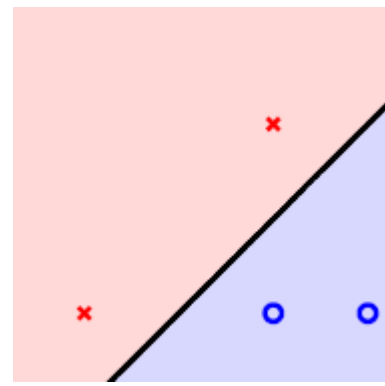
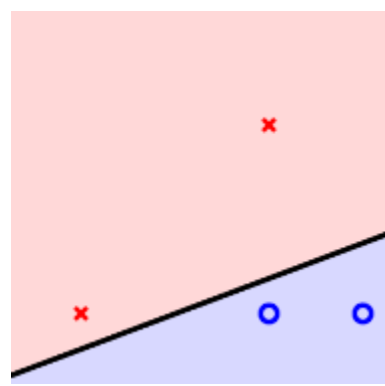
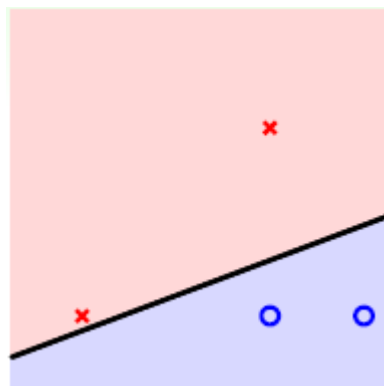
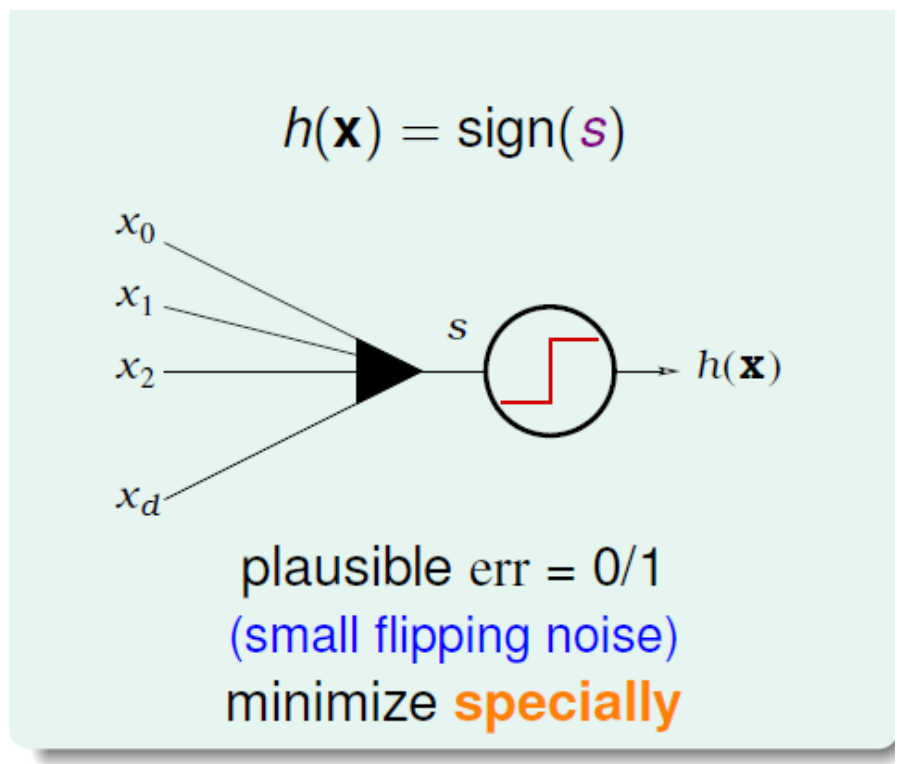
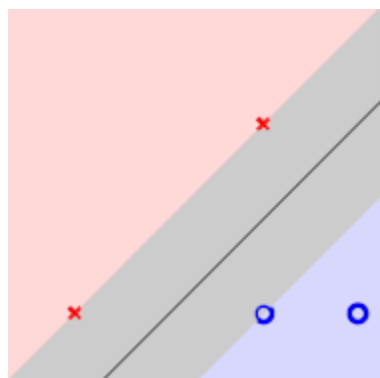
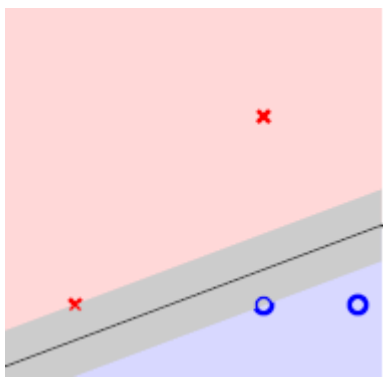
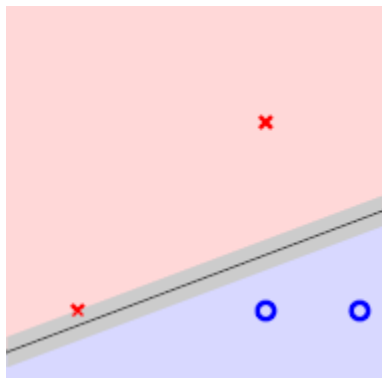
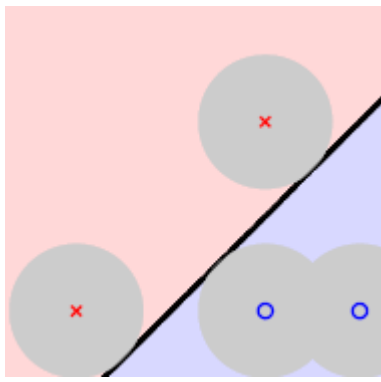
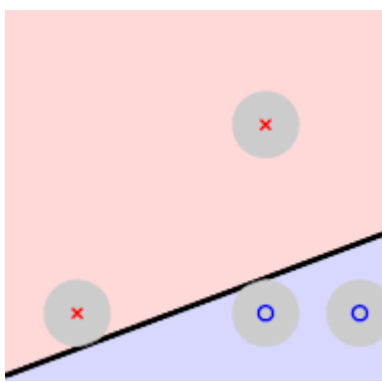
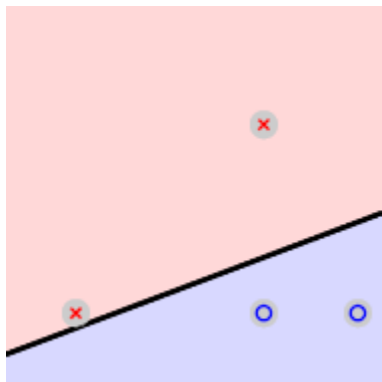


