

INTRODUCTION

- Support Vector Machines (SVM) (máy vecto 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)

INTRODUCTION

- 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.



CONTENTS AT A GLANCE

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SVM: The linearly separable case

02

Soft-margin SVM

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Non-linear SVM





SVM: The linearly separable case

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 rinstances
- Each \mathbf{x}_i is a vector in an n-dimensional space, e.g., $\mathbf{x}_i = (x_{i1}, x_{i2}, ..., x_{in})^\mathsf{T}$. Each dimension represents an attribute.
- Bold characters denote vectors.
- y_i is a class label in $\{-1, 1\}$. '1' is positive class, '-1' is negative class.

Linear separability assumption: there exists a hyperplane (of linear form) that well separates the two classes

LINEAR SVM



SVM finds a hyperplane of the form:

$$d + \langle x \rangle = \langle w \rangle + b$$

- w is the weight of vector; b is a real number (bias)
- <w.x> and <w,x> denote the inner product of two vectors

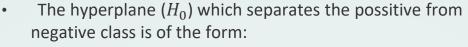


Such that for each x_i

$$y_i = 1 if < w. x_i > + b >= 0$$

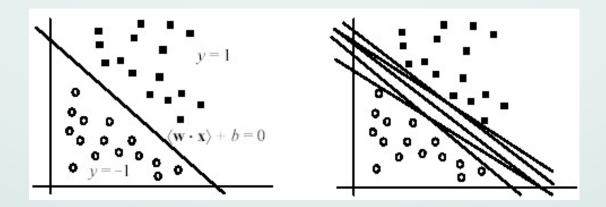
$$y_i = -1 if < w. x_i > + b >= 0$$

SEPERATING HYPERPLANE



$$< w . x > + b = 0$$

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





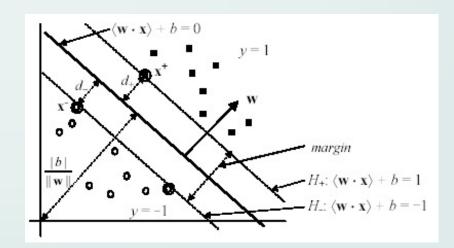
HYPERPLANE & MAX MARGIN OF HYPERPLANE

02

It is proven that the max-margin hyperplane has minimal errors among all possible hyperplanes.

SVM selects the hyperplane with max margin.





HYPERPLANE & MAX MARGIN OF HYPERPLANE

03

Assume that the two classes in our data can be separated clearly by a hyperplane.



Denote $(x^+, 1)$ in possitive class and $(x^-, -1)$ in negative class which are closest to the separating hyperplane H_0 (<w . x> + b = 0)

We define two parallel *marginal hyperplanes* as follows:

- H_+ crosses x^+ and is parallel with H_0 : $(< w . x^+ > + b = 1)$
- H_- crosses x^- and is parallel with H_0 : (<w . x^- > + b = -1

No data point lies between these two marginal hyperplanes. And satisfying:

$$<$$
w . $x_i>$ + b \ge 1, if $y_i=1$
 $<$ w . $x_i>$ + b \le -1, if $y_i=-1$

THE MARGIN





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 x_i to the hyperplane H_0 ($<\mathbf{w} \times \mathbf{x}> + b = 0$) is computed as:

$$\frac{\langle w \cdot x_i \rangle + b}{\|w\|}$$

Where:

$$||w|| = \sqrt{\langle w \cdot w \rangle} = \sqrt{w_1^2 + w_{2+\dots}^2 + w_n^2}$$

THE MARGIN







So the distance d_+ from x^+ to H_0 is

$$d_{+} = \frac{|\langle w \cdot x^{+} \rangle + b|}{\|w\|} = \frac{|1|}{\|w\|} = \frac{1}{\|w\|}$$

So the distance d_- from x^- to H_0 is

$$d_{-} = \frac{|\langle w \cdot x^{-} \rangle + b|}{||w||} = \frac{|-1|}{||w||} = \frac{1}{||w||}$$

As a result, the margin is:

margin =
$$d_+ + d_- = \frac{2}{\|w\|}$$



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

SVM: learning with max margin



Learning SVM is equivalent to the following minimization problem:

- Minimize: $\frac{\langle w \cdot w \rangle}{2}$

- Conditioned on:

$$<$$
w . $x_i>$ + b \geq 1, if y_i = 1 $<$ w . $x_i>$ + b \leq -1, if y_i = -1

Note, it can be reformulated as:

- Minimize:



- Conditioned on:

$$y_i(< w . x_i > + b) \ge 1, \forall i = 1..r$$



This is a *constrained optimization problem*.



