

## How can we expand the Perceptron model to make it more powerful?

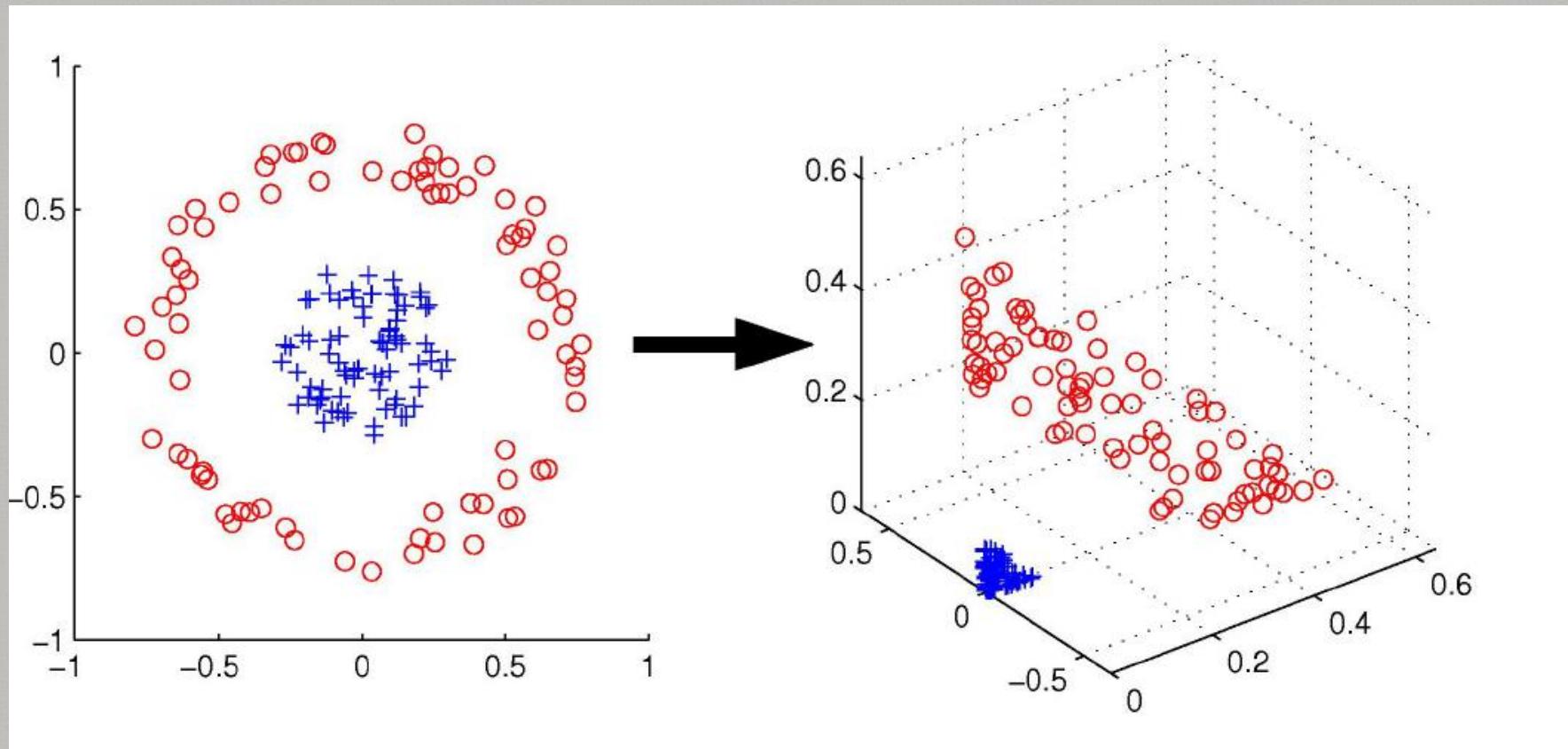
Perceptron 和 SVM 都是用于分类任务的线性模型

Perceptron 目标是找到一个能够分开数据的线性超平面，最小化分类错误次数

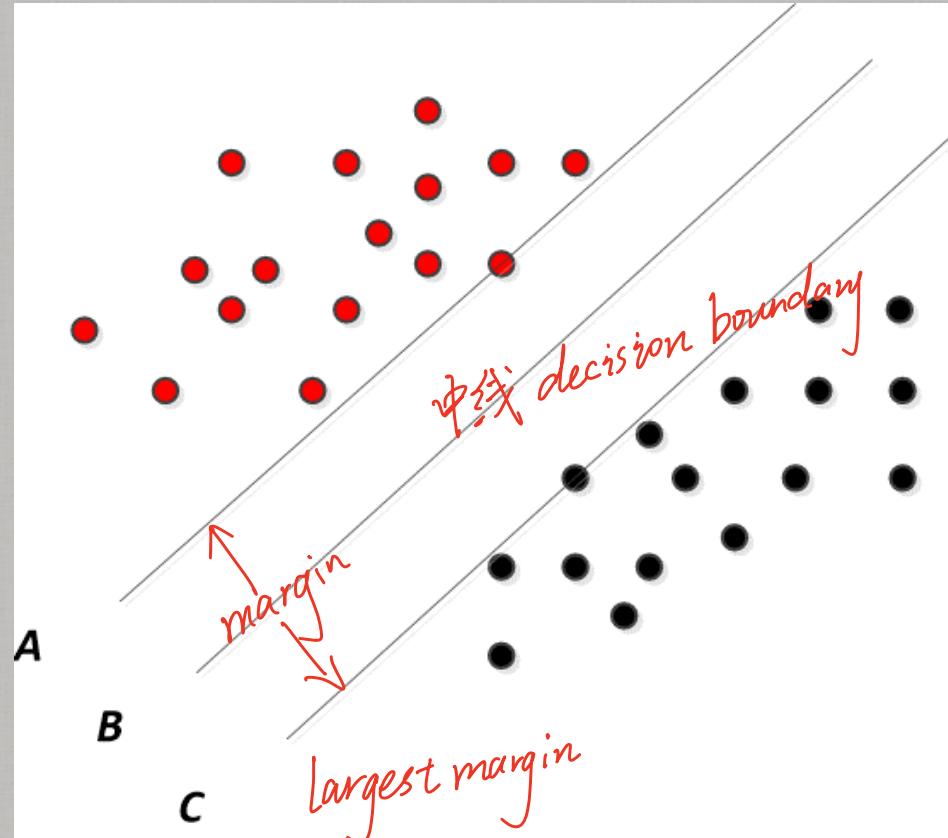
SVM 不仅要找到一个能分开数据的超平面，还要求这个超平面使得两类之间间隔

margin 最大

## Use Nonlinear Feature Mapping



## Introduce the concept of *margin* of a hyperplane



We want a hyperplane with the largest margin. What is the definition of margin of a hyperplane?

# Support Vector Machine Method

- First, consider the **binary linearly separable case: (hard margin)**

硬间隔

Given a training data set  $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N, x_i \in \mathbb{R}^d, y_i \in \{-1, +1\}$ , we are looking for a linear model classifier in the form:

$$y(x) = w^T \phi(x) + b$$

Where  $\phi(x)$  denotes a fixed **feature-space transformation**,  $w$  is the weight vector and we have made the bias (intercept) parameter explicitly. **No expanded feature vector is used.**

- For a binary linearly separable data set, there exists at least one choice of  $w$  and  $b$  to satisfy the following:

$$w^T \phi(x_i) + b > 0, \text{ if } y_i = +1$$

$$w^T \phi(x_i) + b < 0, \text{ if } y_i = -1$$

Which is equivalent to:

$$y_i(w^T \phi(x_i) + b) > 0, \quad i = 1, \dots, N$$

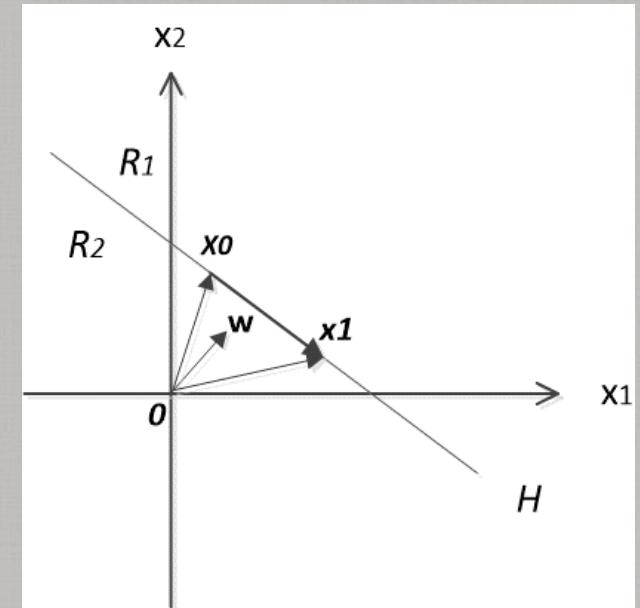
- We look for a hyperplane with the **maximum margin**.

- Consider the hyperplane  $H: \{x: \mathbf{w}^T x + b = 0\}$

First, let's prove that the vector  $\mathbf{w}$  is normal to the hyperplane  $H$ .

Consider two points  $x_0$  and  $x_1$  on  $H$ . We want to show that  $\mathbf{w}$  is perpendicular to the vector  $x_1 - x_0$

$$\mathbf{w}^T(x_1 - x_0) = \mathbf{w}^T x_1 - \mathbf{w}^T x_0 = b - b = 0$$



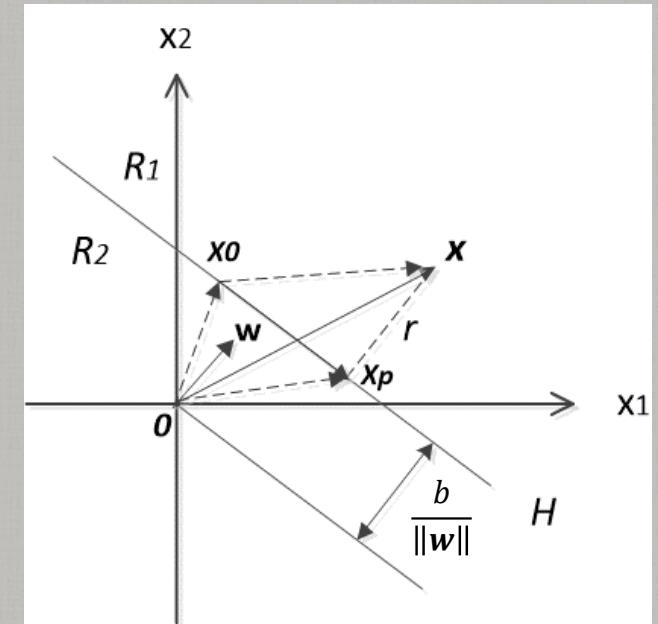
- Consider the hyperplane  $H: \{x: w^T x + b = 0\}$
- Secondly, let's find the ***geometric distance*** from a point  $x$  to hyperplane  $H$ .

Let's take any point  $x_0$  on  $H$ , then, we have,

$$x = x_p + r \frac{w}{\|w\|}$$

Where,  $x_p - x_0$  is the normal projection of  $x - x_0$  to  $H$ .

Hence,  $x_p$  is on  $H$ .  $r$  is the ***algebraic distance*** from  $x$  to the hyperplane  $H$  (positive if  $x$  is on the positive side and negative if  $x$  is on the negative side).



