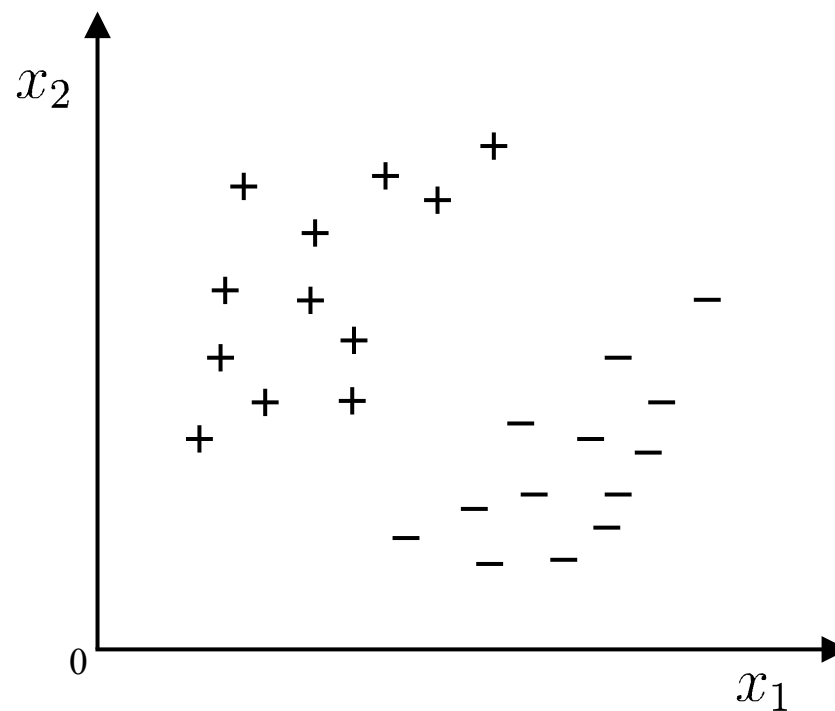


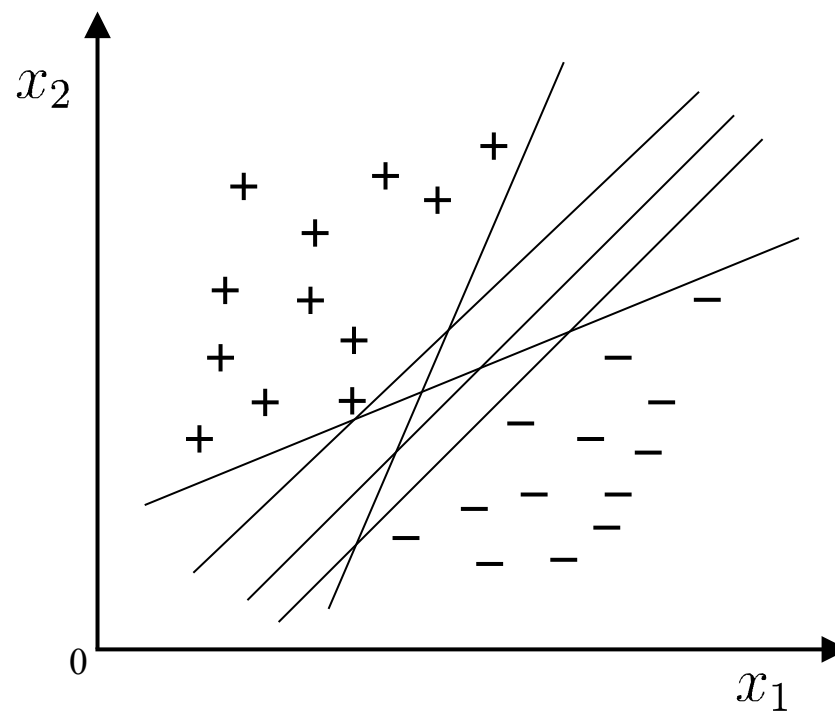


# 二分类问题 Binary Classification



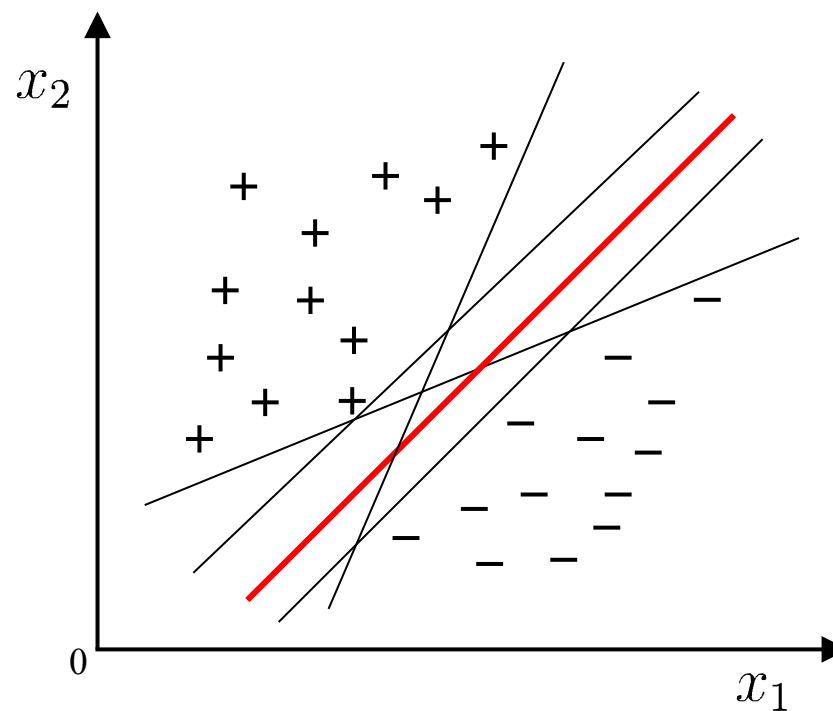
Question: Find a hyperplane in the sample space to separate samples of different categories.

# 二分类问题 Binary Classification



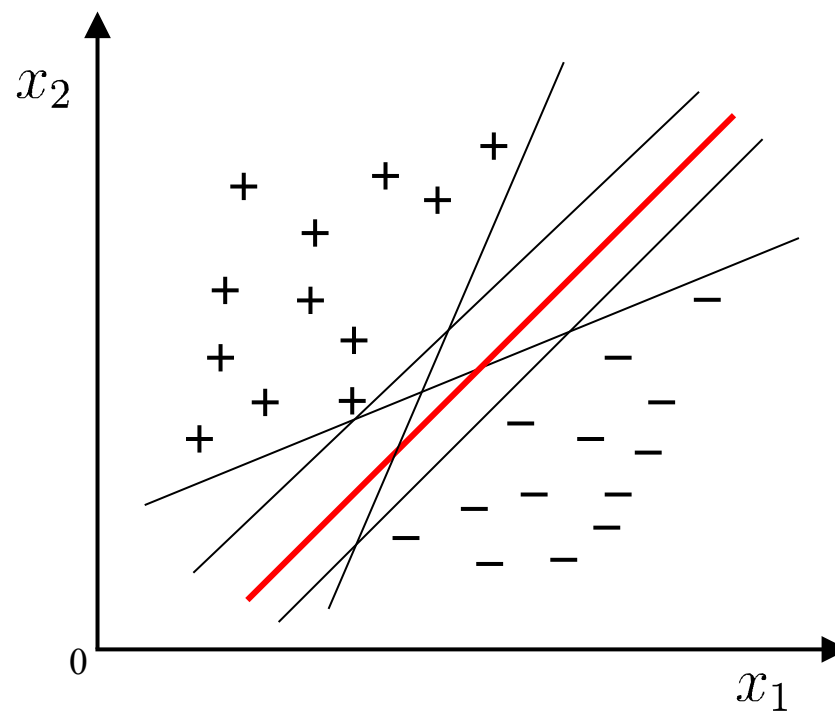