如何选择一条线呢？

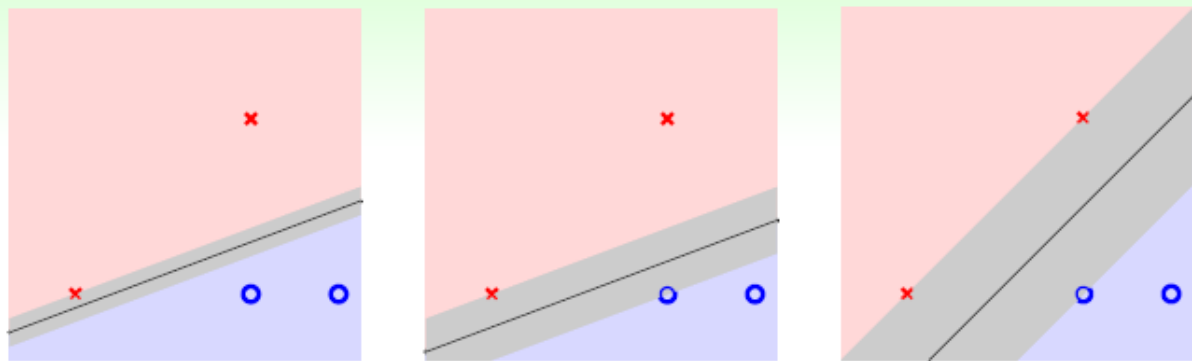


linear (hyperplane) classifiers:
 $h(\mathbf{x}) = \text{sign}(\mathbf{w}^T \mathbf{x})$

越胖越好



目的



$$\begin{aligned} & \max_{\mathbf{w}} \quad \text{fatness}(\mathbf{w}) \\ & \text{subject to} \quad \mathbf{w} \text{ classifies every } (\mathbf{x}_n, y_n) \text{ correctly} \\ & \quad \text{fatness}(\mathbf{w}) = \min_{n=1, \dots, N} \text{distance}(\mathbf{x}_n, \mathbf{w}) \end{aligned}$$

- fatness: formally called **margin**
- correctness: $y_n = \text{sign}(\mathbf{w}^T \mathbf{x}_n)$

goal: find **largest-margin**
separating hyperplane

want: distance(\mathbf{x} , b , \mathbf{w}), with hyperplane $\mathbf{w}^T \mathbf{x}' + b = 0$

