

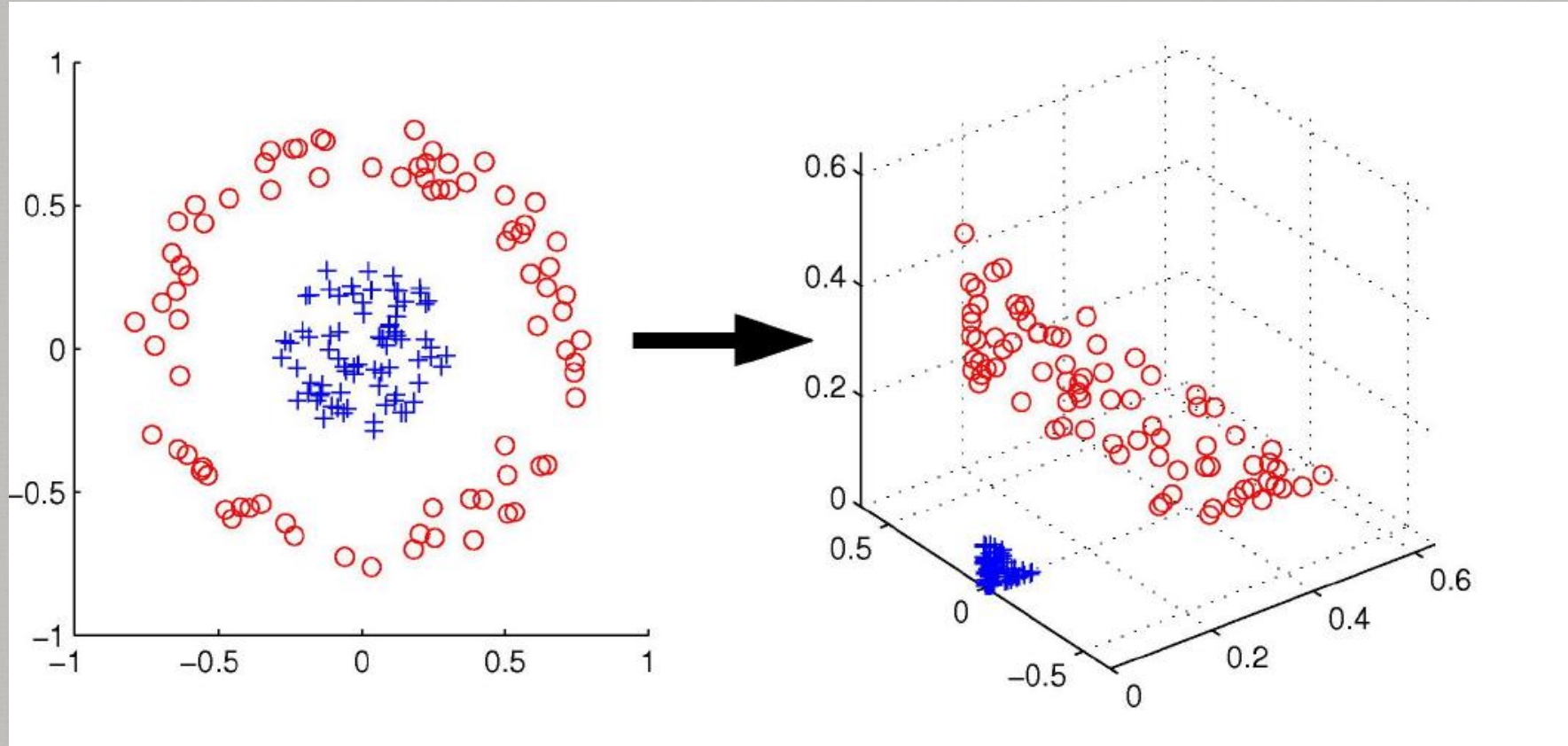
How can we expand the Perceptron model to make it more powerful?

Perceptron 和 SVM 都是用于分类任务的线性模型

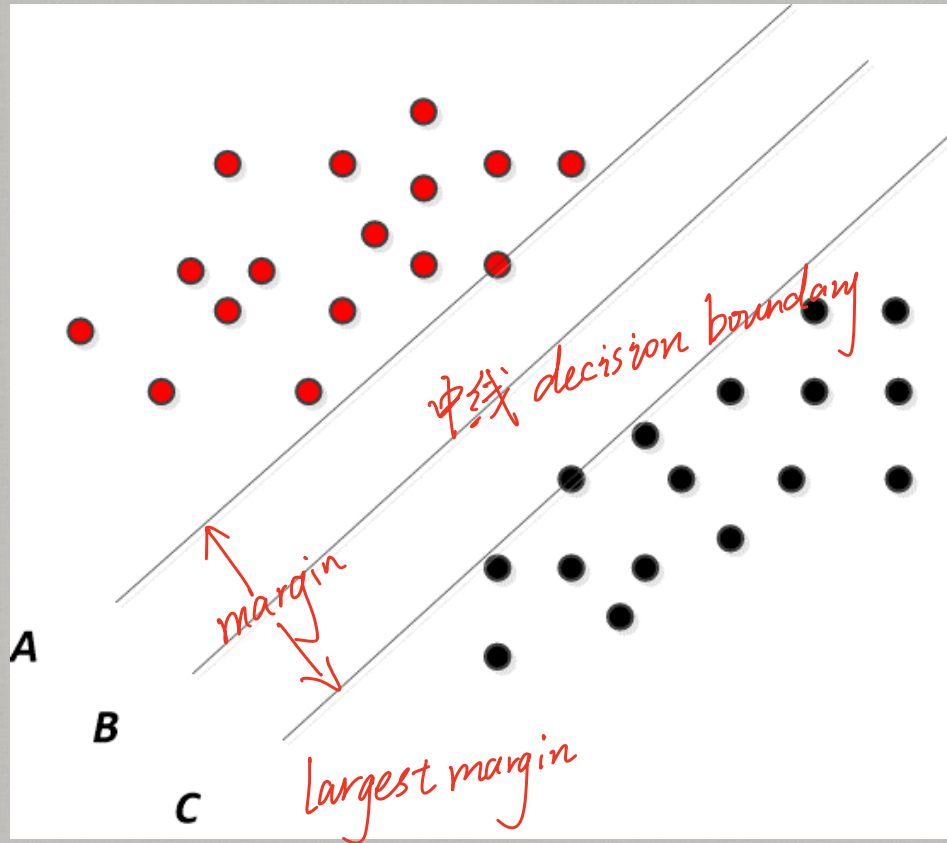
Perceptron 目标是找到一个能够分开数据的线性超平面, 最小化分类错误次数