THE MARGIN







So the distance d_+ from x^+ to H_0 is

$$d_{+} = \frac{|\langle w \cdot x^{+} \rangle + b|}{\|w\|} = \frac{|1|}{\|w\|} = \frac{1}{\|w\|}$$

So the distance d_- from x^- to H_0 is

$$d_{-} = \frac{|\langle w \cdot x^{-} \rangle + b|}{||w||} = \frac{|-1|}{||w||} = \frac{1}{||w||}$$

As a result, the margin is:

margin =
$$d_+ + d_- = \frac{2}{\|w\|}$$

SVM: learning with max margin

The Lagrange function for problem (*) is

$$L(w, b, \alpha) = \frac{1}{2} \langle w \cdot w \rangle - \sum_{i=1}^{r} \alpha_{i} [y_{i} (\langle w \cdot x_{i} \rangle + b)]$$

01

Where each $\alpha_i \ge 0$ is a Lagrange multiplier.

02

Solving (*) is equivalent to the following minimax problem:

$$\arg \min_{\mathbf{w}, b} \max_{\alpha \ge 0} L(\mathbf{w}, b, \alpha)$$

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

The *primal problem* (*) can be derived by solving: $\max_{\alpha \geq 0} L(\mathbf{w}, b, \alpha)$

$$= \max_{\alpha \ge 0} \left(\frac{1}{2} \langle \mathbf{w} \cdot \mathbf{w} \rangle - \sum_{i=1}^{r} \alpha_{i} [y_{i} (\langle \mathbf{w} \cdot \mathbf{x}_{i} \rangle + b) - 1] \right)$$

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

$$\begin{aligned} & \underset{\mathbf{w}, b}{min} L(\mathbf{w}, b, \alpha) \\ &= \min_{\mathbf{w}, b} \left(\frac{1}{2} \langle \mathbf{w} \cdot \mathbf{w} \rangle - \sum_{i=1}^{r} \alpha_{i} [y_{i} (\langle \mathbf{w} \cdot \mathbf{x}_{i} \rangle + b) - 1] \right) \end{aligned}$$

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

SVM: Karush-Kuhn-Tucker

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

$$\alpha_i \ge 0$$

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

$$y_i (\langle \mathbf{w} \cdot \mathbf{x_i} \rangle + b) - 1$$

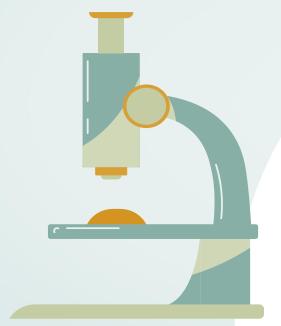
$$\ge 0, \forall \mathbf{x_i} (i = 1..r)$$

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



SVM: Karush-Kuhn-Tucker





- The last equation (5): $\alpha_i(y_i(\langle \mathbf{w} \cdot \mathbf{x_i} \rangle + b) 1) = 0$ comes from a nice result from the duality theory.
- Note: any $\alpha_i > 0$ will imply that the associated point 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

- In general, the KKT conditions do not guarantee the optimality of the solution.
- Fortunately, due to the convexity of the primal problem
 (*), 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 (*) is pretty hard to derive an efficient algorithm. Therefore, its **dual problem** is more preferable.

SVM: the dual form

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 $L(\mathbf{w},b,\alpha)$ in variables (\mathbf{w},b) and zeroing it, we can find the following dual function:

•
$$L_D(\alpha) = \sum_{i=1}^r \alpha_i - \frac{1}{2} \sum_{i,j=1}^r \alpha_i \alpha_j y_i y_j \langle \mathbf{x}_i \cdot \mathbf{x}_j \rangle$$

SVM: the dual form

Solving problem (*) is equivalent to solving its dual problem below:

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

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

The constraints in **(D)** is much more 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 α , we can recover the optimal solution to problem (*) by using the KKT.

Let SV be the set of all support vectors

- SV is a subset of the training data.
- α_i > 0 suggests that x_i is a support vector.

We can compute \mathbf{w}^* by using (1). So:

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

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 (5).
- Hence, $b^* = y_k \langle \mathbf{w}^* \cdot \mathbf{x}_k \rangle$

SVM: classifying new instance

The decision boundary is

$$f(\mathbf{x}) = \langle \mathbf{w}^* \cdot \mathbf{x} \rangle + b^* = \sum_{\mathbf{x_i} \in SV} \alpha_i y_i \langle \mathbf{x_i} \cdot \mathbf{x} \rangle + b^* = 0$$

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

$$\operatorname{sign}(\langle \mathbf{w}^* \cdot \mathbf{z} \rangle + b^*) = \operatorname{sign}\left(\sum_{\mathbf{x_i} \in SV} \alpha_i y_i \langle \mathbf{x_i} \cdot \mathbf{z} \rangle + b^*\right)$$

• 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.