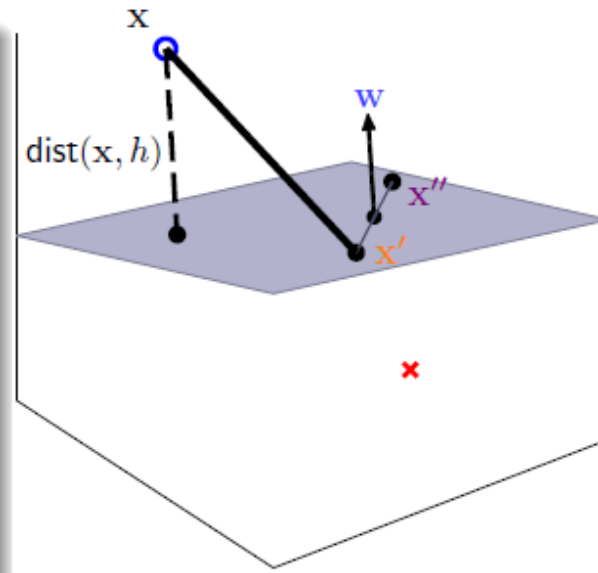
consider \mathbf{x}' , \mathbf{x}'' on hyperplane

① $\mathbf{w}^T \mathbf{x}' = -b$, $\mathbf{w}^T \mathbf{x}'' = -b$

② $\mathbf{w} \perp$ hyperplane:

$$\begin{pmatrix} \mathbf{w}^T & \underbrace{(\mathbf{x}'' - \mathbf{x}')}_{\text{vector on hyperplane}} \end{pmatrix} = 0$$

③ distance = project $(\mathbf{x} - \mathbf{x}')$ to \perp hyperplane



$$\text{distance}(\mathbf{x}, b, \mathbf{w}) = \left| \frac{\mathbf{w}^T}{\|\mathbf{w}\|} (\mathbf{x} - \mathbf{x}') \right| \stackrel{(1)}{=} \frac{1}{\|\mathbf{w}\|} |\mathbf{w}^T \mathbf{x} + b|$$

数据集(X1,Y1)(X2,Y2)到(Xn,Yn)

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

Y为样本的类别:

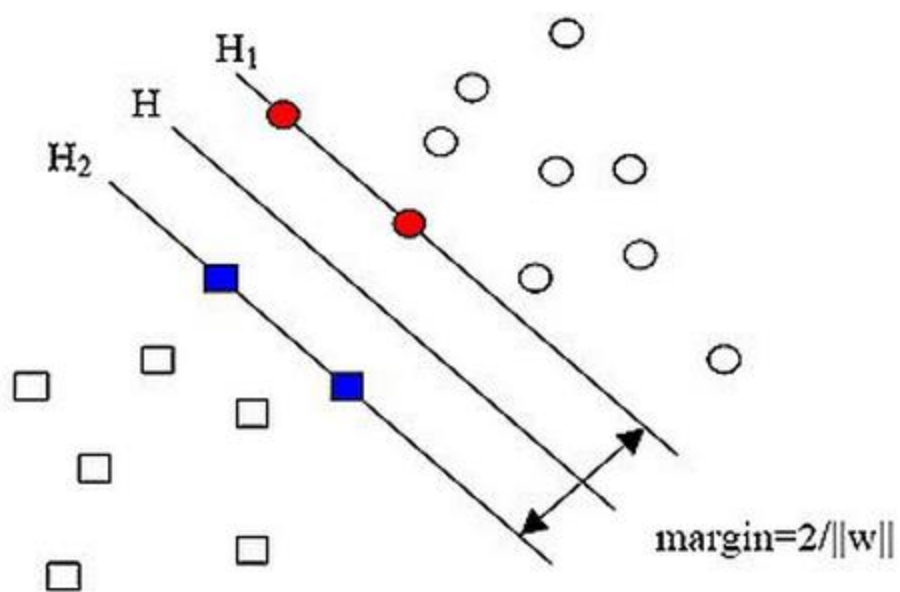
当X为正例时候 $Y = +1$

当X为负例时候 $Y = -1$

$$\begin{aligned} y(x_i) > 0 &\Leftrightarrow y_i = +1 \\ y(x_i) < 0 &\Leftrightarrow y_i = -1 \end{aligned} \quad \text{可推出} \quad y_i \cdot y(x_i) > 0$$

找到一个条线 (w 和 b)，使得离该线最近的点能够最远
 $\text{argmax}(w,b)$ 使得 \min (最近的点到该线的距离)