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)**

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

$$y(\mathbf{x}) = \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}) + b$$

Where $\boldsymbol{\phi}(\mathbf{x})$ denotes a fixed **feature-space transformation**, \mathbf{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 \mathbf{w} and b to satisfy the following:

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

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

Which is equivalent to:

$$y_i(\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_i) + b) > 0, \quad i = 1, \dots, N$$

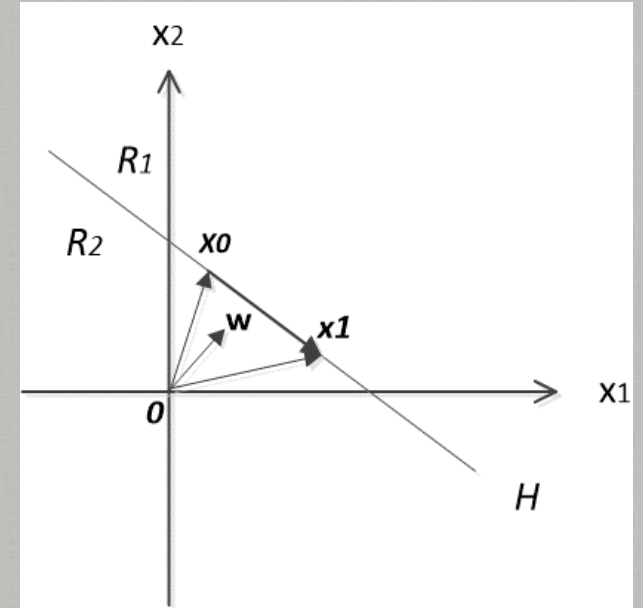
- We look for a hyperplane with the **maximum margin**.

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

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

Consider two points \mathbf{x}_0 and \mathbf{x}_1 on H . We want to show that \mathbf{w} is perpendicular to the vector $\mathbf{x}_1 - \mathbf{x}_0$

$$\mathbf{w}^T (\mathbf{x}_1 - \mathbf{x}_0) = \mathbf{w}^T \mathbf{x}_1 - \mathbf{w}^T \mathbf{x}_0 = b - b = 0$$

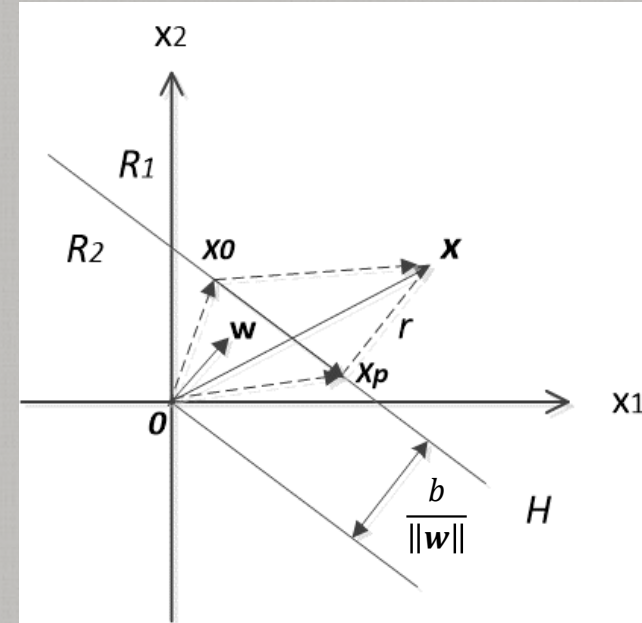


- Consider the hyperplane $H: \{x: w^T x + b = 0\}$
- Secondly, let's find the **geometric distance** from a point x to hyperplane H .

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).



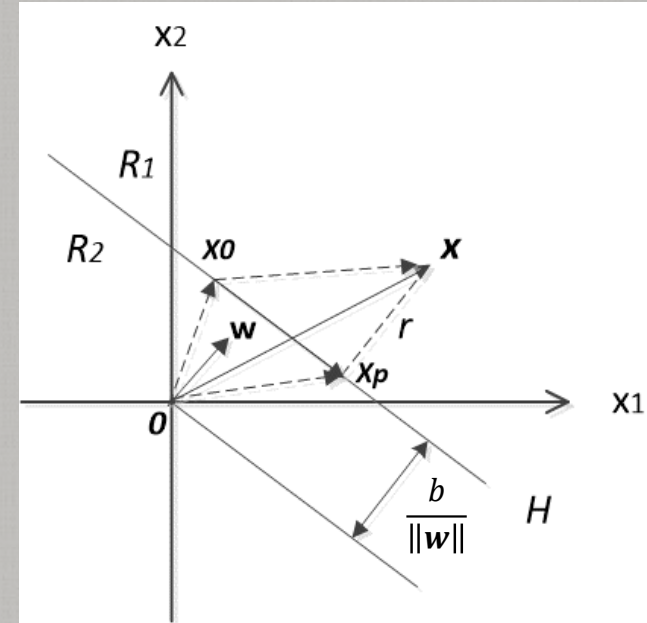
- Hence, we have,

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

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

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

- 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 $H: \{x: w^T x + b = 0\}$