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

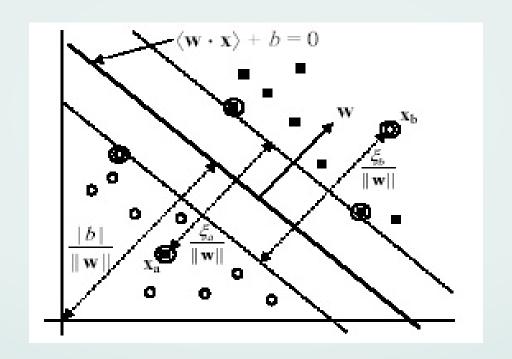


In the cases of **noises** or **overlapping**, those constraints may never meet simutaneously.

It means we cannot solve for **w*** and b*.

Example of inseparability

Noisy points x_a and 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 $\xi_i(\geq 0)$: (Ta sẽ mở rộng ràng buộc về lề bằng cách thêm biến bù)

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

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

- For a noisy/erronous point ξ_i , we have: $\xi_i > 1$
- Otherwise $\xi_i = 0$.



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

$$\begin{aligned} y_i(\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b) &\geq 1 - \xi_i & \textit{for all } i = 1 \dots r \\ \xi_i &\geq 0 & \textit{for all } i = 1 \dots r \end{aligned}$$

Penalty of 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

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

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
$$\frac{\langle \mathbf{w} \cdot \mathbf{w} \rangle}{2} + C \sum_{i=1}^{r} \xi_{i} \binom{*}{*}$$

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

$$\left[\frac{1}{r}\sum_{i=1}^{r} max(0,1-y_i(\langle \boldsymbol{w}\cdot\boldsymbol{x}_i\rangle+b))\right]+\lambda\parallel\boldsymbol{w}\parallel_2^2$$

 $max(0,1-y_i(\langle \boldsymbol{w}\cdot\boldsymbol{x}_i\rangle+b))$ 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

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

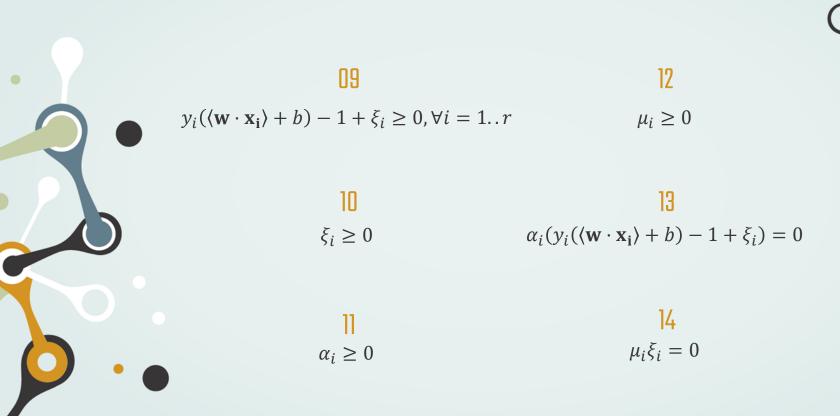
Where $\alpha_i (\geq 0)$ and $\mu_i (\geq 0)$ are Lagrange multipliers.

Karush-Kuhn-Tucker conditions

$$\frac{\partial L_P}{\partial \mathbf{w}} = \mathbf{w} - \sum_{i=1}^r \alpha_i y_i \mathbf{x_i} = 0 \qquad \qquad \frac{\partial L_P}{\partial b} = -\sum_{i=1}^r \alpha_i y_i = 0 \qquad \qquad \frac{\partial L_P}{\partial \xi_i} = C - \alpha_i - \mu_i = 0, \forall i = 1...r$$



Karush-Kuhn-Tucker conditions



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

Note that neither ξ_i nor μ_i appears in the dual problem.





This problem is almost similar with that (**) in the case of linearly separable classification.

The only difference is the constraint: $\alpha_i \leq C$



Soft-margin SVM: the optimal classifier

Once the dual problem is solved for α , we can recover the optimal solution to problem $\binom{*}{*}$

Let SV be the set of all support/noisy vectors

- SV is a subset of the training data.
- α_i > 0 suggests that x_i is a support/noisy vector.

We can compute \mathbf{w}^* by using (1). So:

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

To find b*, we take an index k such that $C > \alpha_k > 0$:

- It means $\xi_k = 0$ due to (8) and (14).
- And $y_k(\langle \mathbf{w}^* \cdot \mathbf{x}_k \rangle + b^*) 1 = 0$ due to (13).
- Hence, $b^* = \frac{1}{v_k} \langle \mathbf{w}^* \cdot \mathbf{x}_k \rangle$

Some notes

From equations (8) to (14), we conclude that:

If
$$\alpha_i = 0$$
 then $y_i(\langle \mathbf{w} \cdot \mathbf{x_i} \rangle + b) \ge 1$ and $\xi_i = 0$
If $0 < \alpha_i < C$ then $y_i(\langle \mathbf{w} \cdot \mathbf{x_i} \rangle + b) = 1$ and $\xi_i = 0$
If $\alpha_i = C$ then $y_i(\langle \mathbf{w} \cdot \mathbf{x_i} \rangle + b) < 1$ and $\xi_i > 0$

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

$$f(\mathbf{x}) = \langle \mathbf{w}^* \cdot \mathbf{x} \rangle + b^* = \sum_{\mathbf{x_i} \in SV} \alpha_i y_i \langle \mathbf{x_i} \cdot \mathbf{x} \rangle + b^* = 0$$

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

$$\operatorname{sign}(\langle \mathbf{w}^* \cdot \mathbf{z} \rangle + b^*) = \operatorname{sign}\left(\sum_{\mathbf{x_i} \in SV} \alpha_i y_i \langle \mathbf{x_i} \cdot \mathbf{z} \rangle + b^*\right)$$

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

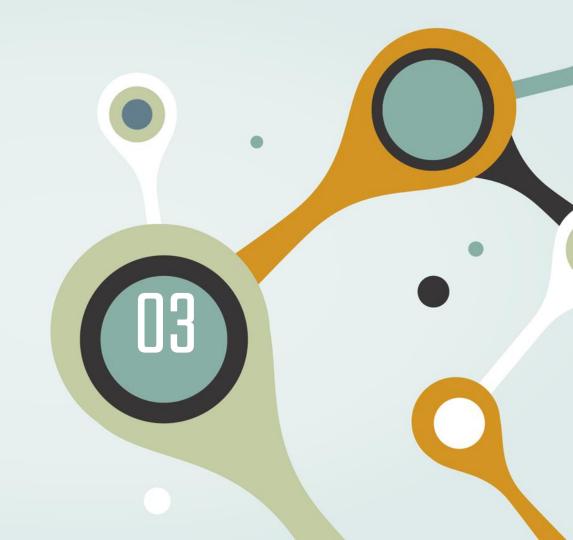
Note: it is important to choose a good value of C, since it significantly affects performance of SVM.

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.

Non-linear SVM



Non-linear SVM: Kernel functions

03

An explicit form of a transformation 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
$$\begin{cases} \sum_{i=1}^r \alpha_i y_i = 0 \\ 0 \leq \alpha_i \leq \mathcal{C}, \forall i = 1..r \end{cases}$$



Classifier:

$$f(\mathbf{z}) = \langle \mathbf{w}^*, \phi(\mathbf{z}) \rangle + b^*$$
$$= \sum_{\mathbf{x}_i \in SV} \alpha_i y_i \langle \phi(\mathbf{x}_i), \phi(\mathbf{z}) \rangle + b^*$$

Both require only the inner product

Kernel trick: Nonlinear SVM can be used by replacing those inner products by evaluations of some *kernel function*

$$K(\mathbf{x}, \mathbf{z}) = \langle \phi(\mathbf{x}), \phi(\mathbf{z}) \rangle$$

Kernel functions: example



Polynomial

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



Consider the polynomial with degree d=2.

For any vectors
$$x = (x_1, x_2)$$
 and $z = (z_1, z_2)$

$$\langle x, z \rangle^{2} = (x_{1}z_{1} + x_{2}z_{2})^{2}$$

$$= x_{1}^{2}z_{1}^{2} + 2x_{1}z_{1}x_{2}z_{2} + x_{2}^{2}z_{2}^{2}$$

$$= \langle (x_{1}^{2}, x_{2}^{2}, \sqrt{2}x_{1}x_{2}), (z_{1}^{2}, z_{2}^{2}, \sqrt{2}z_{1}z_{2}) \rangle$$

$$= \langle \phi(x), \phi(z) \rangle = K(x, z)$$

Where
$$\phi(x) = (x_1^2, x_2^2, \sqrt{2}x_1x_2)$$



Therefore the polynomial is the product of two vectors $\phi(x)$ and $\phi(z)$

Kernel functions: popular choices



Polynomial

$$K(\mathbf{x}, \mathbf{z}) = (\langle \mathbf{x} \cdot \mathbf{z} \rangle + \theta)^d;$$

where $: \theta \in R, d \in N$



Sigmoid

$$K(\mathbf{x}, \mathbf{z}) = \tanh(\beta \langle \mathbf{x} \cdot \mathbf{z} \rangle - \lambda) = \frac{1}{1 + e^{-(\beta(\mathbf{x}.\mathbf{z}) - \lambda)}};$$

$$where: \beta, \lambda \in R$$



Gaussian radial basis function (RBF)

$$K(\mathbf{x},\mathbf{z}) = e^{-\frac{\|\mathbf{x}-\mathbf{z}\|^2}{2\sigma}};$$

where : $\sigma > 0$

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

THANKS

Do you have any questions?







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