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



对于线 (w, b) 可以通过放缩使得其结果值 $|Y| \geq 1$

$$y_i \cdot (w^T \cdot \Phi(x_i) + b) \geq 1$$

$$\arg \max_{w, b} \left\{ \frac{1}{\|w\|} \min_i [y_i \cdot (w^T \cdot \Phi(x_i) + b)] \right\}$$

$$\arg \max_{w, b} \frac{1}{\|w\|} \quad (\text{搞定目标函数})$$

目标函数: $\max_{w,b} \frac{1}{\|w\|} \text{ 且 } y_i(w^T \cdot \Phi(x_i) + b) \geq 1$

转换成求最小值 $\min_{w,b} \frac{1}{2} w^2 \text{ 且 } y_i(w^T \cdot \Phi(x_i) + b) \geq 1$

拉格朗日乘子法标准格式:

$$\begin{array}{ll} \min & f(x) \\ \text{s.t.} & g_i(x) \leq 0, \quad i = 1, \dots, m \end{array}$$

拉格朗日乘子法

$$L(w, b, \alpha) = \frac{1}{2} \|w\|^2 - \sum_{i=1}^n \alpha_i (y_i (w^T \cdot \Phi(x_i) + b) - 1)$$

对偶问题:

$$\min_{w, b} \max_{\alpha} L(w, b, \alpha) \rightarrow \max_{\alpha} \min_{w, b} L(w, b, \alpha)$$

分别对w和b求偏导,分别得到两个条件

$$\frac{\partial L}{\partial w} = 0 \Rightarrow w = \sum_{i=1}^n \alpha_i y_i \Phi(x_n)$$

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

$$L(w, b, \alpha) = \frac{1}{2} \|w\|^2 - \sum_{i=1}^n \alpha_i (y_i (w^T \Phi(x_i) + b) - 1)$$

$$= \frac{1}{2} w^T w - w^T \sum_{i=1}^n \alpha_i y_i \Phi(x_i) - b \sum_{i=1}^n \alpha_i y_i + \sum_{i=1}^n \alpha_i$$

$$= \sum_{i=1}^n \alpha_i - \frac{1}{2} \left(\sum_{i=1}^n \alpha_i y_i \Phi(x_i) \right)^T \sum_{i=1}^n \alpha_i y_i \Phi(x_i)$$

$$= \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n \alpha_i \alpha_j y_i y_j \Phi^T(x_i) \Phi(x_j)$$

$$L(w, b, \alpha) = \frac{1}{2} \|w\|^2 - \sum_{i=1}^n \alpha_i (y_i (w^T \cdot \Phi(x_i) + b) - 1)$$



完成了第一步求解 $\min_{w,b} L(w, b, \alpha)$

$$\sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n \alpha_i \alpha_j y_i y_j \Phi^T(x_i) \Phi(x_j)$$

继续对 α 求极大值 $\max_{\alpha} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j (\Phi(x_i) \cdot \Phi(x_j))$