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

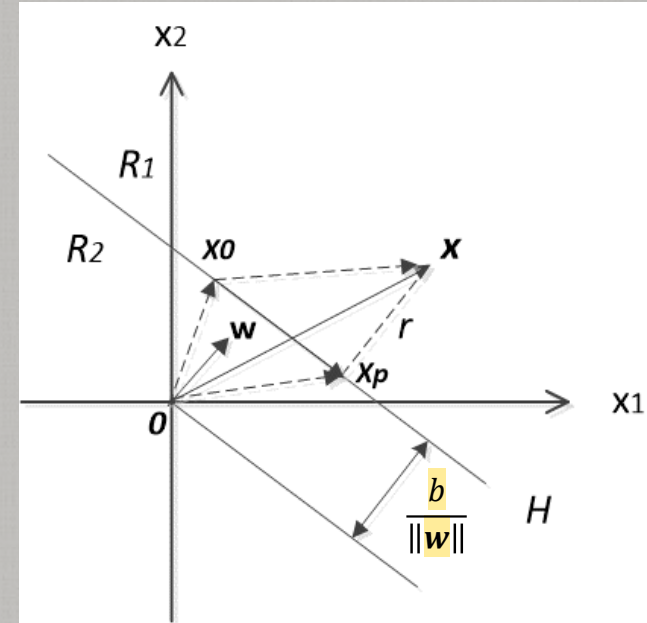
$$r_i = \frac{w^T x_i + b}{\|w\|}$$

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

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

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

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



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

The margin of hyperplane H is,

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

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

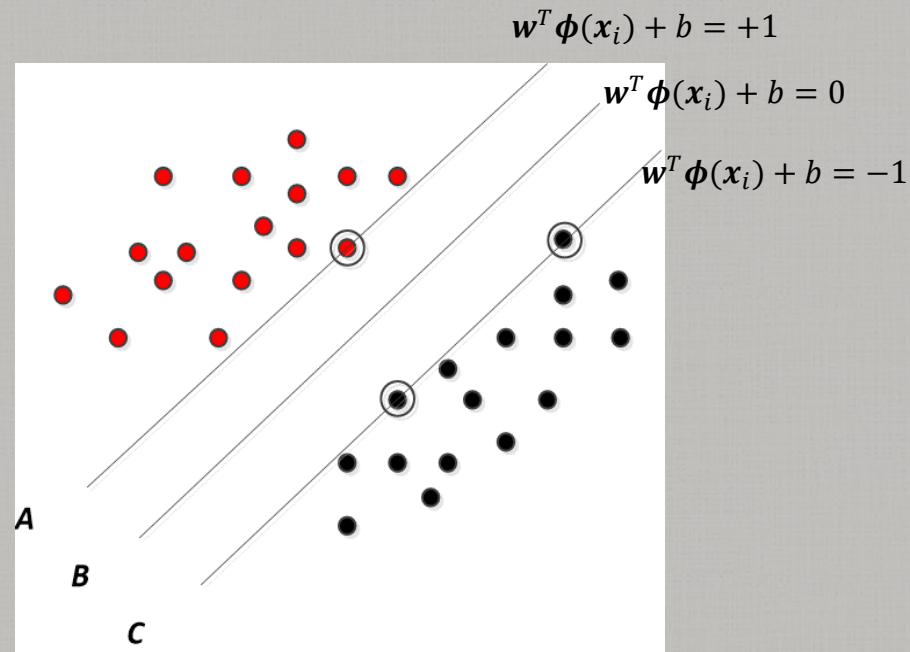
- Suppose all data points in the linearly separable data set satisfy the following constraints:

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

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

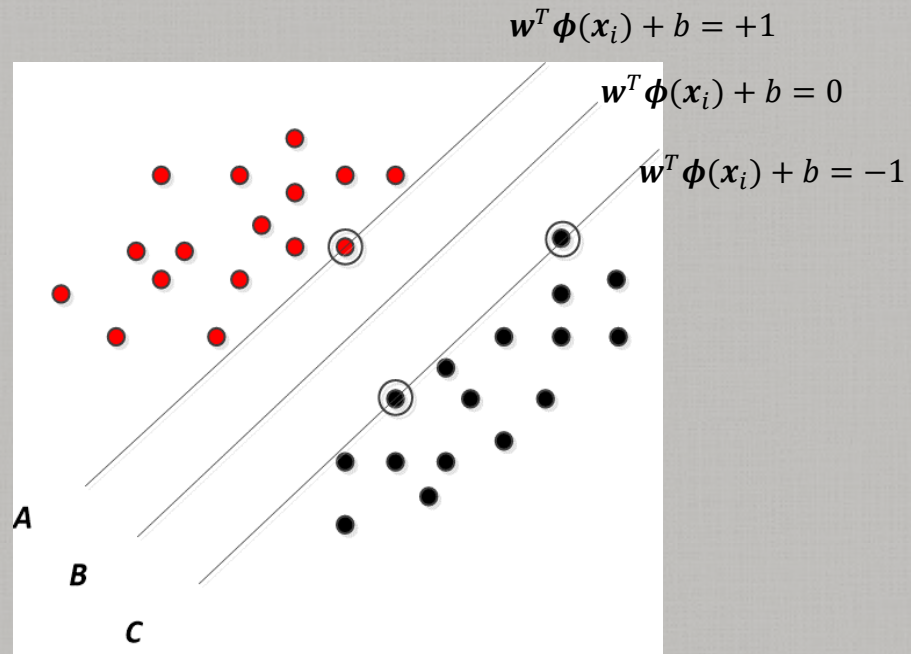
- Which can be combined to a set of inequality:

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



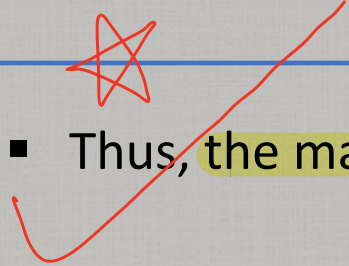
- Those points \mathbf{x}_i that satisfies $\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_i) + b = \pm 1$ are called **support vectors**.

支持向量



- Hence, the margin of H is

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


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

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

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

Which is a ***quadratic programming problem***.

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

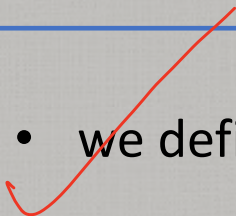


The Lagrange Multiplier Method for Constrained Optimization

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

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

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** Ω to be the set of points \mathbf{x} that satisfy the constraints, that is,

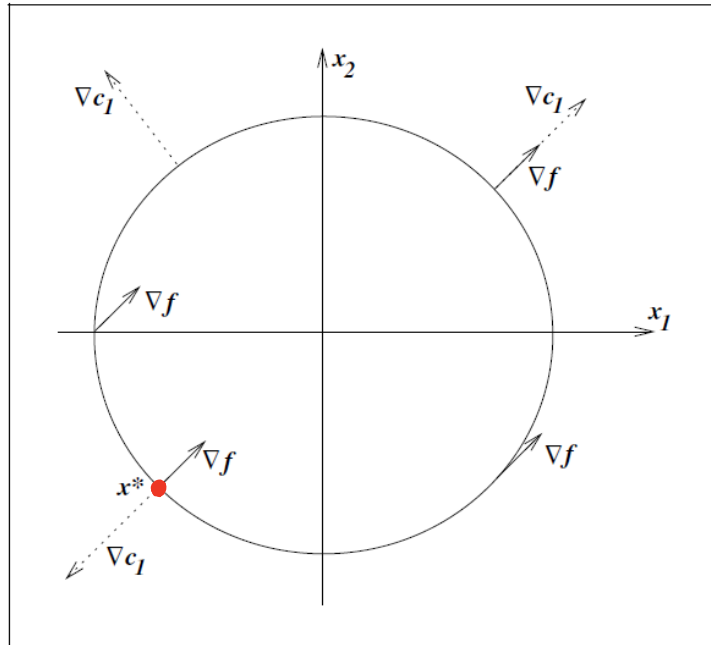
$$\Omega = \{\mathbf{x} | c_i(\mathbf{x}) = 0, i \in \mathcal{E}; c_j(\mathbf{x}) \geq 0, j \in \mathcal{I}\}$$