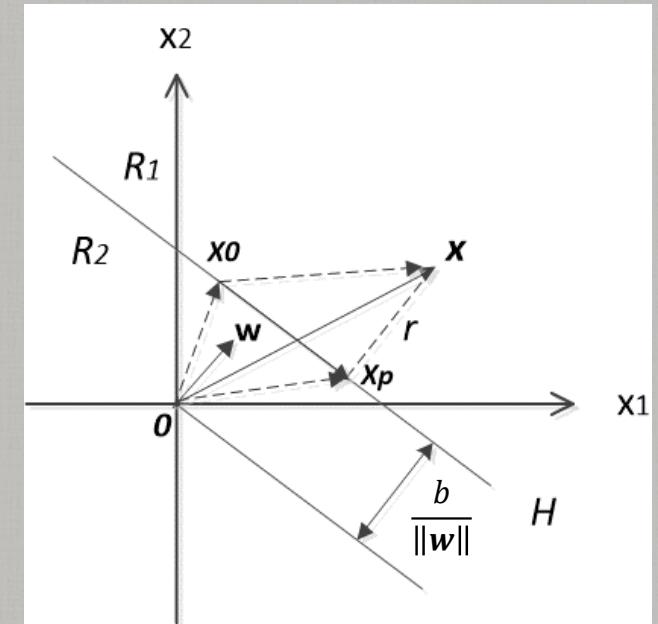
- Hence, we have,

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

$$\Rightarrow \mathbf{w}^T \mathbf{x} + b = r \|\mathbf{w}\|$$

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

- When  $\mathbf{x} = \mathbf{0}$ ,  $r = \frac{b}{\|\mathbf{w}\|}$ , this means the distance from the origin to  $H$  is  $\frac{b}{\|\mathbf{w}\|}$



Consider the hyperplane  $H: \{x: \mathbf{w}^T x + b = 0\}$

- The **algebraic distance** of a point  $x_i$  to hyperplane  $H$  is

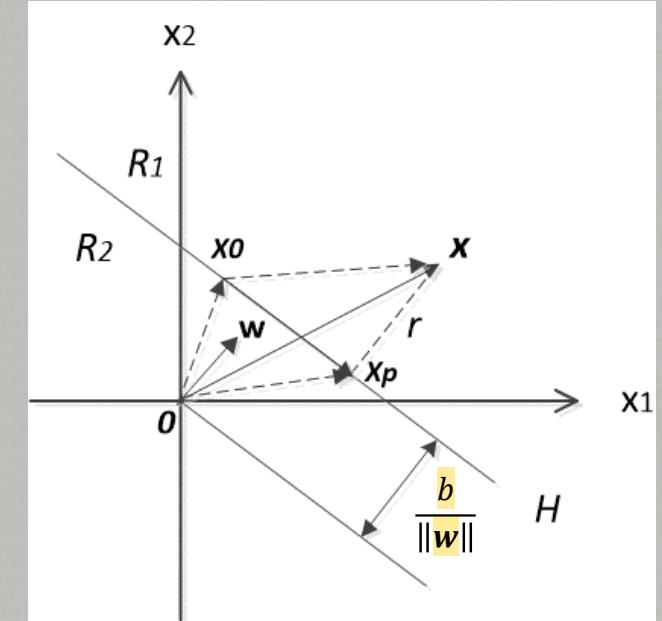
$$r_i = \frac{\mathbf{w}^T x_i + b}{\|\mathbf{w}\|}$$

- Then the **geometric distance** of a point  $x_i$  to hyperplane  $H$  is:

$$\frac{y_i(\mathbf{w}^T x_i + b)}{\|\mathbf{w}\|}$$

- The margin of hyperplane  $H$  is the geometric distance of the closest point in the data set to the hyperplane, i.e.,**

$$\min_i \left\{ \frac{y_i(\mathbf{w}^T x_i + b)}{\|\mathbf{w}\|} \right\}$$



In general, when using feature mapping, let's consider the hyperplane  $H: \{x: \mathbf{w}^T \phi(x) + b = 0\}$

The margin of hyperplane  $H$  is,

$$\min_i \left\{ \frac{y_i(\mathbf{w}^T \phi(x_i) + b)}{\|\mathbf{w}\|} \right\}$$

- Since the rescaling of  $\mathbf{w}$  and  $b$  does not change the hyperplane  $H: \{\mathbf{x}: \mathbf{w}^T \phi(\mathbf{x}) + b = 0\}$ , we can use this freedom to produce the following constraints:

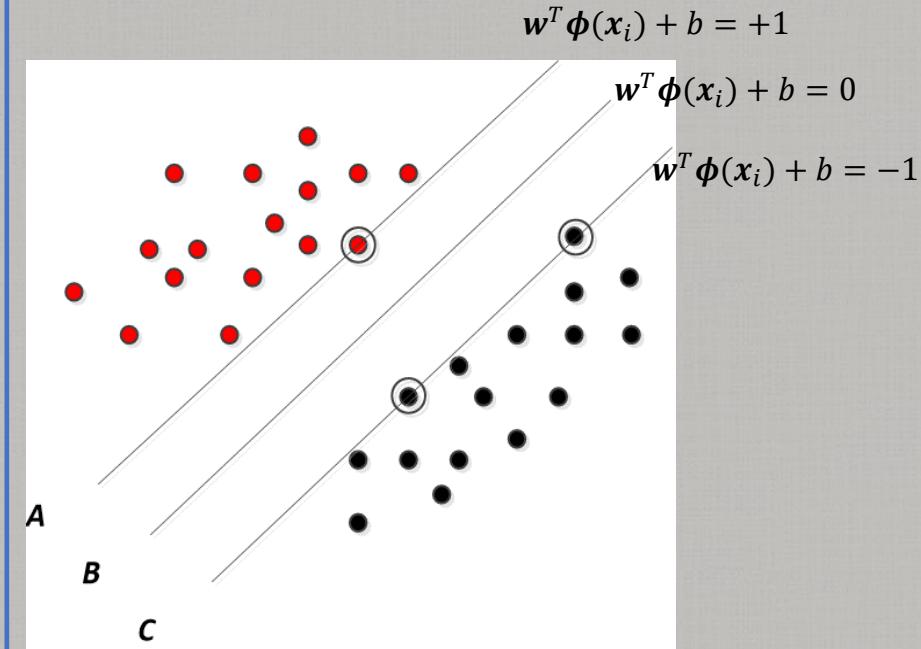
- Suppose all data points in the linearly separable data set satisfy the following constraints:

$$\mathbf{w}^T \phi(\mathbf{x}_i) + b \geq +1, \text{ for } y_i = +1$$

$$\mathbf{w}^T \phi(\mathbf{x}_i) + b \leq -1, \text{ for } y_i = -1$$

- Which can be combined to a set of inequality:

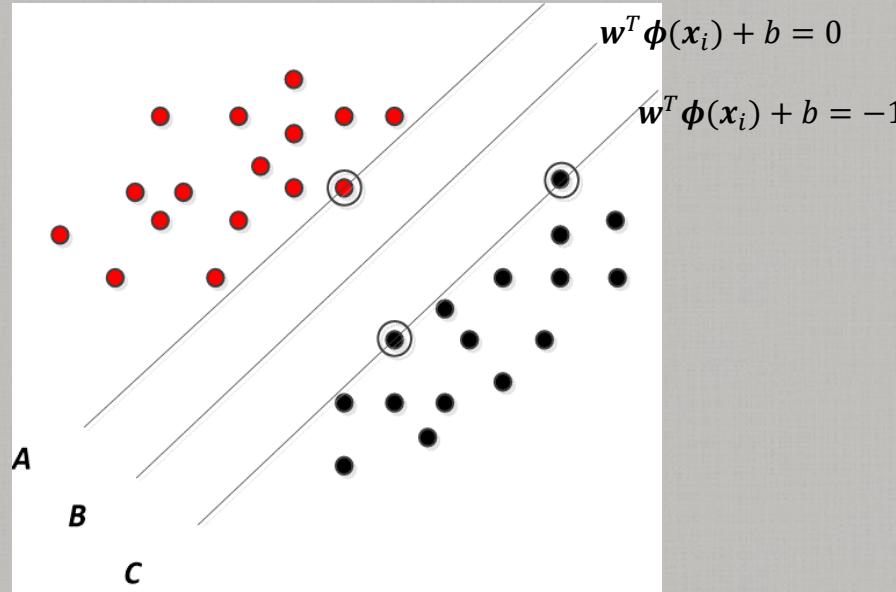
$$y_i(\mathbf{w}^T \phi(\mathbf{x}_i) + b) \geq +1, \quad \forall i$$



- Those points  $\mathbf{x}_i$  that satisfies  $\mathbf{w}^T \phi(\mathbf{x}_i) + b = \pm 1$  are called **support vectors**.

支持向量

$$\mathbf{w}^T \phi(x_i) + b = +1$$



- Hence, the margin of  $H$  is

$$\gamma = \min_i \left\{ \frac{y_i (\mathbf{w}^T \phi(x_i) + b)}{\|\mathbf{w}\|} \right\} = \frac{1}{\|\mathbf{w}\|}$$

- Thus, the maximum margin solution is found by solving the optimization problem:

$$\arg \min_{w,b} \left\{ \frac{1}{2} \|w\|^2 \right\}$$

*subject to (s.t.)*  $y_i(w^T \phi(x_i) + b) \geq 1, i = 1, 2, \dots, N$

Which is a **quadratic programming problem**.

- To solve this problem, we need to review some important results from constrained optimization.



## The Lagrange Multiplier Method for Constrained Optimization

- Let's consider the following *constrained optimization problem*:

$$\min_{x \in \mathbb{R}^n} f(x) \text{ subject to } \begin{cases} c_i(x) = 0, i \in \mathcal{E} \\ c_j(x) \geq 0, j \in \mathcal{I} \end{cases}$$

Where  $f$  and functions  $c_i, c_j$  are all smooth, real valued functions, and  $\mathcal{E}$  and  $\mathcal{I}$  are two finite set of indices. We call  $f$  the **objective function**,  $c_i, i \in \mathcal{E}$  are the **equality constraints** and  $c_j, j \in \mathcal{I}$  are the **inequality constraints**.