条件: $\sum_{i=1}^n \alpha_i y_i = 0$

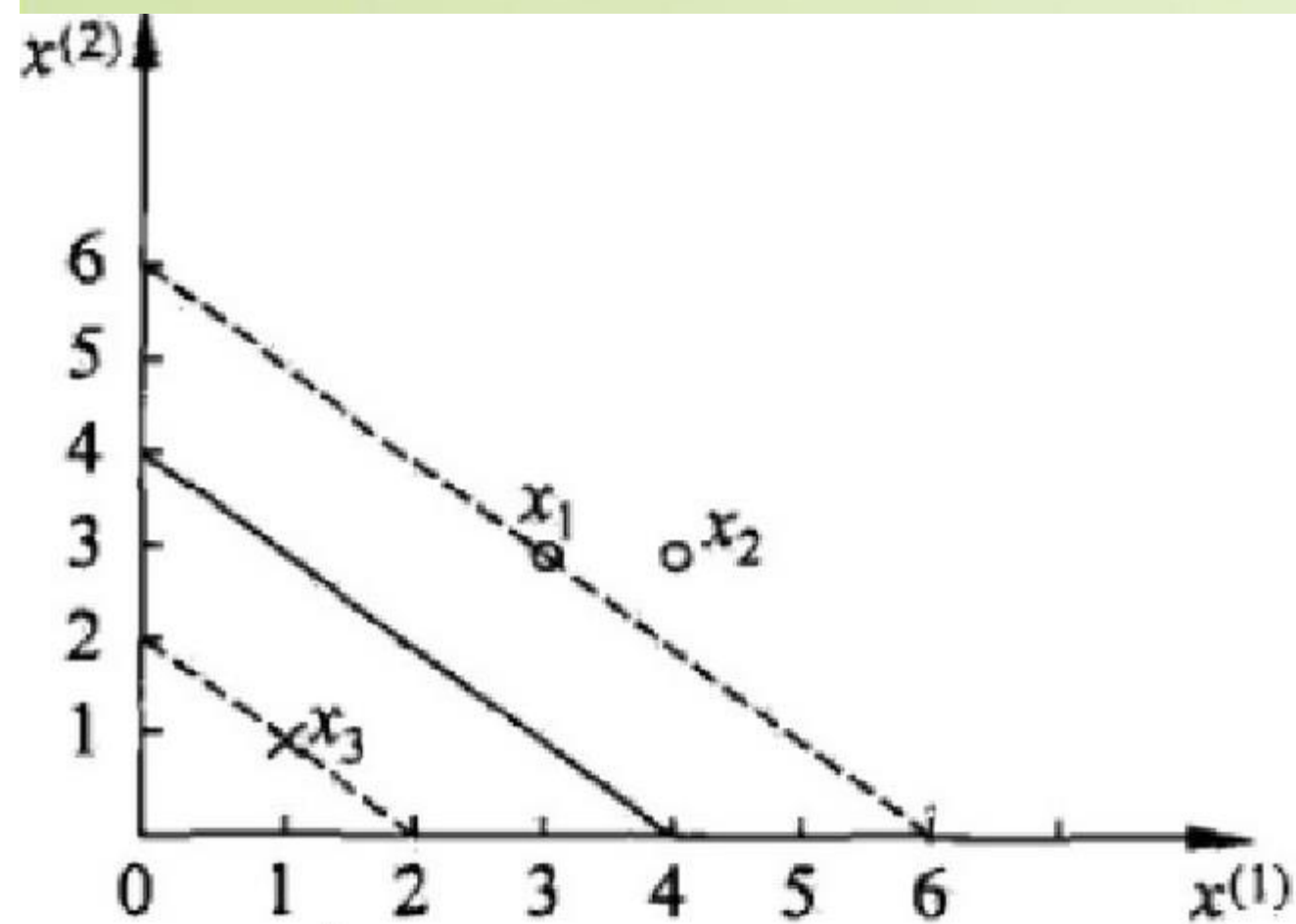
$$\alpha_i \geq 0;$$

极大值转换成求极小值 $\Rightarrow \min_{\alpha} \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j (\Phi(x_i) \cdot \Phi(x_j)) - \sum_{i=1}^n \alpha_i$

条件: $\sum_{i=1}^n \alpha_i y_i = 0$

$$\alpha_i \geq 0;$$

例1. 已知一个如图所示的训练数据集，其正例点是 $x_1 = (3,3)^T$ $x_2 = (4,3)^T$ ，负例点是 $x_3 = (1,1)^T$ ，试求最大间隔分离超平面。



样本: $x_1(3,3,1)$ $x_2(4,3,1)$ $x_3(1,1,1)$

求解: $\frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j (x_i \cdot x_j) - \sum_{i=1}^n \alpha_i$

$$\alpha_1 + \alpha_2 - \alpha_3 = 0$$

$$\alpha_i \geq 0, \quad i = 1, 2, 3$$

$$\frac{1}{2} (18\alpha_1^2 + 25\alpha_2^2 + 2\alpha_3^2 + 42\alpha_1\alpha_2 - 12\alpha_1\alpha_3 - 14\alpha_2\alpha_3) - \alpha_1 - \alpha_2 - \alpha_3$$

$$\frac{1}{2}(18\alpha_1^2 + 25\alpha_2^2 + 2\alpha_3^2 + 42\alpha_1\alpha_2 - 12\alpha_1\alpha_3 - 14\alpha_2\alpha_3) - \alpha_1 - \alpha_2 - \alpha_3$$

$$\alpha_1 + \alpha_2 = \alpha_3 \Rightarrow 4\alpha_1^2 + \frac{13}{2}\alpha_2^2 + 10\alpha_1\alpha_2 - 2\alpha_1 - 2\alpha_2$$

分别对参数进行求导得：
 $\alpha_1 = 1.5$
 $\alpha_2 = -1$ \Rightarrow 不满足条件 $\alpha_i \geq 0, i = 1, 2, 3$

最终的解应该为边界上的点 \Rightarrow $\alpha_1 = 0$
 $\alpha_2 = -2/13$ \Rightarrow 带入原式=-0.153