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

Example : single equality constraint

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

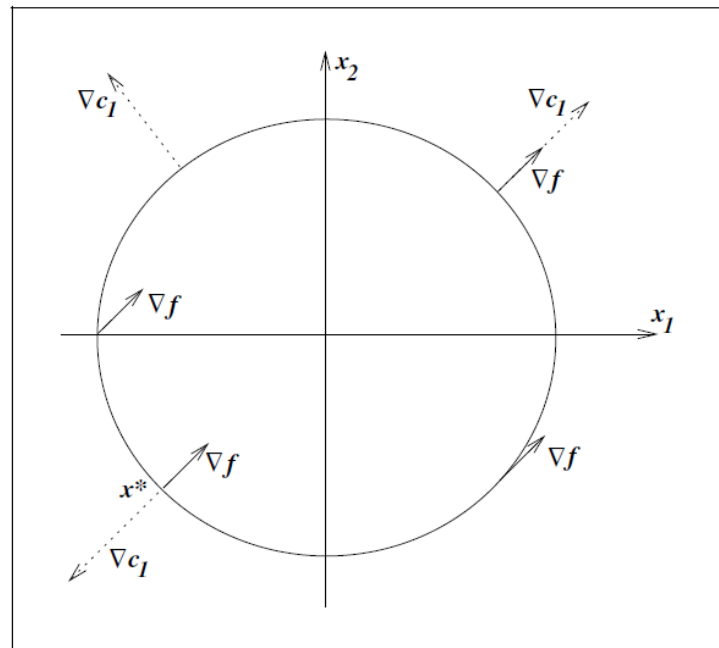
This is a two-variable problem with $f(\mathbf{x}) = x_1 + x_2$ and $c_1(\mathbf{x}) = x_1^2 + x_2^2 - 2$



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 λ_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,

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

- 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 $c_1(\mathbf{x}) = 0$, 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 \mathbf{x}^* , there is no such direction of \mathbf{s} to satisfy

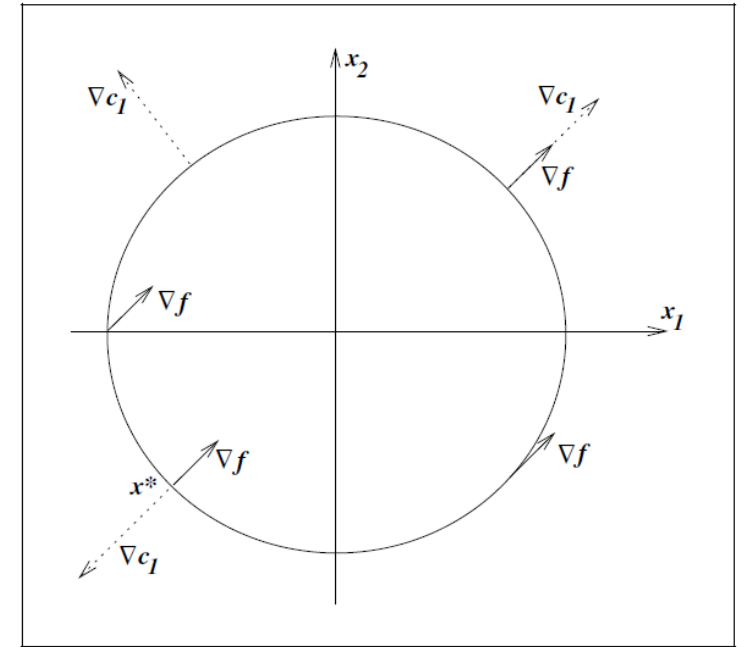
$$\nabla c_1(\mathbf{x})^T \mathbf{s} = 0 \text{ and } \nabla f(\mathbf{x})^T \mathbf{s} < 0$$

Then the point \mathbf{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 $\nabla c_1(\mathbf{x})$ and $\nabla f(\mathbf{x})$ are parallel, that is

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

hold at some \mathbf{x} , for some scalar λ_1 .



Lagrange multiplier method

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

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

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

Notice that,

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

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

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

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

- This means we can search for solutions of the equality-constrained optimization problem by seeking stationary points of the **Lagrangian function**.
- The scalar λ_1 is called the **Lagrange multiplier** for the equation constraint $c_1(\mathbf{x}) = 0$.

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

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

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

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

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

$$\nabla_{x_1} \mathcal{L}(x, \lambda_1) = 1 - 2\lambda_1 x_1 = 0 \Rightarrow x_1 = \frac{1}{2\lambda_1} \quad \begin{pmatrix} 1 - 2\lambda_1 x_1 \\ 1 - 2\lambda_2 x_2 \end{pmatrix} = 0$$

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

$$x_1^2 + x_2^2 - 2 = 0 \Rightarrow \frac{1}{4\lambda_1^2} + \frac{1}{4\lambda_1^2} = 2 \Rightarrow \begin{cases} x_1 = \frac{1}{2\lambda_1} \\ x_2 = \frac{1}{2\lambda_1} \end{cases}$$

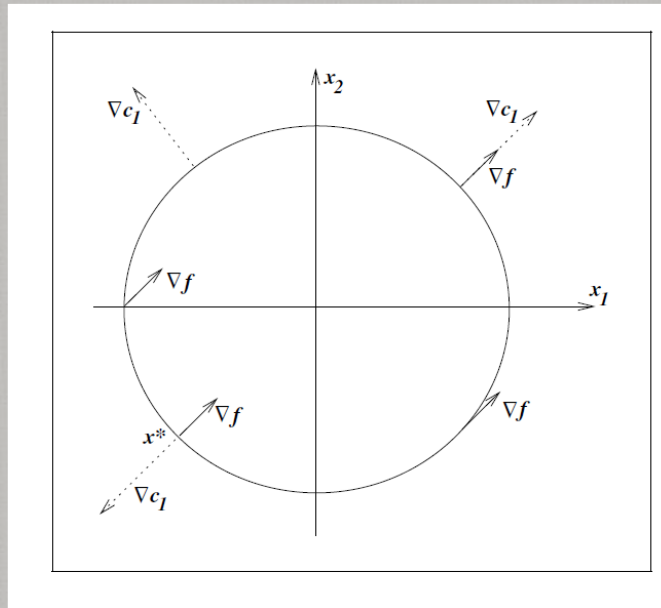
- Substitute these into $C_1(x) = 0$ gives: $\lambda_1 = \frac{1}{2}$ or $-\frac{1}{2}$. $\lambda_1 = \pm \frac{1}{2}$