Question: Find a hyperplane in the sample space to separate samples of different categories.

# 二分类问题 Binary Classification



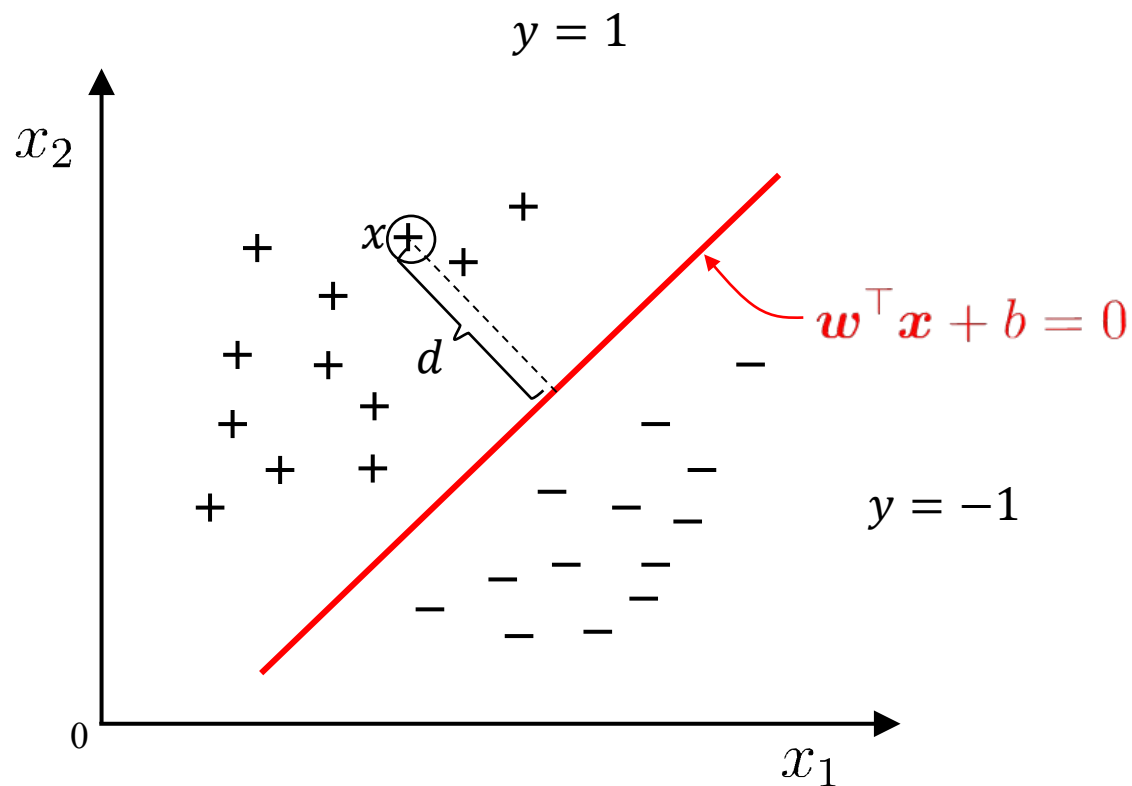
Question: Find a hyperplane in the sample space to separate samples of different categories.