- we define the **feasible set**  $\Omega$  to be the set of points  $x$  that satisfy the constraints, that is,

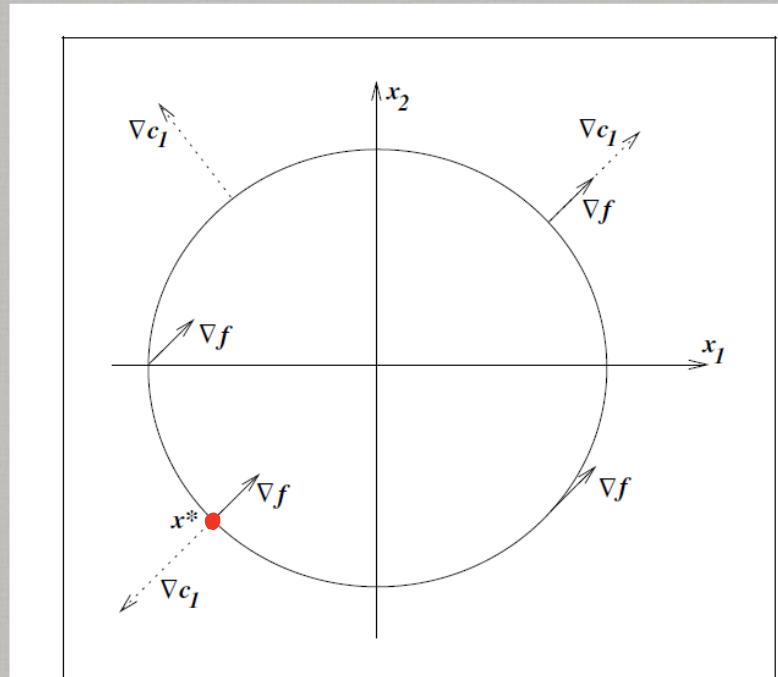
$$\Omega = \{x | c_i(x) = 0, i \in \mathcal{E}; c_j(x) \geq 0, j \in \mathcal{I}\}$$

- At a **feasible point**  $x$ , the inequality constraint  $j \in \mathcal{I}$  is said to be **active** if  $c_j(x) = 0$  and **inactive** if the strict inequality  $c_j(x) > 0$  is satisfied.
- The **active set**  $\mathcal{A}(x)$  at any feasible point  $x$  consists of the equality constraints indices from  $\mathcal{E}$  together with indices of all active inequality constraints.

**Example :** single equality constraint

$$\min_{x_1, x_2} \{x_1 + x_2\} \quad s.t. \quad x_1^2 + x_2^2 - 2 = 0$$

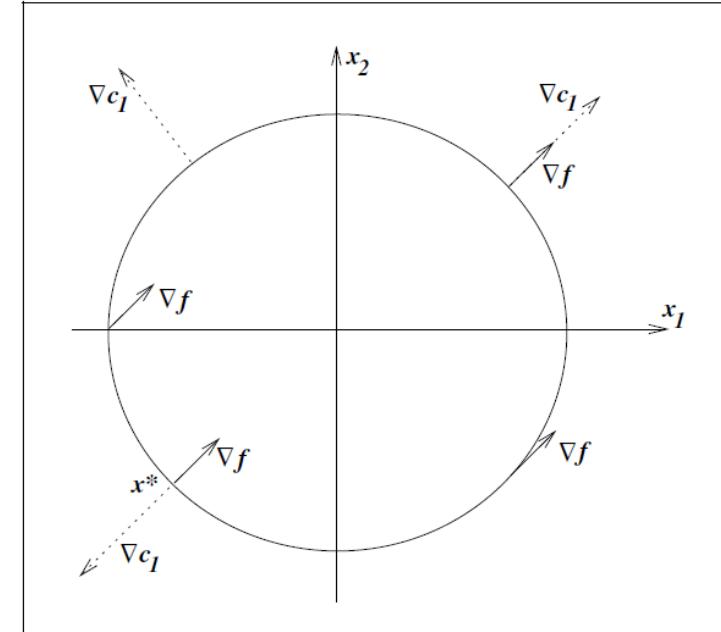
This is a two-variable problem with  $f(\mathbf{x}) = x_1 + x_2$  and  $c_1(\mathbf{x}) = x_1^2 + x_2^2 - 2$



检查

- By inspection, we can find that the feasible set of this problem is the circle of radius  $\sqrt{2}$  centered at the origin (just the boundary of the circle, not its interior). The solution  $\mathbf{x}^*$  is  $(-1, -1)$
- We also see that at the solution  $\mathbf{x}^*$ , the **constraint normal**  $\nabla c_1(\mathbf{x}^*)$  is parallel to  $\nabla f(\mathbf{x}^*)$ . That is, there is a scalar  $\lambda_1^*$  such that

$$\nabla f(\mathbf{x}^*) = \lambda_1^* \nabla c_1(\mathbf{x}^*)$$



$$f(\mathbf{x}) = x_1 + x_2, \quad c_1(\mathbf{x}) = x_1^2 + x_2^2 - 2$$

- Actually,

$$\nabla f(\mathbf{x}) = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \nabla c_1(\mathbf{x}) = 2 \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \quad \nabla f(\mathbf{x}^*) = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \nabla c_1(\mathbf{x}^*) = 2 \begin{bmatrix} -1 \\ -1 \end{bmatrix}, \quad (\lambda_1^* = -\frac{1}{2})$$

- Actually, the necessary condition  $\nabla f(\mathbf{x}^*) = \lambda_1^* \nabla c_1(\mathbf{x}^*)$  is true for the entire class of equality constrained optimization problem. Let's prove this:
- Consider the first order Taylor series approximation of  $f(\mathbf{x})$  and  $c_1(\mathbf{x})$ . To retain feasibility with respect to  $c_i(\mathbf{x}) = 0$ , we require any small step  $\mathbf{s}$  to satisfy that  $c_1(\mathbf{x} + \mathbf{s}) = 0$ , that is,

$$0 = c_1(\mathbf{x} + \mathbf{s}) \approx c_1(\mathbf{x}) + \nabla c_1(\mathbf{x})^T \mathbf{s} = \nabla c_1(\mathbf{x})^T \mathbf{s}$$

- Hence, the step  $\mathbf{s}$  retains feasibility with respect to  $c_1$ , when it satisfies

$$\nabla c_1(\mathbf{x})^T \mathbf{s} = 0$$

- Similarly, if we want  $\mathbf{s}$  to produce a decrease in  $f$ , we should have so that

$$f(\mathbf{x} + \mathbf{s}) - f(\mathbf{x}) \approx \nabla f(\mathbf{x})^T \mathbf{s} < 0$$

i.e.,

$$\nabla f(\mathbf{x})^T \mathbf{s} < 0$$

- If at a point  $x^*$ , there is no such direction of  $s$  to satisfy

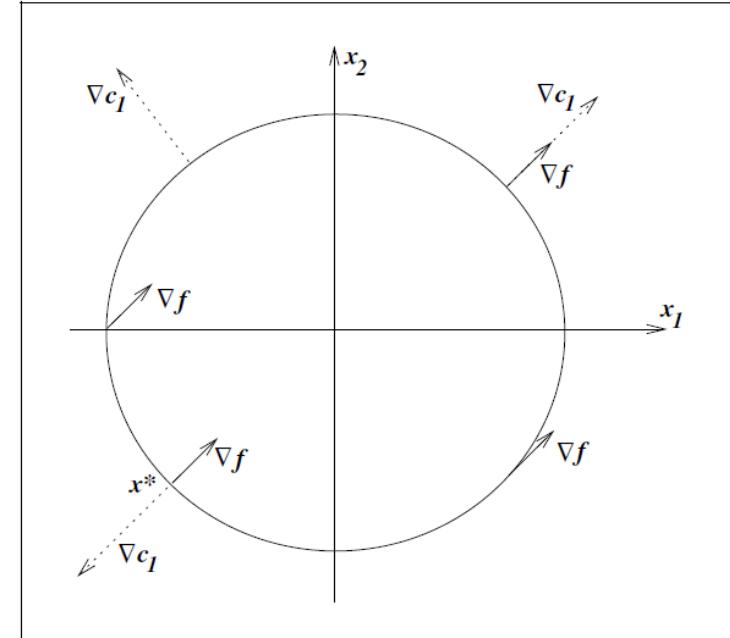
$$\nabla c_1(x)^T s = 0 \text{ and } \nabla f(x)^T s < 0$$

Then the point  $x^*$  appear to be a ***stationary point***

- From the figure, its easy to check that the only way that the above condition can not be met is when  $\nabla c_1(x)$  and  $\nabla f(x)$  are parallel, that is

$$\nabla f(x) = \lambda_1 \nabla c_1(x)$$

hold at some  $x$ , for some scalar  $\lambda_1$ .



## Lagrange multiplier method

- Let's introduce the **Lagrangian function**

$$\mathcal{L}(x, \lambda_1) = f(x) - \lambda_1 c_1(x)$$

$$\nabla f(x) = \begin{pmatrix} \frac{\partial f}{\partial x_1}(x) \\ \vdots \\ \frac{\partial f}{\partial x_n}(x) \end{pmatrix}$$

Notice that,

$$\nabla_x \mathcal{L}(x, \lambda_1) = \nabla f(x) - \lambda_1 \nabla c_1(x)$$

Then, the condition  $\nabla f(x) = \lambda_1 \nabla c_1(x)$  is equivalent to

$$\nabla_x \mathcal{L}(x, \lambda_1) = 0$$

$$c_i(x) = 0$$

- This means we can search for solutions of the equality-constrained optimization problem by seeking stationary points of the **Lagrangian function**.
- The scalar  $\lambda_1$  is called the **Lagrange multiplier** for the equation constraint  $c_1(x) = 0$ .

$$f(x) = x_1 + x_2 \quad C_1(x) = x_1^2 + x_2^2 - 2 = 0$$

Let's go back to the example:  $\min\{x_1 + x_2\} \quad s.t. \quad x_1^2 + x_2^2 - 2 = 0$

$$\mathcal{L}(x, \lambda_1) = f(x) - \lambda_1 C_1(x)$$

- The **Lagrangian function** is  $\mathcal{L}(x, \lambda_1) = x_1 + x_2 - \lambda_1(x_1^2 + x_2^2 - 2)$ . Then,

$$\nabla f(x) = \begin{pmatrix} \frac{\partial f}{\partial x_1}(x) \\ \frac{\partial f}{\partial x_2}(x) \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \nabla_x \mathcal{L}(x, \lambda_1) = \nabla f(x) - \lambda_1 \nabla C_1(x) = \begin{pmatrix} 1 \\ 1 \end{pmatrix} - \lambda_1 \begin{pmatrix} 2x_1 \\ 2x_2 \end{pmatrix}$$

$$\nabla_{x_1} \mathcal{L}(x, \lambda_1) = 1 - 2\lambda_1 x_1 = 0 \Rightarrow x_1 = \frac{1}{2\lambda_1} = \begin{pmatrix} 1 - 2\lambda_1 x_1 \\ 1 - 2\lambda_1 x_2 \end{pmatrix} = 0$$

$$\nabla C_1(x) = \begin{pmatrix} \frac{\partial C_1}{\partial x_1}(x) \\ \frac{\partial C_1}{\partial x_2}(x) \end{pmatrix} = \begin{pmatrix} 2x_1 \\ 2x_2 \end{pmatrix} \quad \nabla_{x_2} \mathcal{L}(x, \lambda_1) = 1 - 2\lambda_1 x_2 = 0 \Rightarrow x_2 = \frac{1}{2\lambda_1}$$

$$x_1^2 + x_2^2 - 2 = 0 \Rightarrow \frac{1}{4\lambda_1^2} + \frac{1}{4\lambda_1^2} = 2 \Rightarrow \left\{ \begin{array}{l} x_1 = \frac{1}{2\lambda_1} \\ x_2 = \frac{1}{2\lambda_1} \end{array} \right.$$

- Substitute these into  $C_1(x) = 0$  gives:  $\lambda_1 = \frac{1}{2}$  or  $-\frac{1}{2}$ .  $\lambda_1 = \pm \frac{1}{2}$

- When  $\lambda_1 = \frac{1}{2}$ , we have the stationary point as  $x^* = [1 \quad 1]^T$

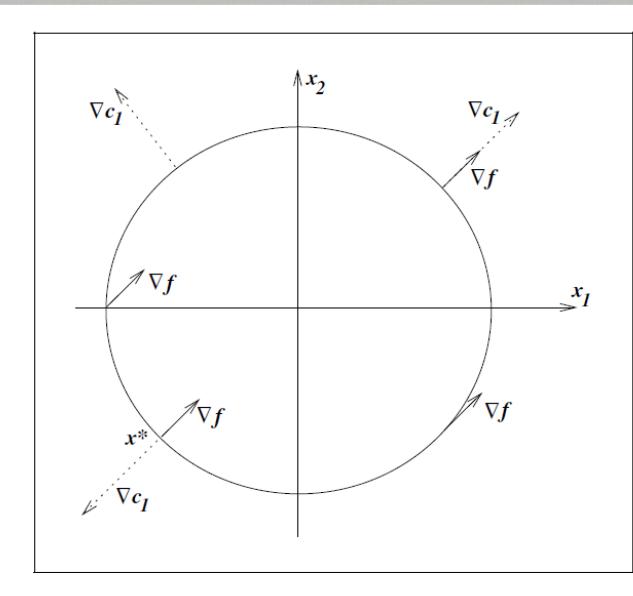
- When  $\lambda_1 = -\frac{1}{2}$ , we have the stationary point as  $x^* = [-1 \quad -1]^T$

- The actual solution is  $x^* = [-1 \quad -1]^T$ .  $\leftarrow \min(x_1 + x_2)$

**Example:** a single inequality constraint

$$\min\{x_1 + x_2\} \quad s.t. \quad 2 - x_1^2 - x_2^2 \geq 0$$

- What is the feasible set?
- What is the solution by visual inspection?