- 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

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

- The step s retains feasibility if

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

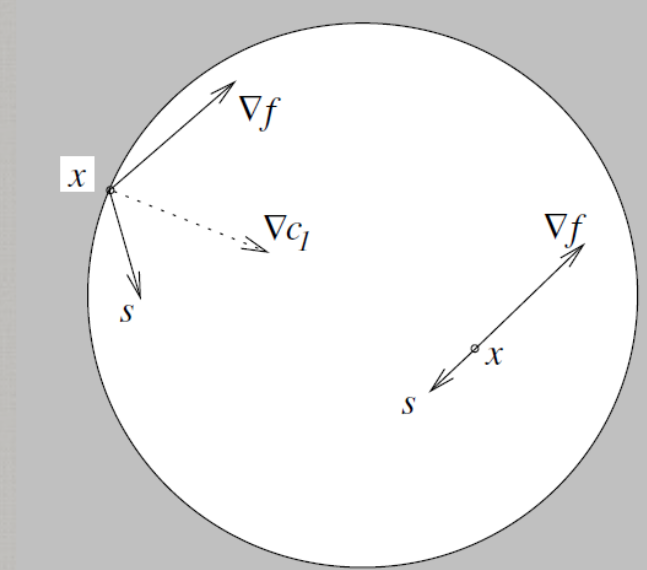
To determine if a step s exists that satisfies both conditions (svm-1) and (svm-2), we consider two cases:

- **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 α 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

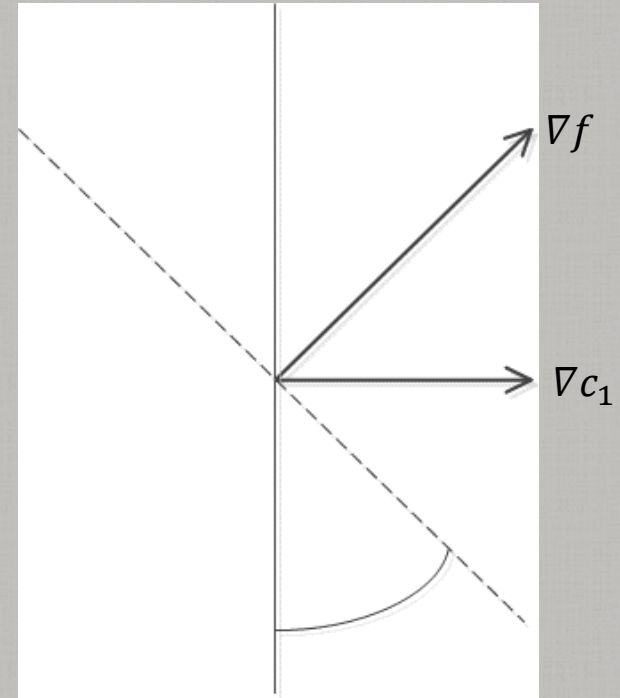
$$\nabla f(x)^T s < 0 \text{ and } \nabla c_1(x)^T s \geq 0 \quad (\text{svm-3})$$

- 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 λ_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

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

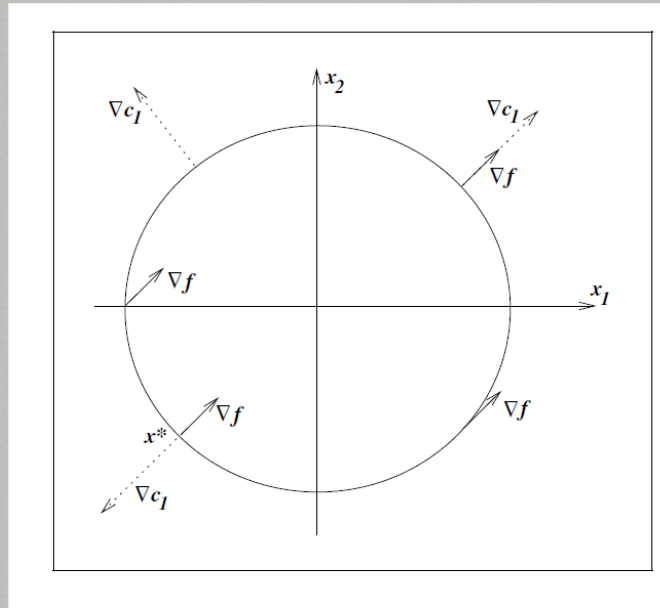
- Condition (svm-6) is known as the **complementarity condition**. It implies that the **Lagrange multiplier λ_1 can be strictly positive only when the corresponding constraint c_1 is active**. 对 $c_1(x) \geq 0$, 当 $c_1(x) = 0$ 时处于边界上, 约束被激活 (active)
当 $c_1(x) > 0$, x 位于可行域内, 约束未被激活 (inactive)
- In case 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 λ_1^* to take a nonnegative value. So (svm-5) becomes equivalent to (svm-4)

Example: a single inequality constraint

$$c_1(x) \geq 0$$

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

Can you find the solution by visual inspection?



Solution:

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

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

- Then,

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

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

Solution (continue):

- With the condition that

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


λ_1 is strictly positive only when $c_1(\mathbf{x})$ is **active**, that is,

$$c_1(\mathbf{x}) = 2 - x_1^2 - x_2^2 = 0$$

(svm-9)

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

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

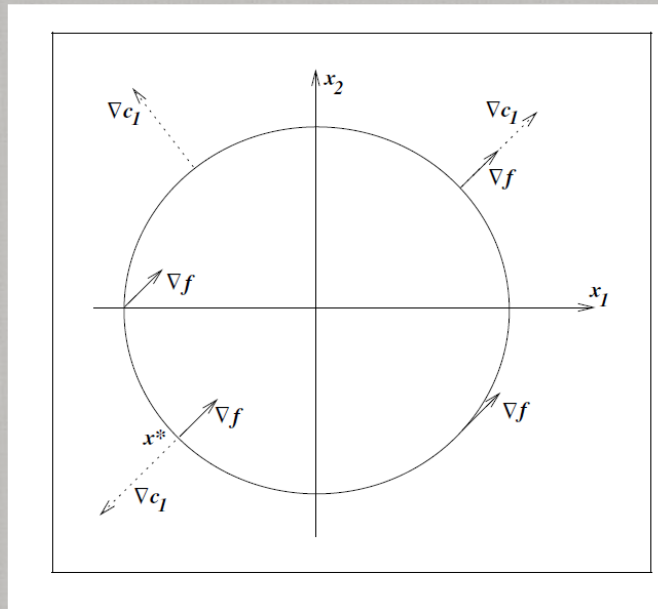
$$\lambda_1 = \pm \frac{1}{2}$$


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

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):