$\alpha_1 = 0.25$
 $\alpha_2 = 0$ \Rightarrow 带入原式=-0.25

最小值在(0.25,0,0.25)处取得

对于 α 值(0.25,0,0.25)

$$w^* = \sum_{i=1}^N \alpha_i^* y_i \Phi(x_i)$$



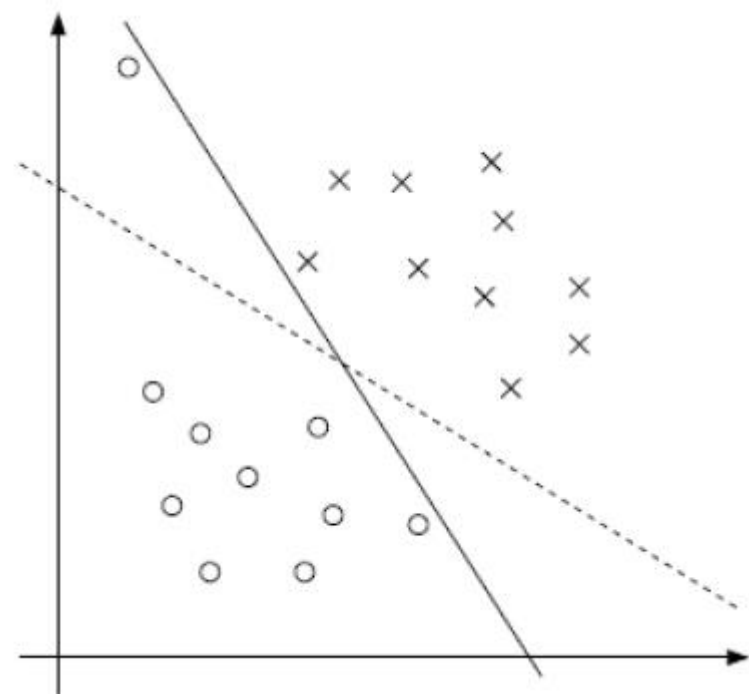
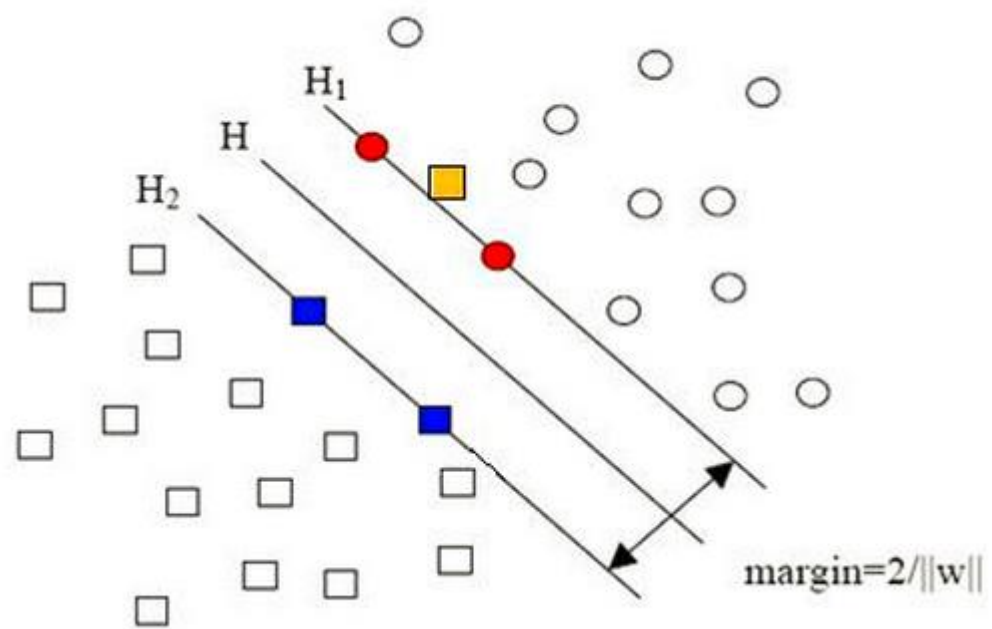
$$w_1 = w_2 = 0.5$$