# 二分类问题 Binary Classification



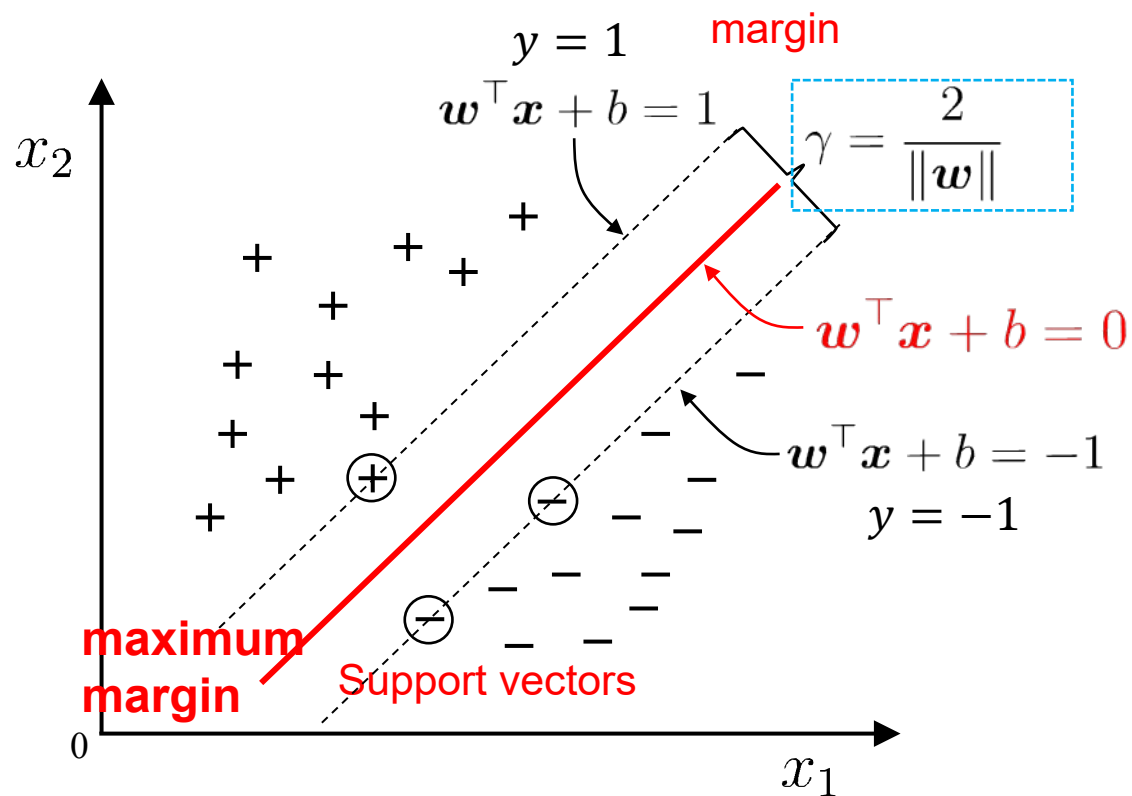
It should choose "**right in the middle**", with good tolerance, high robustness and the strongest generalization ability