- λ_1 is strictly positive only when $c_1(\mathbf{x})$ is active, that is,

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

- λ_2 is strictly positive only when $c_2(\mathbf{x})$ is active, that is,

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

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



The Lagrangian Dual Problem

拉格朗日对偶问题

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

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

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

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

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

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

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

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

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

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

- 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


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

Quiz

$f(x)$

$c_1(x) \geq 0$

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 λ_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,

$$\nabla \mathcal{L}(x, \lambda_1) = \nabla f(x) - \lambda_1 \nabla c_1(x) = 0$$

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

$$\frac{\partial \mathcal{L}}{\partial x_2} = 0 \Rightarrow x_2 = 0$$

$$\Rightarrow \begin{cases} x_1 = \lambda_1 \\ x_2 = 0 \end{cases}$$

- 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:

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



Support Vector Machine Model

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

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

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

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**

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

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

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

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

- 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:

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

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

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

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

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

$$k(\mathbf{x}, \mathbf{x}') = \boldsymbol{\phi}(\mathbf{x})^T \boldsymbol{\phi}(\mathbf{x}')$$

- 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**?
 - $\mathbf{w} = \sum_{i=1}^N a_i y_i \boldsymbol{\phi}(\mathbf{x}_i)$
 - To find the expression for b , we need to revisit the concept of **support vector**

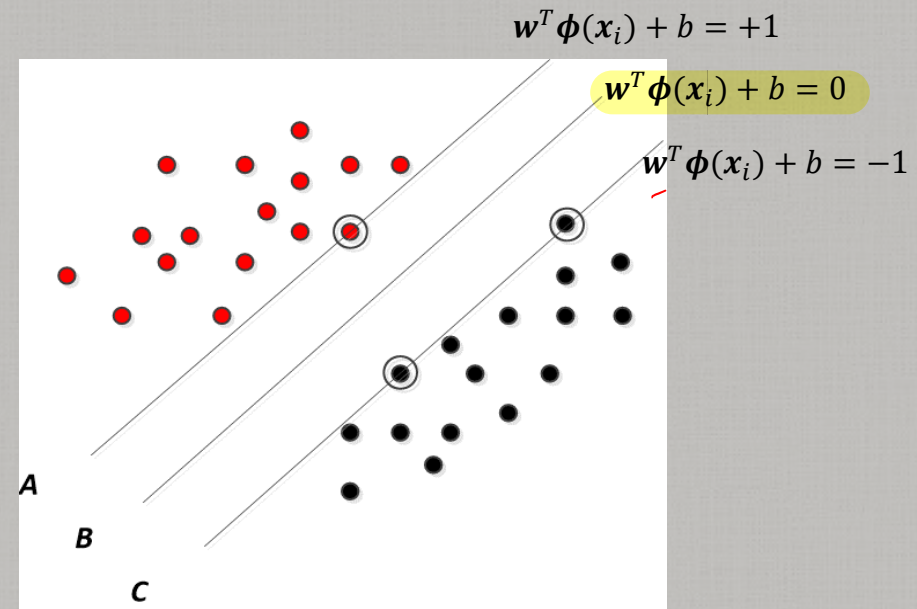
- The Karush-Kuhn-Tucker (**KKT**) conditions play a central role in both the theory and practice of constrained optimization. **KKT conditions are satisfied at the solutions of any constrained optimization problem (convex or not) with any kind of constraints, provided certain conditions.**
- The following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

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

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

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

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



- In order to classify new data point using trained model, we evaluate the sign of the prediction $y(\mathbf{x})$.
Notice that $\mathbf{w} = \sum_{i=1}^N a_i y_i \boldsymbol{\phi}(\mathbf{x}_i)$, we have,

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

- Having solved the quadratic optimization problem and find a value of \mathbf{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**.

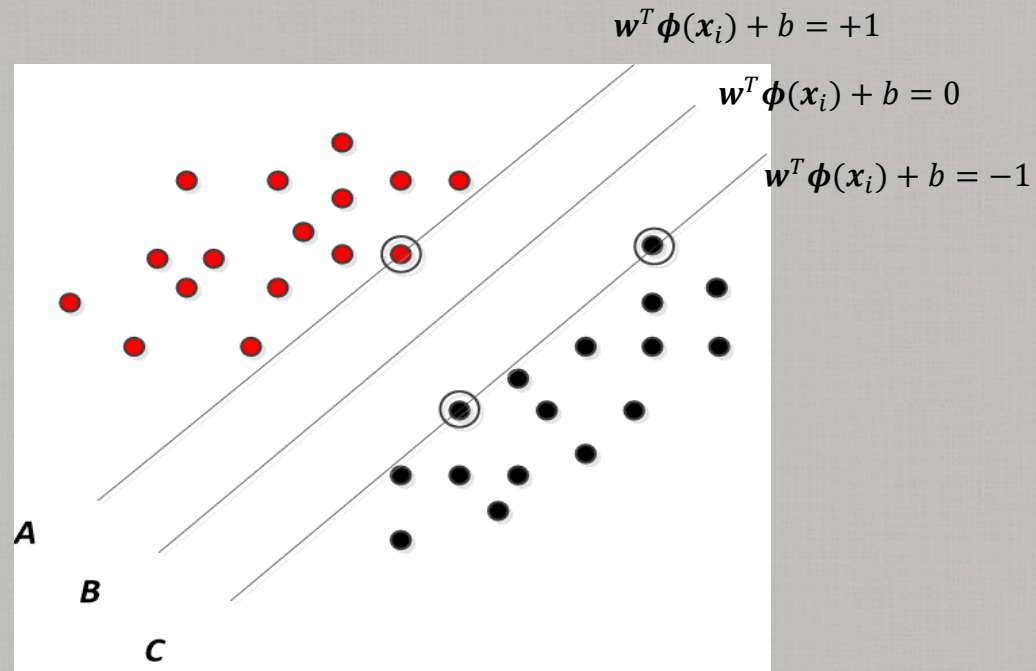
- Multiplying both sides of the above equality by y_i and notice that $y_i^2 = 1$, and then averaging over these equalities, we have,

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

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*:

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

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

- 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**:

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

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

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:

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

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

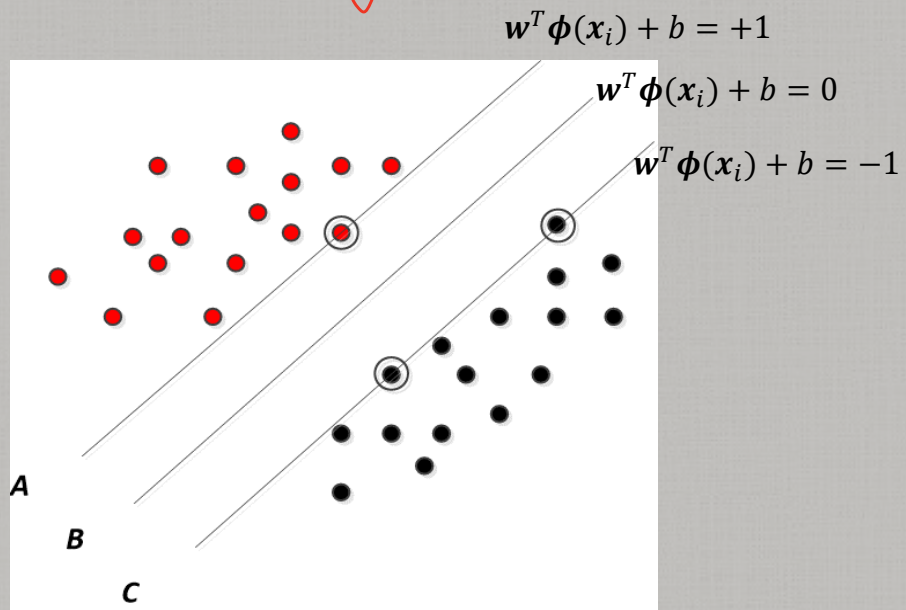
Where $k(\mathbf{x}_i, \mathbf{x}_j) = \boldsymbol{\phi}(\mathbf{x}_i)^T \boldsymbol{\phi}(\mathbf{x}_j)$ is the ***kernel function***. S is the set of all ***support vector*** points.

Support Vector Machine Method (*Soft margin*)

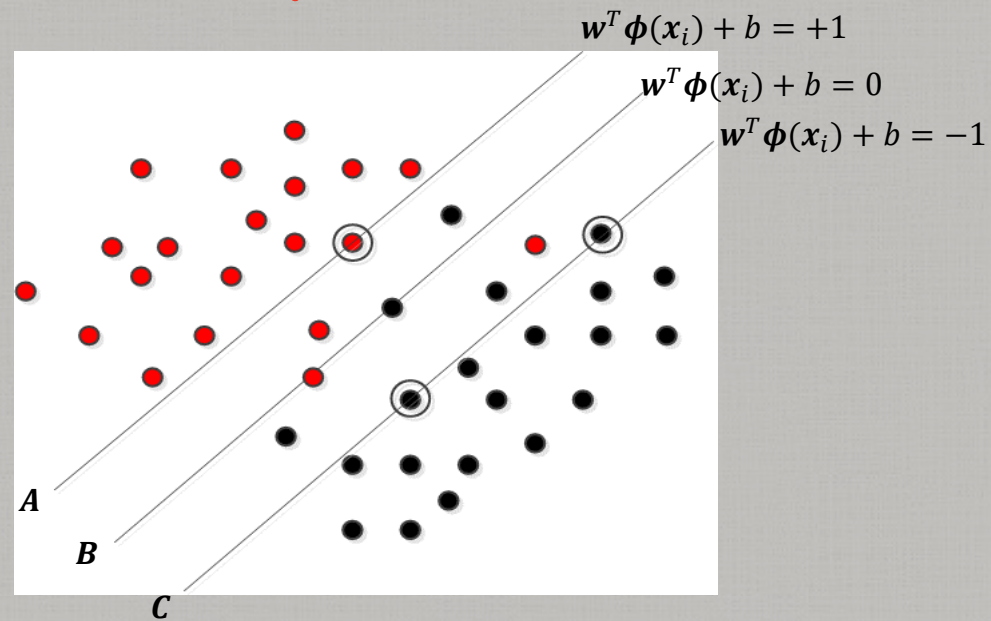
(Non-linearly-separable binary data sets)

- 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



soft margin



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

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

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

- Or equivalently,

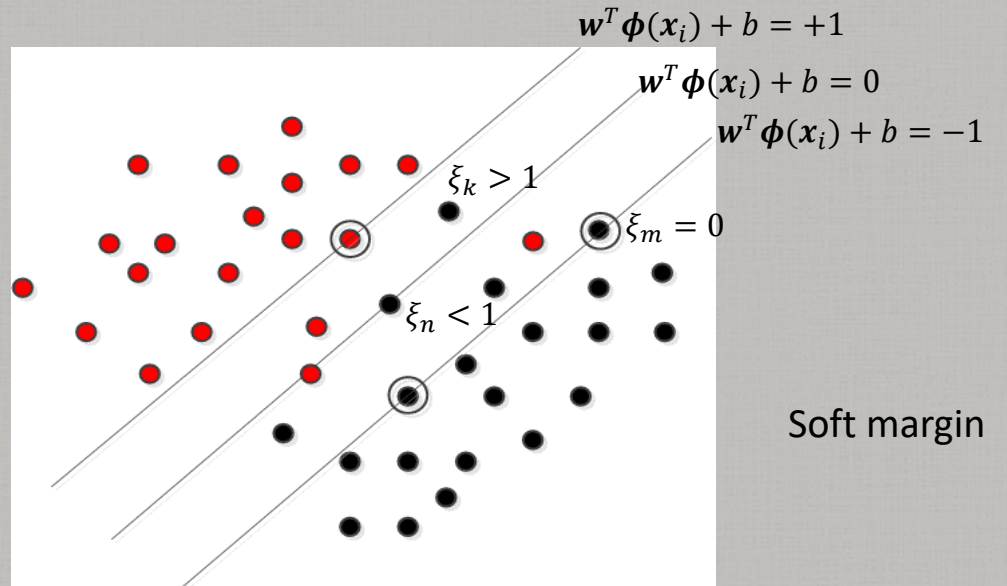
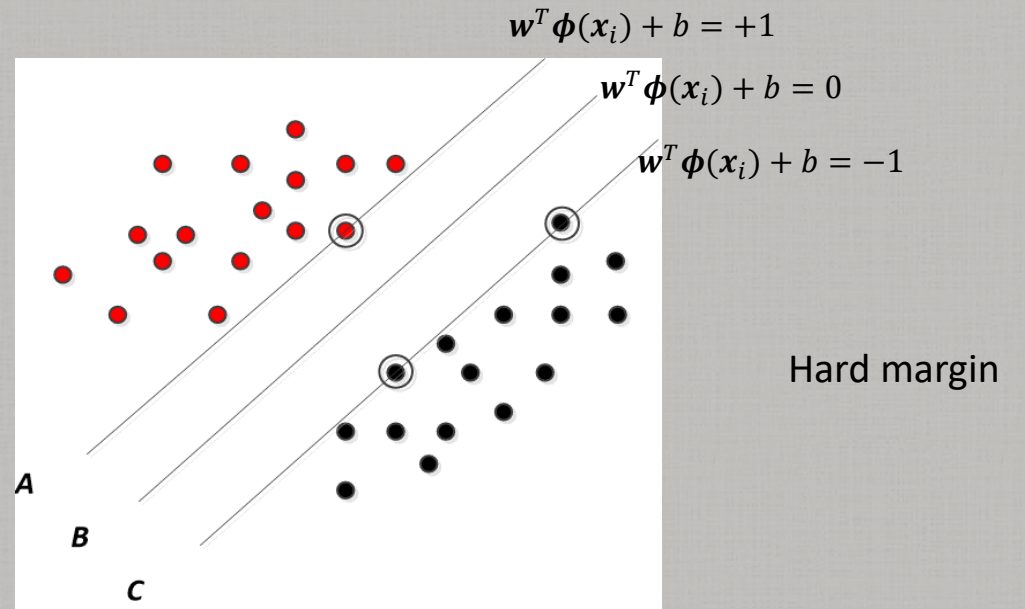
$$y_i \{ \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_i) + b \} \geq 1 - \xi_i, \forall i$$