$$b = -2$$

$$0.5x_1 + 0.5x_2 - 2 = 0$$

$$b^* = y_i - \sum_{i=1}^N \alpha_i^* y_i (\Phi(x_i) \cdot \Phi(x_j))$$



为了解决该问题，引入松弛因子

当C趋近于无穷大时：意味着分类严格不能有错误

当C趋近于很小的时：意味着可以有更大的错误容忍

$$y_i(w \cdot x_i + b) \geq 1 - \xi_i$$

目标函数： $\min \frac{1}{2} \|w\|^2 + C \sum_{i=1}^n \xi_i$

$$L(w, b, \xi, \alpha, \mu) \equiv \frac{1}{2} \|w\|^2 + C \sum_{i=1}^n \xi_i - \sum_{i=1}^n \alpha_i (y_i (w \cdot x_i + b) - 1 + \xi_i) - \sum_{i=1}^n \mu_i \xi_i$$



$$w = \sum_{i=1}^n \alpha_i y_i \phi(x_i)$$

$$0 = \sum_{i=1}^n \alpha_i y_i$$

$$C - \alpha_i - \mu_i = 0$$

帶入原式：

$$-\frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j (x_i \cdot x_j) + \sum_{i=1}^n \alpha_i$$

仍然求对偶问题

$$\sum_{i=1}^n \alpha_i y_i = 0$$

$$C - \alpha_i - \mu_i = 0$$

$$\alpha_i \geq 0$$

$$\mu_i \geq 0$$

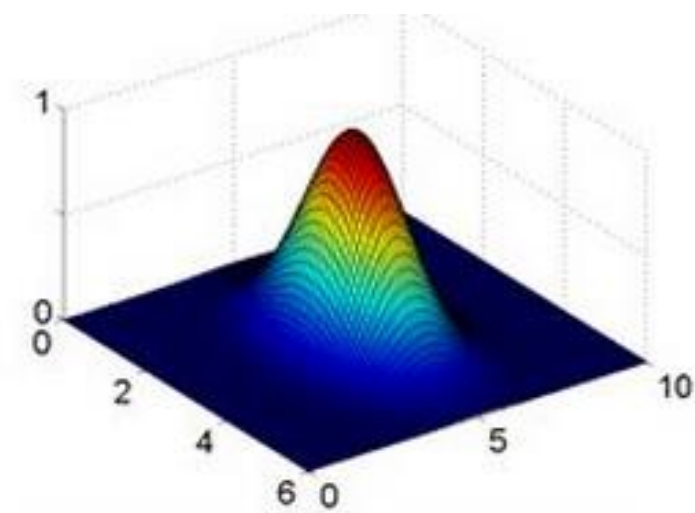
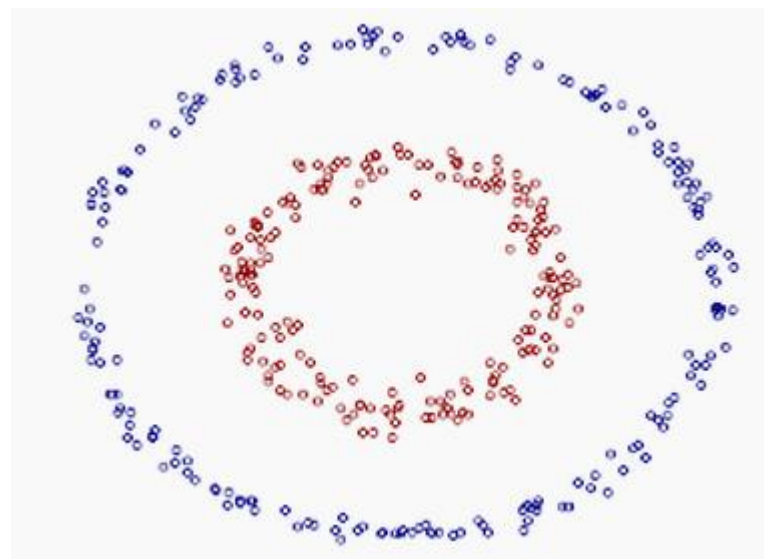
$$0 \leq \alpha_i \leq C$$



$$\min_{\alpha} \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j (x_i \cdot x_j) - \sum_{i=1}^n \alpha_i$$

$$\sum_{i=1}^n \alpha_i y_i = 0$$

$$0 \leq \alpha_i \leq C$$



还是先从小例子来阐述问题。假设我们有俩个数据， $x = (x_1, x_2, x_3)$; $y = (y_1, y_2, y_3)$ ，此时在3D空间已经不能对其经行线性划分了，那么我们通过一个函数将数据映射到更高维的空间，比如9维的话，那么 $f(x) = (x_1x_1, x_1x_2, x_1x_3, x_2x_1, x_2x_2, x_2x_3, x_3x_1, x_3x_2, x_3x_3)$ ，由于需要计算内积，所以在新的数据在9维空间，需要计算 $\langle f(x), f(y) \rangle$ 的内积，需要花费 $O(n^2)$ 。