# 支持向量机 Support Vector Machine

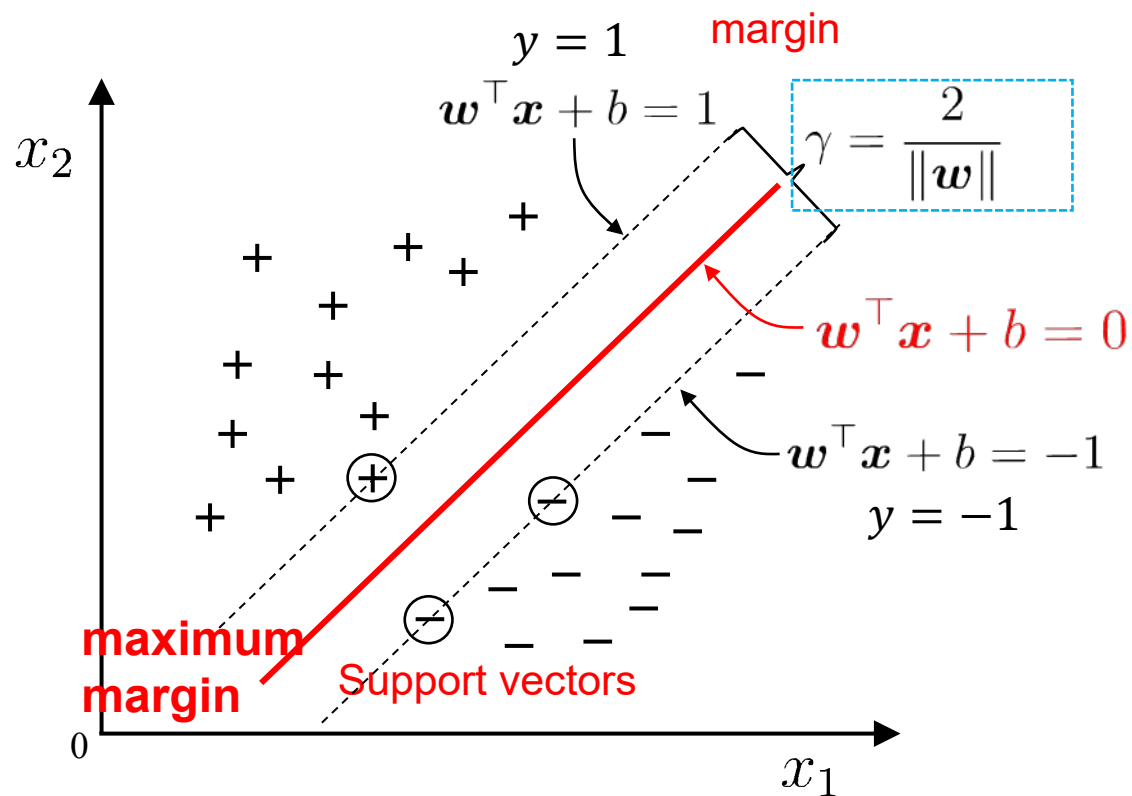


$$d = \frac{|w^T x + b|}{||w||}$$

# 支持向量机 Support Vector Machine



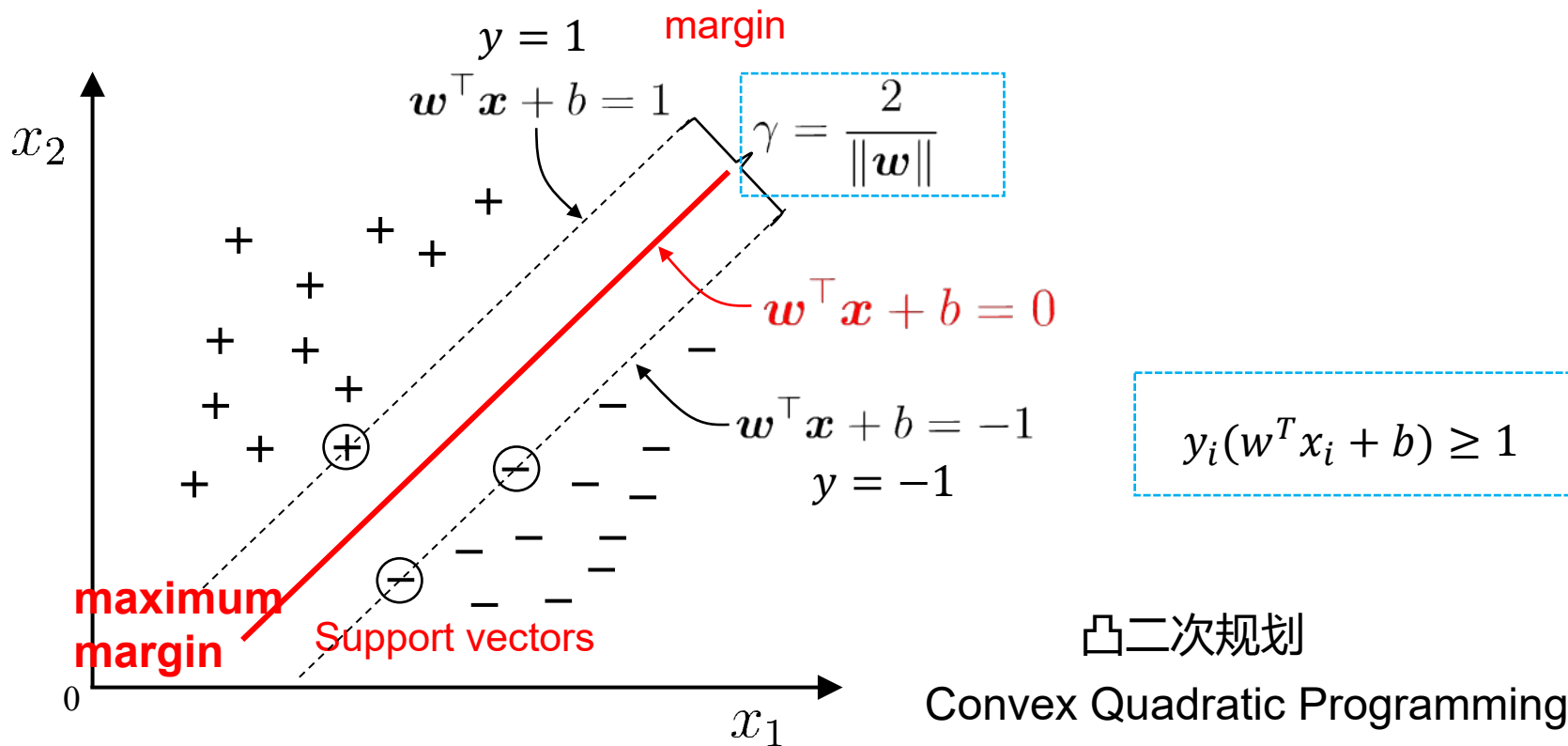
# 支持向量机 Support Vector Machine



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



# 支持向量机 Support Vector Machine



$$\begin{aligned} \arg \max_{w,b} \quad & \frac{2}{\|w\|} \quad \longrightarrow \quad \arg \min_{w,b} \quad \frac{1}{2} \|w\|^2 \\ \text{s.t.} \quad & y_i(w^T x_i + b) \geq 1, \quad i = 1, 2, \dots, m. \end{aligned}$$

# 对偶问题 Dual problem

在数学和优化领域中，对偶问题是与原始优化问题（原始问题）相对应的一个问题。通常，对偶问题是通过原始问题的一种变换来构建的，它可以帮助我们更好地理解原始问题的性质，提供额外的信息，或者用于求解原始问题。

- 对于最小化问题（Minimization Problem）：对偶问题：  $\max g(\lambda, v)$  其中，  $g(\lambda, v) = \inf_x L(x, \lambda, v)$ ，表示对于给定  $L(x, \lambda, v)$  的最小值
- 对于最大化问题（Maximization Problem）：对偶问题：  $\min g(\lambda, v)$  其中，  $g(\lambda, v) = \sup_x L(x, \lambda, v)$ ，表示对于给定  $L(x, \lambda, v)$  的最大值

在这里：

- $\lambda$  和  $v$  是对偶变量（Lagrange Multipliers），它们对应于原始问题的约束条件。
- $L(x, \lambda, v)$  是称为拉格朗日函数（Lagrangian Function）的函数，它由原始问题的目标函数和约束条件组成，通常形式为：