- ***Follow the same argument that a given feasible point  $x$  is not optimal if we can find a small step  $s$  that both retains feasibility and decreases the objective function  $f(x)$  to first order.***
- The step  $s$  improves the objective function, to first order, if

$$f(\mathbf{x} + \mathbf{s}) - f(\mathbf{x}) \approx \nabla f(\mathbf{x})^T \mathbf{s} < 0 \quad (\text{svm-1})$$

- The step  $s$  retains feasibility if

$$\begin{aligned} 0 \leq c_1(\mathbf{x} + \mathbf{s}) &\approx c_1(\mathbf{x}) + \nabla c_1(\mathbf{x})^T \mathbf{s} \\ \Rightarrow c_1(\mathbf{x}) + \nabla c_1(\mathbf{x})^T \mathbf{s} &\geq 0 \end{aligned} \quad (\text{svm-2})$$

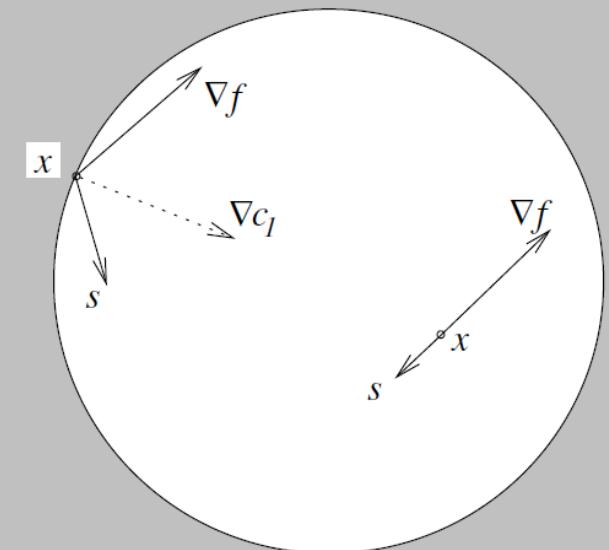
To determine if a step  $s$  exists that satisfies both conditions (svm-1) and (svm-2), we consider two cases:

- **Case I:**  $x$  lies strictly inside the circle so that  $c_1(x) > 0$  holds

In this case, if  $s$  is small enough, the condition (svm-2) can be satisfied!

In fact, whenever  $\nabla f(x) \neq 0$ , we can obtain a step  $s$  that satisfies both (svm-1) and (svm-2) by setting  $s = -\alpha \nabla f(x)$  for any positive scalar  $\alpha$  sufficiently small.

**When  $\nabla f(x) = 0$ , such a  $s$  can not be found.** (svm-1 can not be met)



■ **Case II:**  $x$  lies on the boundary of the circle so that  $c_1(x) = 0$

- In this case, the condition (svm-2) and (svm-1) becomes

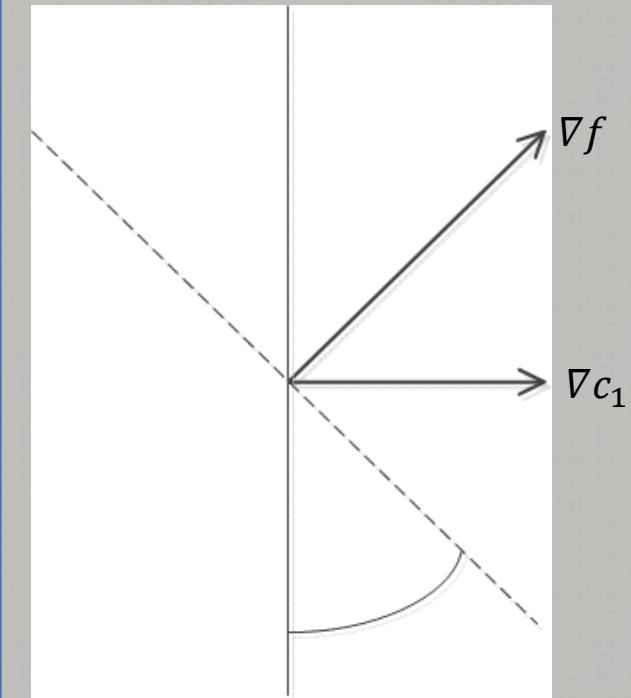
$$\nabla f(x)^T s < 0 \text{ and } \nabla c_1(x)^T s \geq 0 \quad (\text{svm-3})$$

- The first part of the condition defines an open half-space and the second part defines a closed half-space. ***It is clear that the intersection of these two regions is empty only when  $\nabla f(x)$  and  $\nabla c_1(x)$  point in the same direction***, that is, when,

$$\nabla f(x) = \lambda_1 \nabla c_1(x), \text{ for some } \lambda_1 \geq 0 \quad (\text{svm-4})$$

***Notice that the sign of the  $\lambda_1$  is significant here:***

***If  $\lambda_1 < 0$ , then  $\nabla f(x)$  and  $\nabla c_1(x)$  point in the opposite direction and the sets of directions of  $s$  that meet the requirement of (svm-3) will make up an entire open half-plane!***



- Define the **Lagrangian function** as:  $\mathcal{L}(x, \lambda_1) = f(x) - \lambda_1 c_1(x)$
- The optimality conditions for both **case I** and **case II** can be expressed using **Lagrangian function** as: When no first order feasible descent direction exist at some point  $x^*$ , we have that

  $\nabla_x \mathcal{L}(x^*, \lambda_1^*) = 0 \Rightarrow \nabla f(x^*) = \lambda_1^* \nabla c_1(x^*), \text{ for some } \lambda_1^* \geq 0$  (svm-5)

Where we also require that

$$\lambda_1^* c_1(x^*) = 0 \quad (\text{svm-6})$$

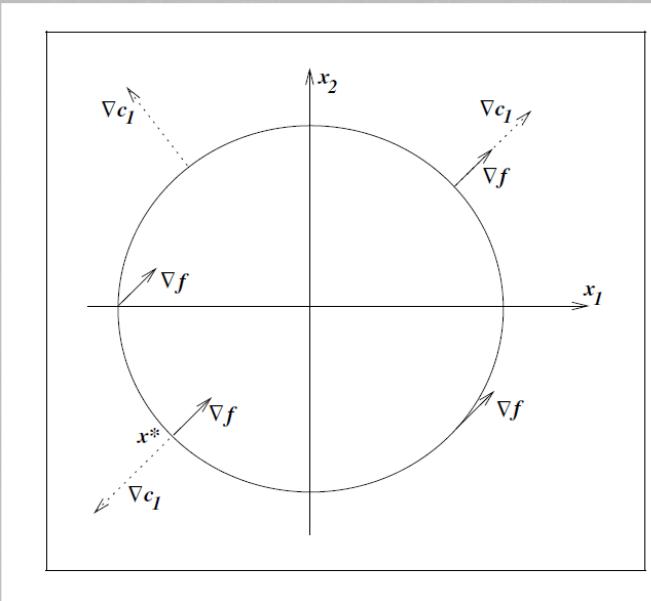
- Condition (svm-6) is known as the **complementarity condition**. It implies that the Lagrange multiplier  $\lambda_1$  can be strictly positive only when the corresponding constraint  $c_1$  is active. 对  $c_1(x) \geq 0$ , 当  $c_1(x)=0$  时处于边界上, 约束被激活(active)  
当  $c_1(x) > 0$ ,  $x$  位于可行域内, 约束未被激活(inactive)
- In case I, we have that  $c_1(x^*) > 0$ , so (svm-6) requires  $\lambda_1^* = 0$ , (svm-5) reduces to  $\nabla f(x^*) = 0$
- In case II, we have that  $c_1(x^*) = 0$ , (svm-6) allows  $\lambda_1^*$  to take a nonnegative value. So (svm-5) becomes equivalent to (svm-4)

~~Example: a single inequality constraint~~

$$c_I(x) \geq 0$$

$$\min\{x_1 + x_2\} \quad s.t. \quad 2 - x_1^2 - x_2^2 \geq 0$$

Can you find the solution by visual inspection?



## Solution:

- We can find the **Lagrangian function** of this problem as:

$$\begin{aligned}\mathcal{L}(\boldsymbol{x}, \lambda_1) &= f(\boldsymbol{x}) - \lambda_1 c_1(\boldsymbol{x}) \\ &= x_1 + x_2 - \lambda_1(2 - x_1^2 - x_2^2) = x_1 + x_2 + \lambda_1(x_1^2 + x_2^2 - 2) \\ &= \lambda_1 x_1^2 + x_1 + \lambda_1 x_2^2 + x_2 - 2\lambda_1\end{aligned}$$

- Then,

$$\nabla_{x_1} \mathcal{L}(\boldsymbol{x}, \lambda_1) = 2\lambda_1 x_1 + 1 = 0 \Rightarrow x_1 = -\frac{1}{2\lambda_1} \quad (\text{svm-7})$$

$$\nabla_{x_2} \mathcal{L}(\boldsymbol{x}, \lambda_1) = 2\lambda_1 x_2 + 1 = 0 \Rightarrow x_2 = -\frac{1}{2\lambda_1} \quad (\text{svm-8})$$

## Solution (continue):

- With the condition that

$$\lambda_1 \geq 0 \text{ and } \lambda_1(x_1^2 + x_2^2 - 2) = 0$$

$\lambda_1$  is strictly positive only when  $c_1(x)$  is **active**, that is,

$$c_1(x) = 2 - x_1^2 - x_2^2 = 0 \quad (\text{svm-9})$$

- Substituting (svm-7) and (svm-8) into (svm-9) gives:

$$\frac{1}{4\lambda_1^2} + \frac{1}{4\lambda_1^2} - 2 = 0 \Rightarrow \lambda_1^* = \frac{1}{2}$$

