the margin is less than 1
- D) At fixed time intervals

Exercises

- **Question 8: Perceptron Gradient** For Perceptron loss with k=0, if the model makes a mistake on example (x_n, y_n), the gradient is:
- A) 0
- B) -y_n x_n
- C) x_n
- D) y_n

Exercises

- **Question 9: Perceptron Limitation** A key limitation of the Perceptron algorithm is:
- A) It cannot learn non-linear boundaries
- B) It doesn't guarantee any margin around the hyperplane
- C) It cannot handle multi-class problems
- D) It is too slow to train

Exercises

- **Question 10: Hard-Margin SVM Objective** In Hard-Margin SVM, maximizing the margin $2\gamma = 2/||w||$ is equivalent to:
- A) Maximizing $||w||$
- B) Minimizing $||w||$
- C) Minimizing $||w||^2$ or $||w||^2/2$
- D) Maximizing $||w||^2$

Exercises

- **Question 11: Hard-Margin SVM Constraint** The constraint in Hard-Margin SVM is:
- A) $y_n(w^T x_n + b) \geq 0$
- B) $y_n(w^T x_n + b) \geq 1$
- C) $y_n(w^T x_n + b) \leq 1$
- D) $|w^T x_n + b| \geq 1$

Exercises

- **Question 12: Hard-Margin SVM Assumption** Hard-Margin SVM assumes:
- A) Data is linearly separable with no points in the margin
- B) Data may have some noise
- C) Some misclassifications are allowed
- D) All training examples are support vectors

Exercises

- **Question 13: Solving Hard-Margin SVM** The Hard-Margin SVM optimization problem is solved using:
- A) Gradient descent only
- B) Lagrange's method with Lagrange multipliers
- C) Newton's method
- D) Random search

Exercises

- **Question 14: Soft-Margin SVM Slack Variables** In Soft-Margin SVM, the slack variable ξ_n represents:
- A) The margin width
- B) The extent of violation of the margin constraint
- C) The number of support vectors
- D) The learning rate

Exercises

- **Question 15: Slack Variable Interpretation** When slack variable $\xi_n > 1$, it means:
- A) The point is correctly classified with large margin
- B) The point is within the margin region
- C) The point is totally on the wrong side of the hyperplane
- D) The point is a support vector

Exercises

- **Question 16: Soft-Margin Constraint** The soft-margin constraint for all training examples is:
- A) y_n(w^T x_n + b) ≥ 1
- B) y_n(w^T x_n + b) ≥ 1 - ξ_n
- C) y_n(w^T x_n + b) ≤ 1 - ξ_n
- D) y_n(w^T x_n + b) = 1 - ξ_n

Exercises

- **Question 17: Hyperparameter C in Soft-Margin SVM** The hyperparameter C in Soft-Margin SVM controls:
- A) The learning rate
- B) The number of iterations
- C) The trade-off between large margin and small training error
- D) The dimensionality of the feature space

Exercises

- **Question 18: Large C Value Effect** When C is very large in Soft-Margin SVM:
- A) Large margin, large training error (bad)
- B) Small training error but also small margin (bad)
- C) Balanced trade-off
- D) No effect on the solution

Exercises

- **Question 19: Loss Functions Comparison** Which loss function is convex and differentiable?
- A) 0-1 Loss
- B) Perceptron Loss
- C) Hinge Loss
- D) Logistic Loss

Exercises

- **Question 20: SVM vs Perceptron** The key advantage of SVM over Perceptron is:
- A) SVM is faster to train
- B) SVM learns the maximum margin hyperplane
- C) SVM uses simpler mathematics
- D) SVM doesn't require hyperparameter tuning

Exercises

- What is the main difference between SVM and KNN?
- How many support vectors are there in the worst case? Why?
- The meaning of the constant C in SVM? Compare the role of C in SVM with that of λ in Ridge regression.

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THANK YOU !