$$L(x, \lambda, v) = \text{目标函数} - \lambda^T \cdot (\text{不等式约束}) - v^T \cdot (\text{等式约束})$$

通过求解对偶问题，我们可以获得原始问题的最优值的一个下界或上界。

# 拉格朗日乘数法的例子

- **问题：**假设你需要在平面上找到距离原点最近的点，但这个点必须位于直线  $y=2x+3$  上。
- **解决方法：**

# 拉格朗日乘数法的例子

- **问题：**假设你需要在平面上找到距离原点最近的点，但这个点必须位于直线  $y=2x+3$  上。
- **解决方法：**
  1. **目标函数：**需要最小化的目标函数是到原点的距离的平方， $f(x, y) = x^2 + y^2$ 。
  2. **约束：**点必须位于  $y=2x+3$  上，因此约束条件为  $g(x, y) = y - 2x - 3 = 0$ 。
  3. **构建拉格朗日函数：**构建拉格朗日函数  $L(x, y, \lambda) = x^2 + y^2 + \lambda (y - 2x - 3)$ 。
  4. **求解：**通过  $L(x, y, \lambda)$  关于  $x, y, \lambda$  的偏导数求解并置为零，可以得到最优解。

# KKT (Karush-Kuhn-Tucker) 条件的例子



- **问题：**假设你需要在一个盒子中放置最大体积的长方体，但其长、宽、高的和不能超过某个值，例如10
- **解决方法：**



# KKT (Karush-Kuhn-Tucker) 条件的例子

- **问题：**假设你需要在一个盒子中放置最大体积的长方体，但其长、宽、高的和不能超过某个值，例如10
- **解决方法：**
  1. **目标函数：**最大化长方体的体积，即  $f(x,y,z)=xyz$ 。
  2. **约束：**长、宽、高的和不超过10，即  $g(x,y,z)=x+y+z-10\leq 0$ 。  
这是一个不等式约束。
  3. **构建拉格朗日函数：**拉格朗日函数  $L(x,y,z,\lambda)$  结合了目标函数和约束条件，通过引入拉格朗日乘子  $\lambda$ ：  
$$L(x,y,\lambda)=xyz-\lambda(x+y+z-10)$$