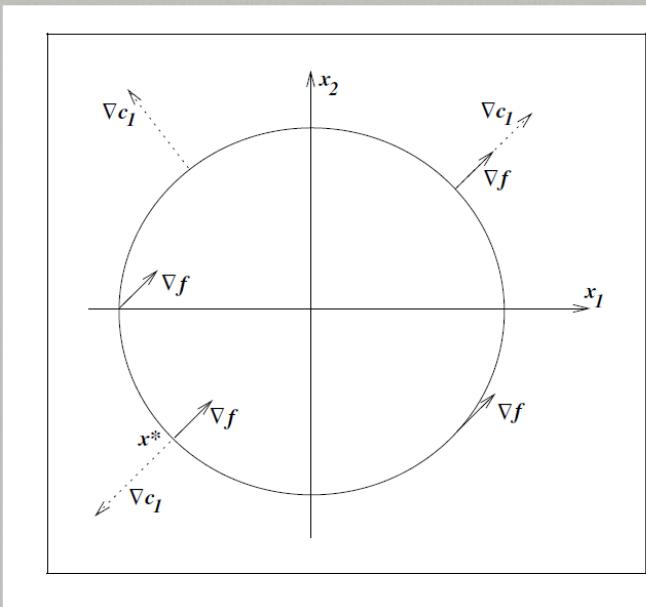
$$\lambda_1 = \pm \frac{1}{2}$$

- Then we have the solution  $x^* = \begin{bmatrix} -\frac{1}{2\lambda_1} \\ -\frac{1}{2\lambda_1} \end{bmatrix} = \begin{bmatrix} -1 \\ -1 \end{bmatrix}$

~~Example:~~ two inequality constraints

$$\min\{x_1 + x_2\} \quad s.t. \quad 2 - x_1^2 - x_2^2 \geq 0, x_2 \geq 0$$

Can you find the solution by visual inspection?



## Solution:

- We can find the **Lagrangian function** of this problem as:

$$\begin{aligned}\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}) &= f(\mathbf{x}) - \lambda_1 c_1(\mathbf{x}) - \lambda_2 c_2(\mathbf{x}) \\ &= x_1 + x_2 - \lambda_1(2 - x_1^2 - x_2^2) - \lambda_2 x_2 \\ &= \lambda_1 x_1^2 + x_1 + \lambda_1 x_2^2 + (1 - \lambda_2) x_2 - 2\lambda_1\end{aligned}$$

Where  $\boldsymbol{\lambda} = [\lambda_1 \quad \lambda_2]^T$  is the vector of *Lagrange multipliers*.

- The extension of condition (svm-5) becomes:

$$\nabla_{\mathbf{x}} \mathcal{L}(\mathbf{x}^*, \boldsymbol{\lambda}^*) = 0, \text{ for some } \boldsymbol{\lambda}^* \geq 0$$

- That is,

$$\nabla_{x_1} \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}) = 2\lambda_1 x_1 + 1 = 0 \Rightarrow x_1 = -\frac{1}{2\lambda_1} \quad (\text{svm-10})$$

$$\nabla_{x_2} \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}) = 2\lambda_1 x_2 + 1 - \lambda_2 = 0 \Rightarrow x_2 = \frac{\lambda_2 - 1}{2\lambda_1} \quad (\text{svm-11})$$

## Solution (continue):

- $\lambda_1$  is strictly positive only when  $c_1(x)$  is active, that is,

$$c_1(x) = 2 - x_1^2 - x_2^2 = 0 \quad (\text{svm-12})$$

- $\lambda_2$  is strictly positive only when  $c_2(x)$  is active, that is,

$$c_2(x) = x_2 = 0 \quad (\text{svm-13})$$

- Substituting (svm-13) into (svm-12) gives:

$$2 - x_1^2 = 0 \Rightarrow x_1^2 = 2 \quad (\text{svm-14})$$

- Substituting (svm-10) into (svm-14) gives:  $\frac{1}{4\lambda_1^2} = 2 \Rightarrow \lambda_1 = \frac{1}{2\sqrt{2}}$

- Substituting (svm-11) into (svm-13) gives:  $\frac{\lambda_2 - 1}{2\lambda_1} = 0 \Rightarrow \lambda_2 = 1$

## Solution (continue):

- Hence, we have,

$$\lambda^* = \begin{bmatrix} 1 \\ \frac{1}{2\sqrt{2}} \\ 1 \end{bmatrix}$$

- The corresponding solution point  $x^* = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} -\frac{1}{2\lambda_1} \\ \frac{\lambda_2 - 1}{2\lambda_1} \end{bmatrix} = \begin{bmatrix} -\sqrt{2} \\ 0 \end{bmatrix}$



## The Lagrangian Dual Problem

拉格朗日对偶问题

- Let's restate the constrained optimization problem (the ***primal problem***):

$$\min_{x \in \mathbb{R}^n} f(x) \text{ subject to } c_i(x) \geq 0, i = 1, \dots, m$$

- Let's define the ***Lagrangian function*** as:

$$\mathcal{L}(x, \lambda) = f(x) - \sum_{i=1}^m \lambda_i c_i(x)$$

Where,  $\lambda = [\lambda_1 \dots \lambda_m] \in \mathbb{R}^m$  is the *Lagrange multiplier vector*.

- Then we have the following first-order optimality conditions (***KKT conditions***) of the primal problem:

$$\nabla \mathcal{L}(x, \lambda) = \nabla f(x) - \sum_{i=1}^m \lambda_i \nabla c_i(x) = 0$$

$$\nabla f(x) = \lambda_1 \nabla c_1(x) + \lambda_2 \nabla c_2(x) + \dots + \lambda_m \nabla c_m(x)$$

$$c_i(x) \geq 0, \quad i = 1, \dots, m$$

$$\lambda_i c_i(x) = 0, \quad i = 1, \dots, m$$

- Let's define the ***dual objective function***  $q: \mathcal{R}^n \rightarrow \mathcal{R}$  as:

$$q(\lambda) = \inf_x \mathcal{L}(x, \lambda)$$

下确界

Notice that the calculation of the infimum requires finding the global minimizer of the function  $\mathcal{L}(x, \lambda)$ . This is not a problem when the function is convex.

- The ***dual problem*** is defined as:

$$\max_{\lambda} q(\lambda) \text{ subject to } \lambda \geq 0$$

- The ***dual problem*** provides a lower bound to the solution of the ***primal problem***. The difference between the optimal value of ***primal problem*** and ***dual problem*** is called the ***duality gap***. For convex optimization problem, the duality gap is zero.

~~Example:~~ consider the problem



$$\min_{x_1, x_2} \left\{ \frac{1}{2} (x_1^2 + x_2^2) \right\} \text{ s.t. } x_1 - 1 \geq 0$$

Quiz

*f(x)*

*c<sub>1</sub>(x) ≥ 0*

**Solution:**

- The **Lagrangian function** is:

$$\mathcal{L}(x, \lambda_1) = f(x) - \lambda_1 C_1(x)$$

$$\mathcal{L}(x_1, x_2, \lambda_1) = \frac{1}{2}(x_1^2 + x_2^2) - \lambda_1(x_1 - 1)$$

- If we hold  $\lambda_1$  fixed, this is a convex function of  $x = [x_1 \ x_2]^T$ . Hence, the infimum with respect to  $x$  is achieved when the partial derivatives with respect to  $x_1$  and  $x_2$  are zero, that is,

$$\nabla \mathcal{L}(x, \lambda_1) = \nabla f(x) - \lambda_1 \nabla C_1(x) = 0$$

$$\frac{\partial \mathcal{L}}{\partial x_1} = 0 \Rightarrow x_1 - \lambda_1 = 0 \Rightarrow x_1 = \lambda_1;$$

$$\frac{\partial \mathcal{L}}{\partial x_2} = 0 \Rightarrow x_2 = 0 \quad \Rightarrow \quad \begin{cases} x_1 = \lambda_1 \\ x_2 = 0 \end{cases}$$

- By substituting these infimal values into  $\mathcal{L}(x_1, x_2, \lambda_1)$ , we obtain the **dual objective** function:

$$q(\lambda_1) = \frac{1}{2}(\lambda_1^2 + 0) - \lambda_1(\lambda_1 - 1) = -\frac{1}{2}\lambda_1^2 + \lambda_1$$

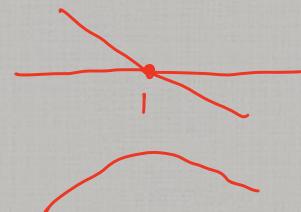
## Solution (continue):

- Hence the **dual problem** is:

$$\max_{\lambda_1 \geq 0} \left( -\frac{1}{2} \lambda_1^2 + \lambda_1 \right)$$

To solve this problem, we let

$$\frac{d \left( -\frac{1}{2} \lambda_1^2 + \lambda_1 \right)}{d \lambda_1} = 0 \Rightarrow \lambda_1 = 1$$



This is the solution of the **dual problem**!!!

- Therefore, we have the solution of the **primal problem** as:

$$x^* = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} \lambda_1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

## ~~Support Vector Machine Model~~

- Thus, the maximum margin solution is found by solving the optimization problem:

$$\underset{\mathbf{w}, b}{\operatorname{argmin}} \left\{ \frac{1}{2} \|\mathbf{w}\|^2 \right\}$$

$$\text{subject to } y_i(\mathbf{w}^T \phi(\mathbf{x}_i) + b) \geq 1, \quad i = 1, 2, \dots, N$$

Which is a quadratic programming problem.

- This quadratic optimization problem is called the ***primal problem*** of the support vector machine model and can be solved using standard optimization algorithms.

Instead of directly work on the ***primal problem***, we will solve the ***dual problem*** first.

- To solve this problem, we introduce *Lagrange multipliers*  $a_i \geq 0$ , with one multiplier for each constraint, giving the **Lagrangian function**

$$L_P(\mathbf{w}, b, \mathbf{a}) = \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^N a_i \{y_i(\mathbf{w}^T \boldsymbol{\phi}(x_i) + b) - 1\}$$

Where  $\mathbf{a} = [a_1, a_2, \dots, a_N]^T$  is the *Lagrange multiplier vector*.