在具体点，令 $x = (1, 2, 3)$; $y = (4, 5, 6)$ ，那么 $f(x) = (1, 2, 3, 2, 4, 6, 3, 6, 9)$ ， $f(y) = (16, 20, 24, 20, 25, 36, 24, 30, 36)$ ，

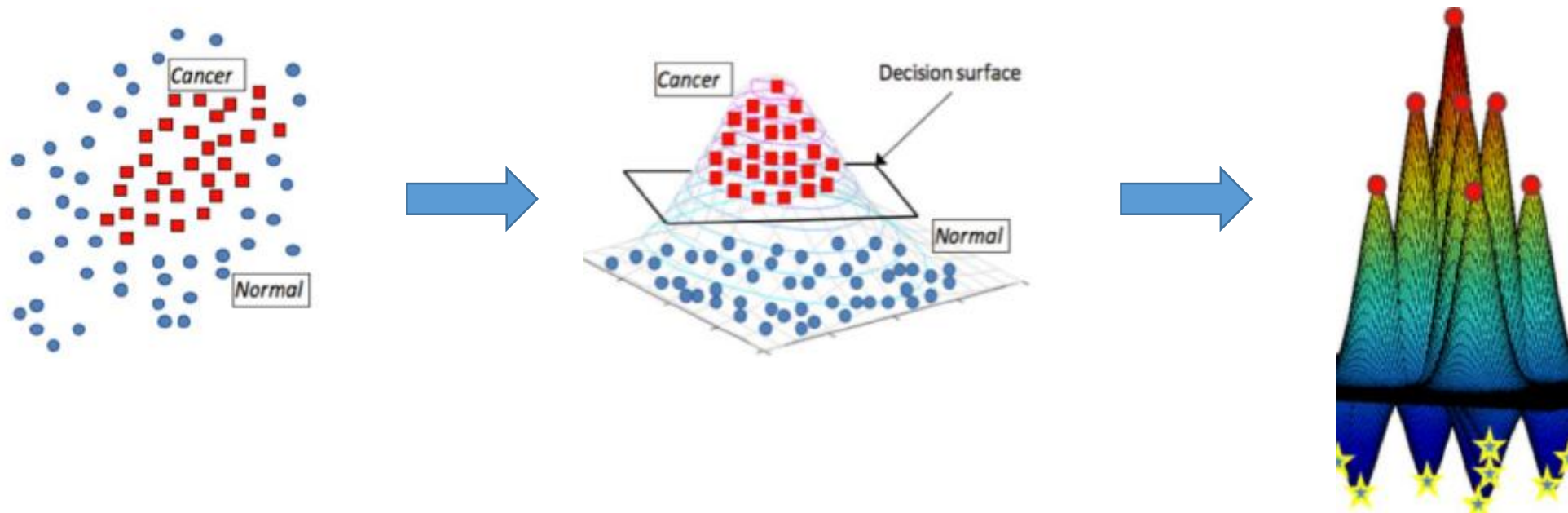
此时 $\langle f(x), f(y) \rangle = 16 + 40 + 72 + 40 + 100 + 180 + 72 + 180 + 324 = 1024$

似乎还能计算，但是如果将维数扩大到一个非常大数时候，计算起来可不是一丁点问题了。

但是发现， $K(x, y) = (\langle x, y \rangle)^2$

$K(x, y) = (4 + 10 + 18)^2 = 32^2 = 1024$

两者相等， $K(x, y) = (\langle x, y \rangle)^2 = \langle f(x), f(y) \rangle$ ，但是 $K(x, y)$ 计算起来却比 $\langle f(x), f(y) \rangle$ 简单的多，也就是说只要用 $K(x, y)$ 来计算，效果 and $\langle f(x), f(y) \rangle$ 是一样的，但是计算效率却大幅度提高了，如： $K(x, y)$ 是 $O(n)$ ，而 $\langle f(x), f(y) \rangle$ 是 $O(n^2)$ 。所以使用核函数的好处就是，可以在一个低维空间去完成高维度（或者无限维度）样本内积的计算，比如 $K(x, y) = (4 + 10 + 18)^2$ 的3D空间对比 $\langle f(x), f(y) \rangle = 16 + 40 + 72 + 40 + 100 + 180 + 72 + 180 + 324$ 的9D空间。



高斯核函数:

$$K(X, Y) = \exp \left\{ -\frac{\|X - Y\|^2}{2\sigma^2} \right\}$$