# KKT (Karush-Kuhn-Tucker) 条件的例子



$$L(x, y, \lambda) = xyz - \lambda(x + y + z - 10)$$

## 4. 应用KKT条件

- **梯度为零**：对  $L(x, y, z, \lambda)$  对  $x, y, z, \lambda$  的偏导数应为零。

$$\bullet \quad \frac{\partial L}{\partial x} = yz - \lambda = 0 \quad \frac{\partial L}{\partial y} = xz - \lambda = 0 \quad \frac{\partial L}{\partial z} = xy - \lambda = 0$$

$$\bullet \quad \frac{\partial L}{\partial \lambda} = -x - y - z + 10 = 0$$

- **约束条件**：  $x + y + z \leq 10$ 。
- **拉格朗日乘子非负**：  $\lambda \geq 0$ 。
- **互补松弛性**：  $\lambda(x + y + z - 10) = 0$ 。

5. **求解**：通过解上述方程组，我们可以找到满足约束的最优解。

# 最优超平面求解

## Optimal hyperplane Solution

- Using Lagrangian Multiplier Method and KKT Condition to solve the Optimal Value

$$\begin{aligned} \arg \min_{\mathbf{w}, b} \quad & \frac{1}{2} \|\mathbf{w}\|^2 \\ \text{s.t.} \quad & y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1, \quad i = 1, 2, \dots, m. \end{aligned}$$

- Integrated into: (Where  $\alpha_i \geq 0$  is a Lagrangian multiplier)

$$L(\mathbf{w}, b, \alpha) = \frac{1}{2} \|\mathbf{w}\|^2 + \sum_{i=1}^m \alpha_i (1 - y_i(\mathbf{w}^\top \mathbf{x}_i + b))$$

- Let the partial derivative=0

$$\frac{\partial L(\mathbf{w}, b, \alpha)}{\partial \mathbf{w}} = \mathbf{w} - \sum_{i=1}^m \alpha_i y_i \mathbf{x}_i = 0 \quad \frac{\partial L(\mathbf{w}, b, \alpha)}{\partial b} = \sum_{i=1}^m \alpha_i y_i = 0$$

- then

$$\mathbf{w} = \sum_{i=1}^m \alpha_i y_i \mathbf{x}_i, \quad \sum_{i=1}^m \alpha_i y_i = 0.$$



# 最优超平面求解 Optimal hyperplane Solution

$$\begin{aligned}
 L(w, b, a) &= \frac{1}{2} \|w\|^2 + \sum_{i=1}^m \alpha_i (1 - y_i(w^T x_i + b)) \\
 &= \frac{1}{2} w^T w - \sum_{i=1}^m \alpha_i y_i w^T x_i - b \sum_{i=1}^m \alpha_i y_i + \sum_{i=1}^m \alpha_i \\
 &= \frac{1}{2} w^T \sum_{i=1}^m \alpha_i y_i x_i - \sum_{i=1}^m \alpha_i y_i w^T x_i + \sum_{i=1}^m \alpha_i \\
 &= \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i=1}^m \alpha_i y_i w^T x_i
 \end{aligned}$$

Dual problem:

$$\begin{aligned}
 \max_a \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j y_i y_j x_i^T x_j &= \min_a \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j y_i y_j x_i^T x_j - \sum_{i=1}^m \alpha_i \\
 \text{s.t. } \sum_{i=1}^m \alpha_i y_i &= 0, \alpha_i \geq 0, i = 1, 2, \dots, m
 \end{aligned}$$

KKT Condition

Obtain the optima  $\alpha$  (SMO, Sequential Minimal Optimization) algorithm

The optimal solution can be obtained

$$f(x) = w^T x + b = \sum_{i=1}^m \alpha_i y_i x_i^T x + b$$

$$\begin{cases} \alpha_i \geq 0, \\ y_i f(x_i) \geq 1, \\ \alpha_i (y_i f(x_i) - 1) = 0. \end{cases}$$

$y_i f(x_i) > 1 \implies \alpha_i = 0$   
 $\alpha_i > 0 \implies y_i f(x_i) = 1$