- To find the **dual problem**, we have,

$$\begin{aligned} L_P(\mathbf{w}, b, \mathbf{a}) &= \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^N a_i \{y_i(\mathbf{w}^T \boldsymbol{\phi}(x_i) + b) - 1\} \\ &= \frac{1}{2} \mathbf{w}^T \mathbf{w} - \sum_{i=1}^N \{a_i y_i (\mathbf{w}^T \boldsymbol{\phi}(x_i)) + a_i y_i b - a_i\} \\ &= \frac{1}{2} \mathbf{w}^T \mathbf{w} - \sum_{i=1}^N a_i y_i (\mathbf{w}^T \boldsymbol{\phi}(x_i)) - \sum_{i=1}^N a_i y_i b + \sum_{i=1}^N a_i \end{aligned}$$

- Setting the derivatives of  $L_P(\mathbf{w}, b, \mathbf{a})$  with respect to  $\mathbf{w}$  and  $b$  equal to zero, we obtain the following conditions:

$$\frac{\partial L_P}{\partial \mathbf{w}} = 0 \Rightarrow \mathbf{w} = \sum_{i=1}^N a_i y_i \boldsymbol{\phi}(x_i)$$

$$\frac{\partial L_P}{\partial b} = 0 \Rightarrow \sum_{i=1}^N a_i y_i = 0$$

- Eliminating  $w$  and  $b$  from  $L_P(w, b, a)$  using these conditions then gives the dual representation of the maximum margin problem in which we **maximize**

$$\begin{aligned} L_D(a) &= \sum_{i=1}^N a_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N a_i a_j y_i y_j \phi(x_i)^T \phi(x_j) \\ &= \sum_{i=1}^N a_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N a_i a_j y_i y_j k(x_i, x_j) \end{aligned}$$

Subject to the constraints:

$$a_i \geq 0, \text{ all } i \text{ and } \sum_{i=1}^N a_i y_i = 0$$

- Here the **kernel function** is defined by

$$k(x, x') = \phi(x)^T \phi(x')$$

- This convex optimization problem is called the ***dual problem*** of the support vector machine method and can be solved using standard optimization software.
- Assuming that ***dual problem*** of SVM is solved and the solution  $\mathbf{a} = [a_1 \ a_2 \ \dots \ a_N]^T$  is obtained, how can we determine the solution  $(\mathbf{w}, b)$  of the ***primal problem***?
  - $\mathbf{w} = \sum_{i=1}^N a_i y_i \phi(\mathbf{x}_i)$
  - To find the expression for  $b$ , we need to revisit the concept of ***support vector***

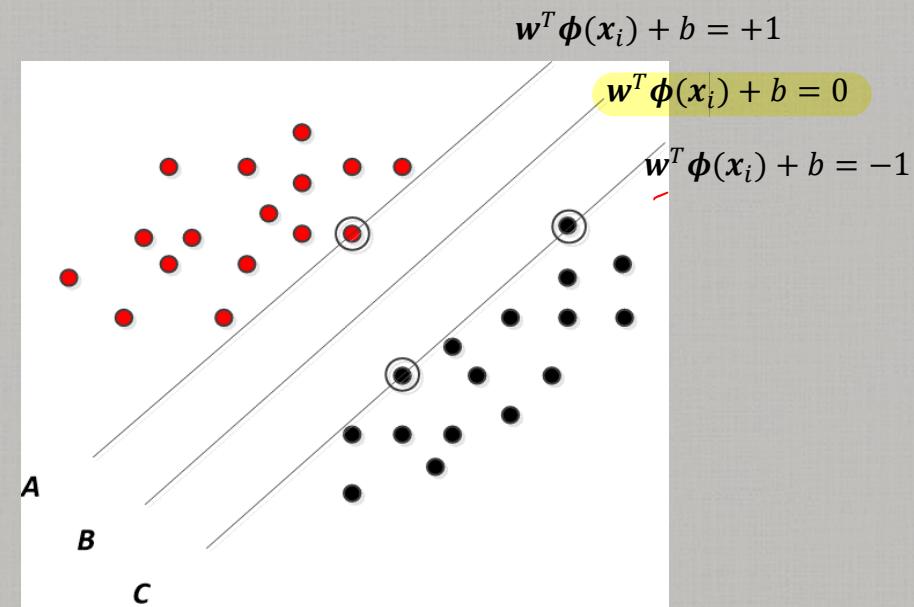
- The Karush-Kuhn-Tucker (**KKT**) conditions play a central role in both the theory and practice of constrained optimization. **KKT conditions are satisfied at the solutions of any constrained optimization problem (convex or not) with any kind of constraints, provided certain conditions.**
- The following are the **KKT** conditions derived from the **primal problem**:

$$a_i \geq 0, i = 1, 2, \dots, N$$

$$y_i[\mathbf{w}^T \phi(\mathbf{x}_i) + b] - 1 \geq 0$$

$$a_i\{y_i[\mathbf{w}^T \phi(\mathbf{x}_i) + b] - 1\} = 0$$

- Thus, for any data point, either  $a_i = 0$  or  $y_i(\mathbf{w}^T \phi(\mathbf{x}_i) + b) = 1$ .
- Those data points satisfying  $y_i(\mathbf{w}^T \phi(\mathbf{x}_i) + b) = 1$  are called **support vectors** and they correspond to points on the hyperplanes  $\mathbf{w}^T \phi(\mathbf{x}_i) + b = +1$  and  $\mathbf{w}^T \phi(\mathbf{x}_i) + b = -1$ .



- In order to classify new data point using trained model, we evaluate the sign of the prediction  $y(\mathbf{x})$ . Notice that  $\mathbf{w} = \sum_{i=1}^N a_i y_i \phi(\mathbf{x}_i)$ , we have,
- $$y(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x}) + b = \sum_{i=1}^N a_i y_i k(\mathbf{x}, \mathbf{x}_i) + b$$
- Having solved the quadratic optimization problem and find a value of  $a$ , we can then determine the value of the intercept parameter  $b$  by noting that any **support vector**  $\mathbf{x}_i$  satisfies

$$y_i y(\mathbf{x}_i) = 1 \Rightarrow y_i \left( \sum_{j=1}^N a_j y_j k(\mathbf{x}_i, \mathbf{x}_j) + b \right) = 1$$

Where  $S$  is the set of indices of the **support vectors**.

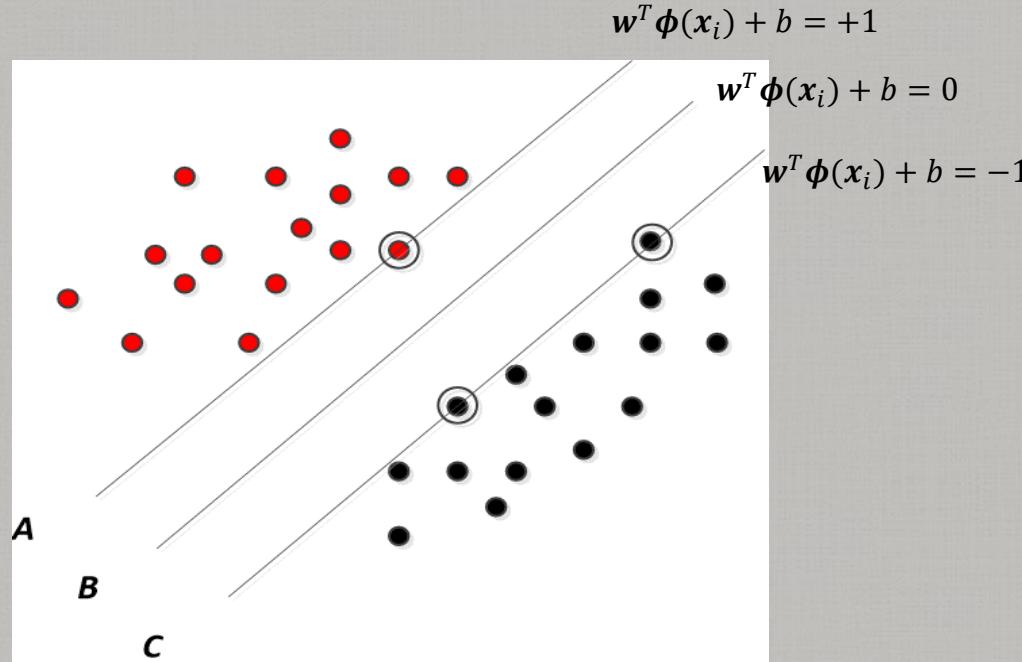
- Multiplying both sides of the above equality by  $y_i$  and notice that  $y_i^2 = 1$ , and then averaging over these equalities, we have,

$$b = \frac{1}{N_S} \sum_{i \in S} \left( y_i - \sum_{j=1}^N a_j y_j k(\mathbf{x}_i, \mathbf{x}_j) \right)$$

Where  $N_S$  is the total number of support vectors.

# Support Vector Machine Method (hard margin)

## (Linearly separable binary data set)



## Support Vector Machine Method (hard margin)

- The *primal problem*:

$$\underset{\mathbf{w}, b}{\operatorname{argmin}} \left\{ \frac{1}{2} \|\mathbf{w}\|^2 \right\}$$

*subject to*     $y_i(\mathbf{w}^T \phi(\mathbf{x}_i) + b) \geq 1, \quad i = 1, 2, \dots, N$

- The Lagrangian function of the primal problem is:

$$L_P(\mathbf{w}, b, \mathbf{a}) = \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^N a_i \{y_i (\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_i) + b) - 1\}$$

- The ***dual problem***:

$$\underset{\mathbf{a}}{\operatorname{argmax}} \left\{ L_D(\mathbf{a}) = \sum_{i=1}^N a_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N a_i a_j y_i y_j \boldsymbol{\phi}(\mathbf{x}_i)^T \boldsymbol{\phi}(\mathbf{x}_j) \right\}$$

subject to  $a_i \geq 0$ , all  $i$  and  $\sum_{i=1}^N a_i y_i = 0$

The solution of the ***dual problem*** can be found using some optimization software:

$$\mathbf{a} = [a_1, a_2, \dots, a_N]^T$$

## Support Vector Machine Method (hard margin)

- With the solution  $a_i, i = 1, 2, \dots, N$ , of the dual problem found, the ***decision function*** for a new input  $\mathbf{x}$  is:

$$y(\mathbf{x}) = \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}) + b = \sum_{i=1}^N a_i y_i \boldsymbol{\phi}(\mathbf{x}_i)^T \boldsymbol{\phi}(\mathbf{x}) + b = \sum_{i=1}^N a_i y_i k(\mathbf{x}_i, \mathbf{x}) + b$$

$$b = \frac{1}{N_S} \sum_{i \in S} \left( y_i - \sum_{j=1}^N a_j y_j k(\mathbf{x}_i, \mathbf{x}_j) \right)$$

Where  $k(\mathbf{x}_i, \mathbf{x}_j) = \boldsymbol{\phi}(\mathbf{x}_i)^T \boldsymbol{\phi}(\mathbf{x}_j)$  is the ***kernel function***.  $S$  is the set of all ***support vector*** points.

## Support Vector Machine Method (*Soft margin*) *(Non-linearly-separable binary data sets)*

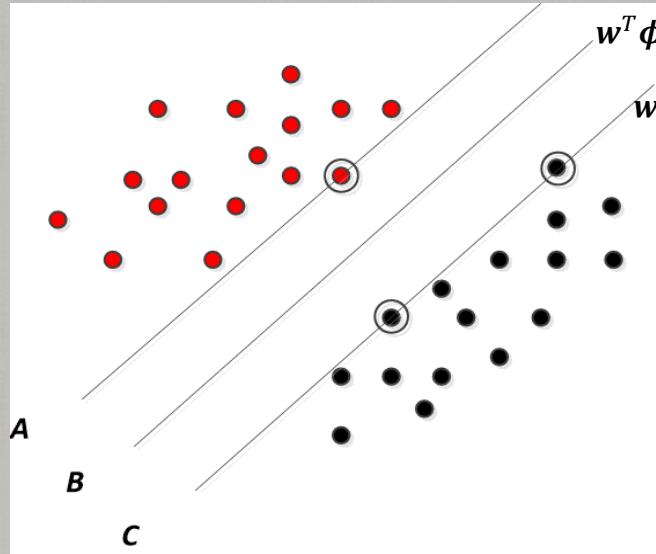
- The hard margin SVM method will find no feasible solution on non-linearly separable data set!
- How can we extend the ideas of hard margin SVM to handle non-linearly separable data set?