- $\xi_i = 0$: 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:

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

- $\xi_i = 0$: 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: $y_i \{\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_i) + b\} \geq +1 - \xi_i, \forall i$ 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:

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

- Using these results to eliminate \mathbf{w} , b and ξ_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:

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

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

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

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

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

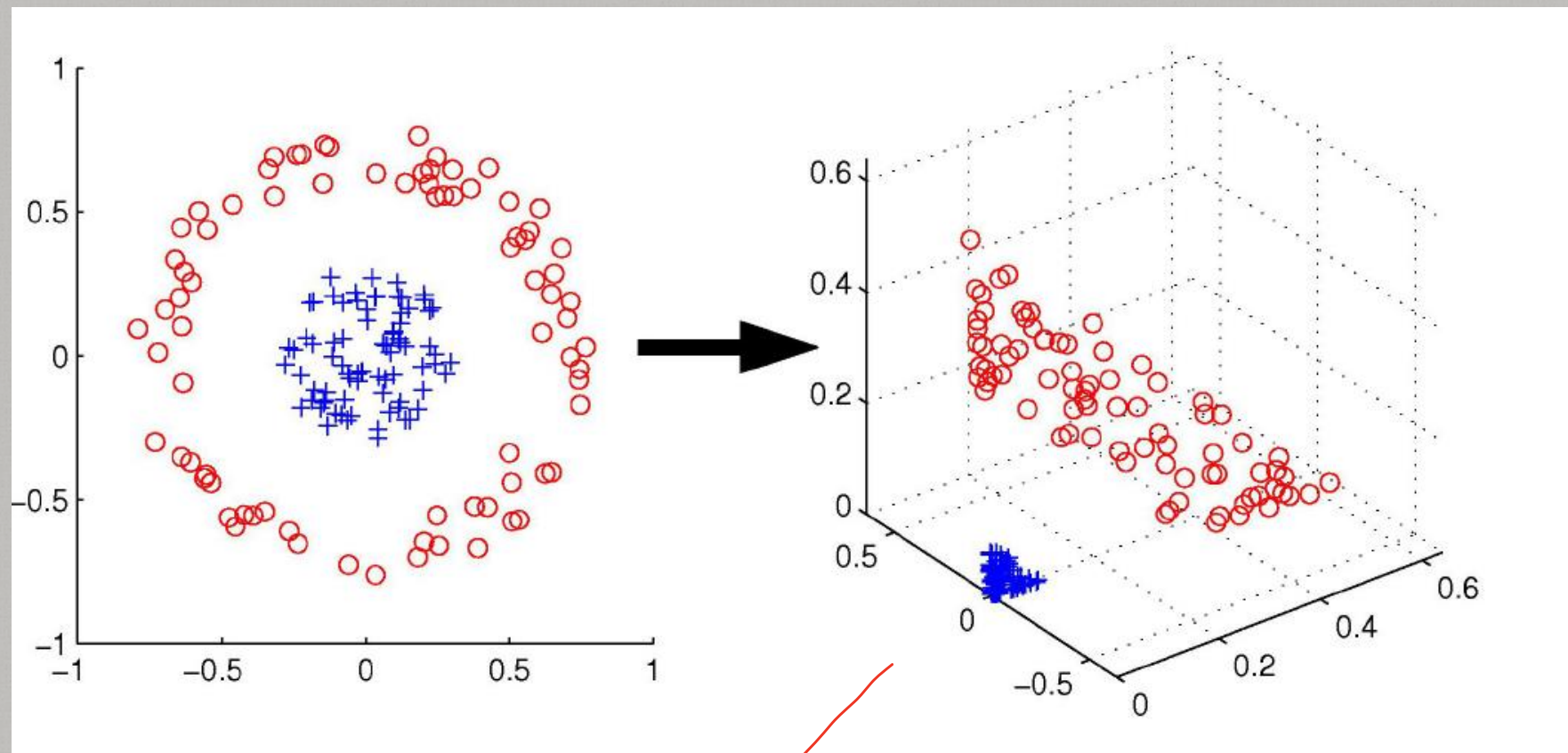
- Originally we define the ***kernel function*** as:

$$k(\mathbf{x}, \mathbf{x}') = \boldsymbol{\phi}(\mathbf{x})^T \boldsymbol{\phi}(\mathbf{x}')$$

Which involve transforming the input \mathbf{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.,

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

Which is an ellipse in the original input space.

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

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

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

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

- 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 $\boldsymbol{\phi}(\mathbf{x})^T \boldsymbol{\phi}(\mathbf{x}')$ 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 $\mathcal{R}^d \times \mathcal{R}^d \rightarrow \mathcal{R}$:

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

- 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 $\{\mathbf{x}_i\}_{i=1}^N$:

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

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
 - $k(\mathbf{x}, \mathbf{y}) = k_1(\mathbf{x}, \mathbf{y}) + k_2(\mathbf{x}, \mathbf{y})$
 - $k(\mathbf{x}, \mathbf{y}) = \alpha k_1(\mathbf{x}, \mathbf{y})$
 - $k(\mathbf{x}, \mathbf{y}) = k_1(\mathbf{x}, \mathbf{y}) k_2(\mathbf{x}, \mathbf{y})$
 - $k(\mathbf{x}, \mathbf{y}) = k_3(\boldsymbol{\phi}(\mathbf{x}), \boldsymbol{\phi}(\mathbf{y}))$
- 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:***

$$k(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^T \mathbf{x}_j$$

- ***Polynomial Kernel:***

$$k(\mathbf{x}_i, \mathbf{x}_j) = (\mathbf{x}_i^T \mathbf{x}_j + \theta)^d$$

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

$$k(\mathbf{x}_i, \mathbf{x}_j) = e^{-\gamma \|\mathbf{x}_i - \mathbf{x}_j\|^2}$$

- ***Sigmoid Kernel:***

$$k(\mathbf{x}_i, \mathbf{x}_j) = \tanh(\eta \mathbf{x}_i^T \mathbf{x}_j + \theta)$$

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)