# 最优超平面求解

## Optimal hyperplane Solution



$$\begin{aligned} L(w, b, a) &= \frac{1}{2} \|w\|^2 + \sum_{i=1}^m \alpha_i (1 - y_i (w^T x_i + b)) \\ &= \frac{1}{2} w^T w - \sum_{i=1}^m \alpha_i y_i w^T x_i - b \sum_{i=1}^m \alpha_i y_i + \sum_{i=1}^m \alpha_i \\ &= \frac{1}{2} w^T \sum_{i=1}^m \alpha_i y_i x_i - \sum_{i=1}^m \alpha_i y_i w^T x_i + \sum_{i=1}^m \alpha_i \\ &= \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i=1}^m \alpha_i y_i w^T x_i \end{aligned}$$

Dual problem:

$$\begin{aligned} \max_a \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j y_i y_j x_i^T x_j &= \min_a \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j y_i y_j x_i^T x_j - \sum_{i=1}^m \alpha_i \\ \text{s.t. } \sum_{i=1}^m \alpha_i y_i &= 0, \alpha_i \geq 0, i = 1, 2, \dots, m \end{aligned}$$

KKT Condition

Obtain the optima  $\alpha$  (SMO, Sequential Minimal Optimization) algorithm

The optimal solution can be obtained

$$f(x) = w^T x + b = \sum_{i=1}^m \alpha_i y_i x_i^T x + b$$

$$\begin{cases} \alpha_i \geq 0, \\ y_i f(\mathbf{x}_i) \geq 1, \\ \alpha_i (y_i f(\mathbf{x}_i) - 1) = 0. \end{cases}$$

$$\begin{aligned} y_i f(\mathbf{x}_i) > 1 &\implies \alpha_i = 0 \\ \alpha_i > 0 &\implies y_i f(\mathbf{x}_i) = 1 \end{aligned}$$

# 最优超平面求解

## Optimal hyperplane Solution



$$\begin{aligned}
 L(w, b, a) &= \frac{1}{2} \|w\|^2 + \sum_{i=1}^m \alpha_i (1 - y_i(w^T x_i + b)) \\
 &= \frac{1}{2} w^T w - \sum_{i=1}^m \alpha_i y_i w^T x_i - b \sum_{i=1}^m \alpha_i y_i + \sum_{i=1}^m \alpha_i \\
 &= \frac{1}{2} w^T \sum_{i=1}^m \alpha_i y_i x_i - b \sum_{i=1}^m \alpha_i y_i + \sum_{i=1}^m \alpha_i \\
 &= \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i=1}^m \alpha_i (w^T x_i + b - 1)
 \end{aligned}$$

Dual problem:

$$\max_a \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j y_i y_j x_i^T x_j$$

$$\text{s.t. } \sum_{i=1}^m \alpha_i = 1$$

若  $\alpha_i = 0$ , 则该样本将不会在左式的求和中出现, 也就不会对  $f(x)$  有任何影响;  
若  $\alpha_i > 0$ , 则必有  $f(x_i) = 1$ , 所对应的样本点位于最大间隔边界上, 是一个支持向量。