*hard margin*

$$\mathbf{w}^T \phi(x_i) + b = +1$$

$$\mathbf{w}^T \phi(x_i) + b = 0$$

$$\mathbf{w}^T \phi(x_i) + b = -1$$

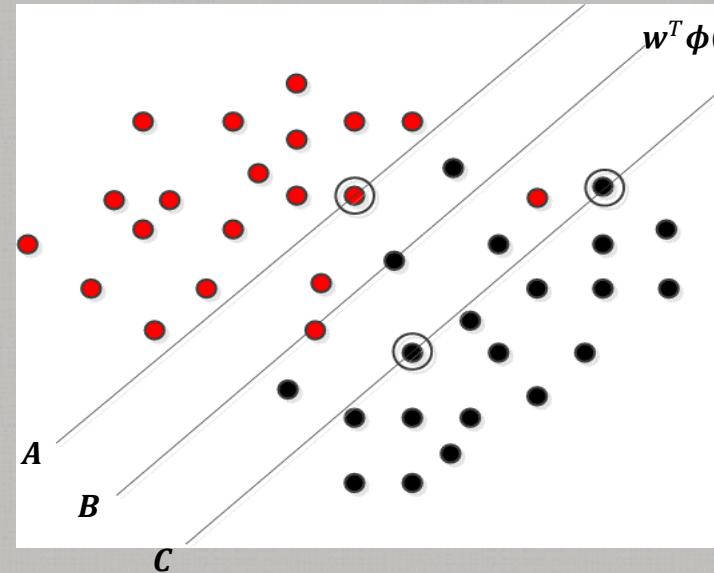


*soft margin*

$$\mathbf{w}^T \phi(x_i) + b = +1$$

$$\mathbf{w}^T \phi(x_i) + b = 0$$

$$\mathbf{w}^T \phi(x_i) + b = -1$$



- This can be done by introducing positive ***slack variables***  $\xi_i \geq 0, i = 1, \dots, N$  in the constraints on the data set:

$$\mathbf{w}^T \phi(\mathbf{x}_i) + b \geq +1 - \xi_i, \quad \text{for } y_i = +1$$

$$\mathbf{w}^T \phi(\mathbf{x}_i) + b \leq -1 + \xi_i, \quad \text{for } y_i = -1$$

- Or equivalently,

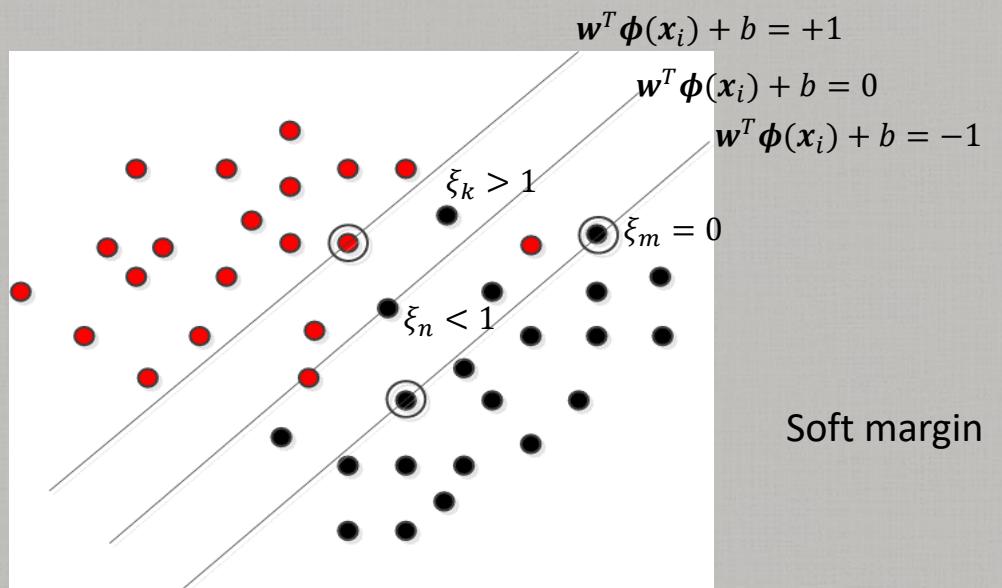
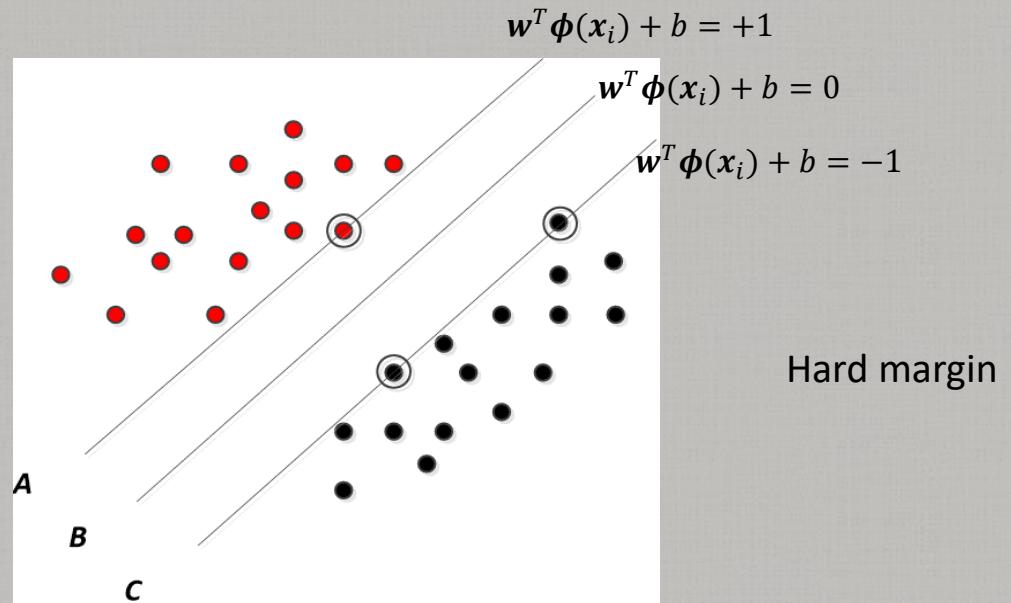
$$y_i \{\mathbf{w}^T \phi(\mathbf{x}_i) + b\} \geq 1 - \xi_i, \forall i$$

- $\xi_i = 0$ : the data point  $\mathbf{x}_i$  is out of the margin and is properly classified;
- $0 < \xi_i \leq 1$ : the data point  $\mathbf{x}_i$  is inside the margin but on the correct side of the decision boundary;
- $\xi_i > 1$ : the data point  $\mathbf{x}_i$  is on the wrong side of the decision boundary.

## Soft margin:

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

- $\xi_i = 0$ : the data point  $\mathbf{x}_i$  is properly classified;
- $0 < \xi_i \leq 1$ : the data point  $\mathbf{x}_i$  is inside the margin but on the correct side of the decision boundary;
- $\xi_i > 1$ : the data point  $\mathbf{x}_i$  is on the wrong side of the decision boundary (miss-classified).
- $\sum_{i=1}^N \xi_i$  is the ***upper bound*** of the number of misclassified instances



### Soft margin method:

- Our goal is now to maximize the margin while softly penalizing points that lie on the wrong side of the margin boundary. We therefore minimize:

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

Subject to the constraints:  $y_i \{\mathbf{w}^T \phi(\mathbf{x}_i) + b\} \geq +1 - \xi_i, \forall i$  and  $\xi_i \geq 0$ .

- Where the parameter  $C$  control the tradeoff between the slack variable penalty and the margin.
- When  $C \rightarrow \infty$ , this becomes the hard margin method.
- The corresponding **Lagrangian function** is given by:

$$L_P(\mathbf{w}, b, \mathbf{a}) = \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^N \xi_i - \sum_{i=1}^N a_i \{y_i y(\mathbf{x}_i) - 1 + \xi_i\} - \sum_{i=1}^N \mu_i \xi_i$$

Where,  $a_i \geq 0$  and  $\mu_i \geq 0$  are **Lagrange multipliers**.

- This is the **primal problem** of soft margin method.

# Support Vector Machine Method

## *Soft margin method:*

- The **KKT conditions** of the primal problem are given by:

$$\begin{aligned} a_i &\geq 0 \\ y_i y(\mathbf{x}_i) - 1 + \xi_i &\geq 0 \\ a_i \{y_i y(\mathbf{x}_i) - 1 + \xi_i\} &= 0 \\ \mu_i &\geq 0 \\ \xi_i &\geq 0 \\ \mu_i \xi_i &= 0 \end{aligned}$$

Where  $i = 1, \dots, N$

- $a_i > 0$ , for points of  $\mathbf{x}_i$  that satisfy  $y_i y(\mathbf{x}_i) - 1 + \xi_i = 0 \Rightarrow y_i y(\mathbf{x}_i) = 1 - \xi_i$ . These points of  $\mathbf{x}_i$  are **support vectors**. (includes all the data points on the margin boundary as well as those on the wrong side of the margin boundary)

### Soft margin method:

- The dual problem can be derived as:

$$\frac{\partial L_p}{\partial \mathbf{w}} = 0 \Rightarrow \mathbf{w} = \sum_{i=1}^N a_i y_i \phi(\mathbf{x}_i); \quad \frac{\partial L_p}{\partial b} = 0 \Rightarrow \sum_{i=1}^N a_i y_i = 0; \quad \frac{\partial L_p}{\partial \xi_i} = 0 \Rightarrow a_i = C - \mu_i$$

- Using these results to eliminate  $\mathbf{w}, b$  and  $\xi_i$  from  $L_p(\mathbf{w}, b, \mathbf{a})$ , we obtain the **dual Lagrangian** as:

$$L_D(\mathbf{a}) = \sum_{i=1}^N a_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N a_i a_j y_i y_j k(\mathbf{x}_i, \mathbf{x}_j)$$

Subject to the following constraints:

$$0 \leq a_i \leq C$$

$$\sum_{i=1}^N a_i y_i = 0$$

Where  $i = 1, \dots, N$

- This is the **dual problem** of the soft margin method. This is a quadratic programming problem.

- Prediction on new instance  $\mathbf{x}$  is again made by the sign of  $y(\mathbf{x})$ :

$$y(\mathbf{x}) = \sum_{i=1}^N a_i y_i k(\mathbf{x}, \mathbf{x}_i) + b$$

- To determine the value of  $b$ , we note that those support vectors  $\mathbf{x}_i$  have  $\xi_i = 0$ , so that  $y_i y(\mathbf{x}_i) = 1$ , and hence will satisfy

$$y_i y(\mathbf{x}_i) = 1 \Rightarrow y_i \left( \sum_{j=1}^N a_j y_j k(\mathbf{x}_i, \mathbf{x}_j) + b \right) = 1$$

Where  $S$  is the set of indices of the **support vectors**.

- Multiplying both sides of the above equality by  $y_i$  and notice that  $y_i^2 = 1$ , and then averaging over these equalities, we have ,

$$b = \frac{1}{N_S} \sum_{i \in S} \left( y_i - \sum_{j=1}^N a_j y_j k(\mathbf{x}_i, \mathbf{x}_j) \right)$$

Where  $N_S$  is the total number of support vectors.

# **Kernels and Kernel Trick**

- Recall the ***dual optimization problem*** of SVM:

$$\max_{\boldsymbol{a}} \left\{ L_D(\boldsymbol{a}) = \sum_{i=1}^N a_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N a_i a_j y_i y_j k(\boldsymbol{x}_i, \boldsymbol{x}_j) \right\}$$

- With the solution  $a_i, i = 1, 2, \dots, N$ , of the dual problem found, the ***dual decision function***:

$$y(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{x} + b = \sum_{i=1}^N a_i y_i k(\boldsymbol{x}, \boldsymbol{x}_i) + b$$

$$b = \frac{1}{N_S} \sum_{i \in S} \left( y_i - \sum_{j \in S} a_j y_j k(\boldsymbol{x}_i, \boldsymbol{x}_j) \right)$$

Where  $k(\boldsymbol{x}_i, \boldsymbol{x}_j) = \boldsymbol{\phi}(\boldsymbol{x}_i)^T \boldsymbol{\phi}(\boldsymbol{x}_j)$  is the ***kernel function***.

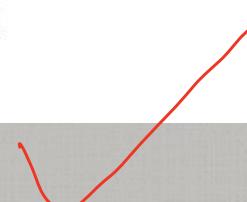
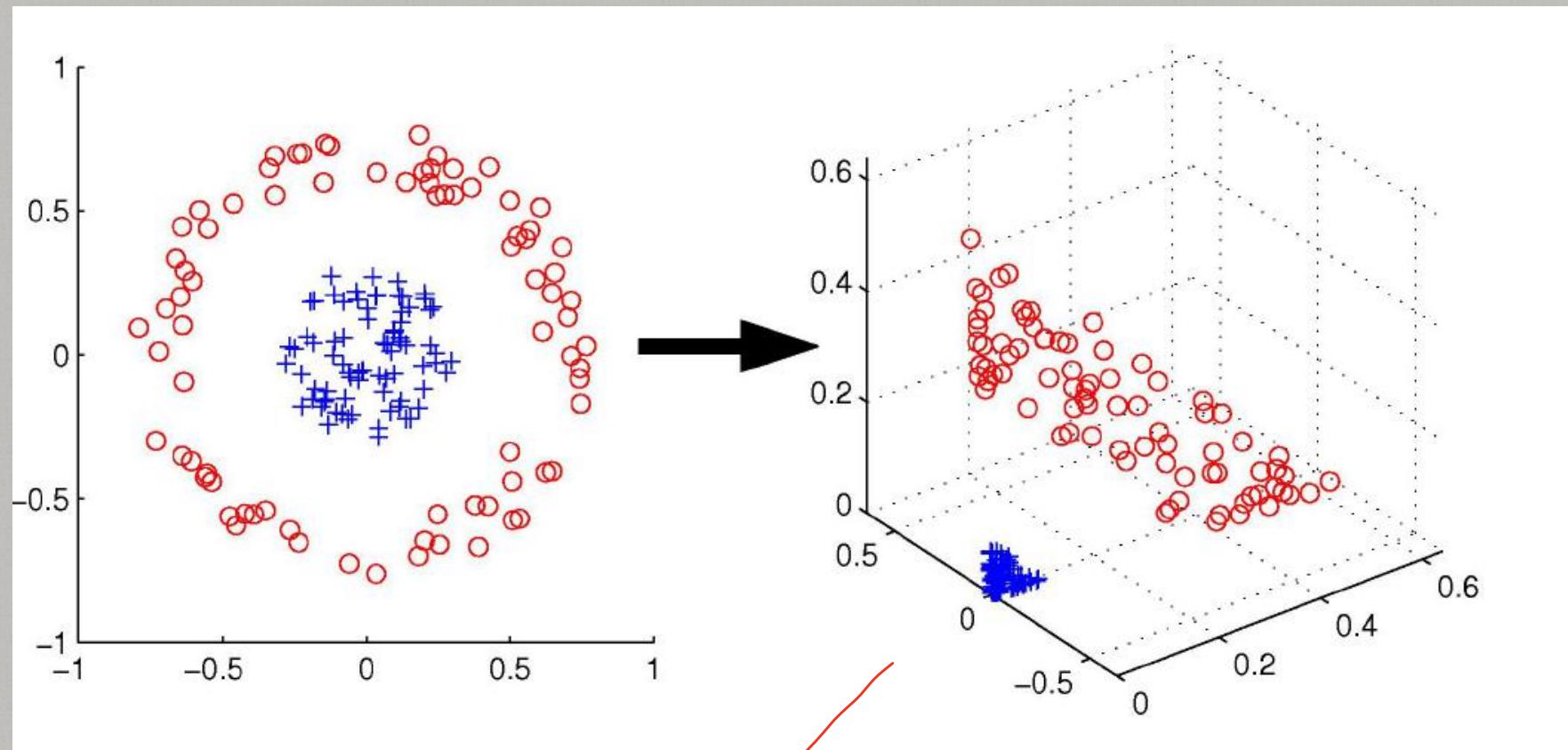
- Originally we define the ***kernel function*** as:

$$k(x, x') = \phi(x)^T \phi(x')$$

Which involve transforming the input  $x$  from original input space to higher dimensional feature space and then carry out inner product operation.

- By using the kernel function with some properties, we can make the operations in ***input space*** and leave the mapping completely ***implicit***.

核函数将低维空间中的数据映射到高维空间中



- Clearly, the data in the left is not linearly separable.
- If we map it to a 3-dimensional feature space using

$$\phi: \mathcal{R}^2 \rightarrow \mathcal{R}^3$$

$$(x_1, x_2) \rightarrow (z_1, z_2, z_3) = (x_1^2, \sqrt{2}x_1x_2, x_2^2)$$

- Then, in the new feature space, the data set is linearly separable by a hyperplane  $\mathbf{w}^T \mathbf{Z} + b = 0$ ,

$$w_1 z_1 + w_2 z_2 + w_3 z_3 + b = 0$$

i.e.,

$$w_1 x_1^2 + w_2 \sqrt{2}x_1x_2 + w_3 x_2^2 = -b$$

Which is an ellipse in the original input space.

- Consider two vectors  $\mathbf{x} = [x_1 \quad x_2]^T$  and  $\mathbf{x}' = [x'_1 \quad x'_2]^T$  in original feature space. We have,

$$\phi(\mathbf{x})^T \phi(\mathbf{x}') = [x_1^2 \quad \sqrt{2}x_1x_2 \quad x_2^2] \begin{bmatrix} (x'_1)^2 \\ \sqrt{2}x'_1x'_2 \\ (x'_2)^2 \end{bmatrix} = (x_1x'_1)^2 + 2(x_1x'_1)(x_2x'_2) + (x_2x'_2)^2$$

- Now, let's define  $k(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^T \mathbf{x}')^2$ , then,

$$\begin{aligned} k(\mathbf{x}, \mathbf{x}') &= (\mathbf{x}^T \mathbf{x}')^2 = \left( [x_1 \quad x_2] \begin{bmatrix} x'_1 \\ x'_2 \end{bmatrix} \right)^2 = (x_1x'_1 + x_2x'_2)^2 \\ &= (x_1x'_1)^2 + 2(x_1x'_1)(x_2x'_2) + (x_2x'_2)^2 \end{aligned}$$

- This means, with the kernel function  $k(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^T \mathbf{x}')^2$ , instead of carry out the mapping on the data set and then calculate  $\phi(\mathbf{x})^T \phi(\mathbf{x}')$  in ***transformed high-dimensional feature space***, we only need to calculate  $k(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^T \mathbf{x}')^2$  in the ***input space!!!***

## Important properties of *kernel functions*:

A kernel is a two arguments real-valued function over  $\mathcal{R}^d \times \mathcal{R}^d \rightarrow \mathcal{R}$ :

$$k(\mathbf{x}, \mathbf{y}) = \phi(\mathbf{x})^T \phi(\mathbf{y})$$

- A *kernel* must be *symmetric*, that is,

$$k(\mathbf{x}, \mathbf{y}) = k(\mathbf{y}, \mathbf{x})$$

- The *kernel matrix* is *positive semi-definite*:

A kernel matrix  $K$  is the matrix results from applying kernel  $k$  to all pairs of data points in data set  $\{\mathbf{x}_i\}_{i=1}^N$ :

$$K = \begin{bmatrix} k(\mathbf{x}_1, \mathbf{x}_1) & k(\mathbf{x}_1, \mathbf{x}_2) & \dots & k(\mathbf{x}_1, \mathbf{x}_N) \\ k(\mathbf{x}_2, \mathbf{x}_1) & k(\mathbf{x}_2, \mathbf{x}_2) & \ddots & k(\mathbf{x}_2, \mathbf{x}_N) \\ \vdots & \vdots & \ddots & \vdots \\ k(\mathbf{x}_N, \mathbf{x}_1) & k(\mathbf{x}_N, \mathbf{x}_2) & \dots & k(\mathbf{x}_N, \mathbf{x}_N) \end{bmatrix}$$

## **Kernel construction rules:**

- Clearly, the linear kernel defined as  $k(\mathbf{x}, \mathbf{y}) = \mathbf{x}^T \mathbf{y}$  is a valid kernel.
- For any positive semi-definite matrix  $\mathbf{B}_{d \times d}$ ,  $k(\mathbf{x}, \mathbf{y}) = \mathbf{x}^T \mathbf{B} \mathbf{y}$  is a valid kernel.
- Suppose  $k_1, k_2$  and  $k_3$  are valid kernels, then, the following are all valid kernels
  - $k(\mathbf{x}, \mathbf{y}) = k_1(\mathbf{x}, \mathbf{y}) + k_2(\mathbf{x}, \mathbf{y})$
  - $k(\mathbf{x}, \mathbf{y}) = \alpha k_1(\mathbf{x}, \mathbf{y})$
  - $k(\mathbf{x}, \mathbf{y}) = k_1(\mathbf{x}, \mathbf{y})k_2(\mathbf{x}, \mathbf{y})$
  - $k(\mathbf{x}, \mathbf{y}) = k_3(\phi(\mathbf{x}), \phi(\mathbf{y}))$
- Suppose  $k_1$  is a kernel and  $p$  is a polynomial with **non-negative** coefficients, then the following are kernels
  - $k(\mathbf{x}, \mathbf{y}) = p(k_1(\mathbf{x}, \mathbf{y}))$
  - $k(\mathbf{x}, \mathbf{y}) = e^{k_1(\mathbf{x}, \mathbf{y})}$

The following are some of the commonly used kernels in Machine Learning:

- **Linear Kernel:**

$$k(x_i, x_j) = x_i^T x_j$$

- **Polynomial Kernel:**

$$k(x_i, x_j) = (x_i^T x_j + \theta)^d$$

- **Gaussian Radial Basis Function (RBF): (universal kernel)**

$$k(x_i, x_j) = e^{-\gamma \|x_i - x_j\|^2}$$

- **Sigmoid Kernel:**

$$k(x_i, x_j) = \tanh(\eta x_i^T x_j + \theta)$$

### ***Advantages of kernel based methods:***

- Kernel methods learn nonlinear functions with the algorithms for learning linear function
- Kernel allows for learning in high-dimensional feature spaces without explicit mapping into feature space
- Kernels make learning in high-dimensional feature space computationally feasible
- Kernels provide an abstraction that separates data representations and learning

Power of SVM = linear model with max margin + nonlinear feature mapping (kernel functions)