这显示出支持向量机的一个重要性质: 训练完成后, 大部分的训练样本都不需保留, 最终模型仅与支持向量有关。

Obtain the optima  $\alpha$  (SMO, Sequential Minimal Optimization) algorithm

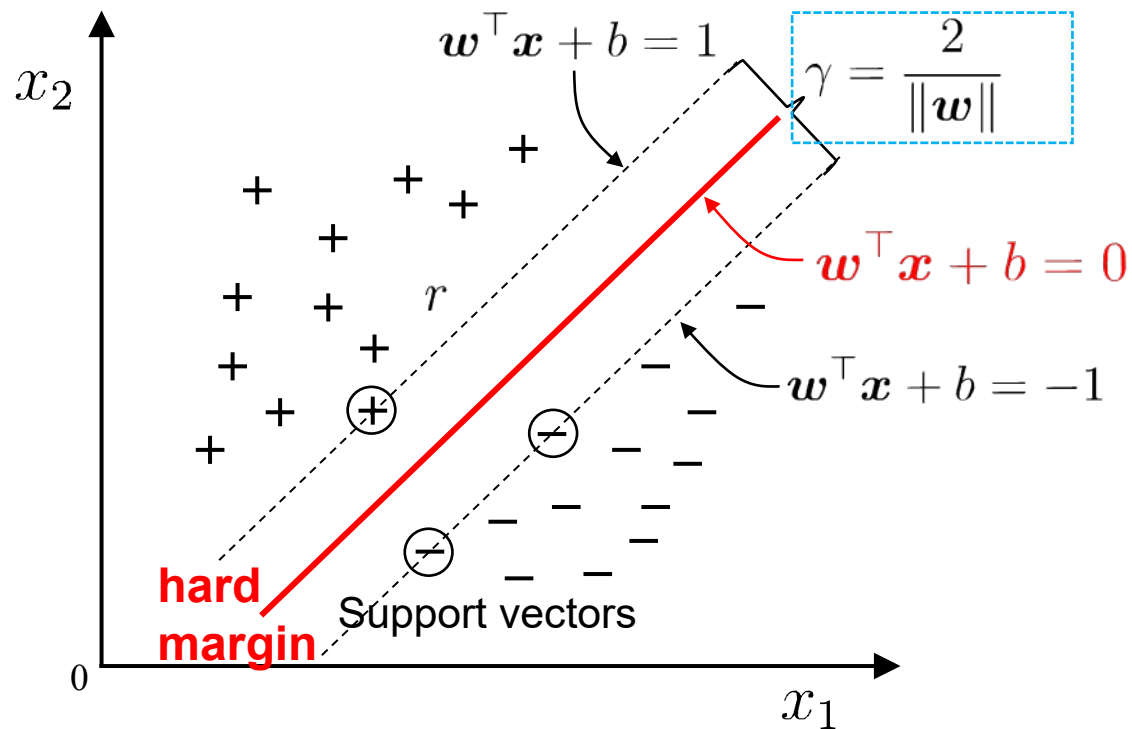
The optimal solution can be obtained

$$f(x) = w^T x + b = \sum_{i=1}^m \alpha_i y_i x_i^T x + b$$

$$\begin{cases} \alpha_i \geq 0, \\ y_i f(x_i) \geq 1, \\ \alpha_i (y_i f(x_i) - 1) = 0. \end{cases}$$

$$\begin{aligned}
 y_i f(x_i) > 1 &\longrightarrow \alpha_i = 0 \\
 \alpha_i > 0 &\longrightarrow y_i f(x_i) = 1
 \end{aligned}$$

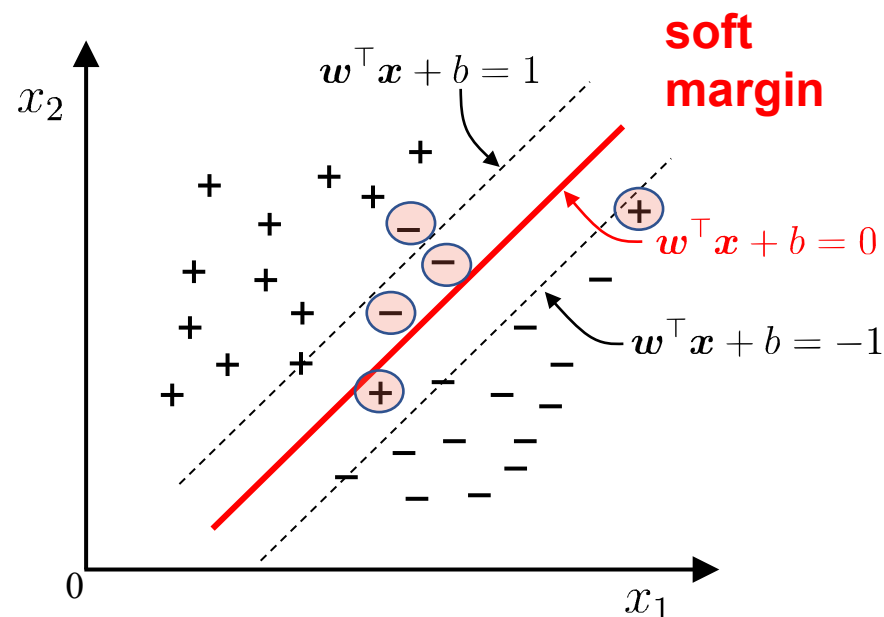
# 支持向量机 Support Vector Machine



$$\begin{aligned} \arg \max_{w,b} \quad & \frac{2}{\|w\|} \quad \longrightarrow \quad \arg \min_{w,b} \quad \frac{1}{2} \|w\|^2 \\ \text{s.t.} \quad & y_i(w^T x_i + b) \geq 1, \quad i = 1, 2, \dots, m. \end{aligned}$$

# 软间隔 Soft Margin

- Q: It is difficult to determine a linearly separable hyperplane in the feature space; At the same time, it is difficult to determine whether a linearly separable result is caused by over fitting
- A: The concept of "soft margin" is introduced to allow the support vector machine to not meet the constraints on some samples



# 软间隔支持向量机 Soft Margin Support Vector Machine

The slack variable  $\varepsilon$  can be introduced :

$$\min_{w,b} \frac{1}{2} \|w\|_2^2 + C \sum_i \varepsilon_i \quad \text{s.t.} \quad y_i(w^T x_i + b) \geq 1 - \varepsilon_i$$
$$\varepsilon_i \geq 0, i=1,2,\dots,m$$

Integrated into: (Where  $\alpha_i$  ,  $\varepsilon_i$  are Lagrangian multipliers)

$$L(w, b, a, \varepsilon, \mu) = \frac{1}{2} \|w\|^2 + C \sum_{i=1}^m \varepsilon_i + \sum_{i=1}^m \alpha_i (1 - \varepsilon_i - y_i(w^T x_i + b)) - \sum_{i=1}^m \mu_i \varepsilon_i$$

Let the partial derivative=0

$$\frac{\partial L(w, b, a, \varepsilon, \mu)}{\partial w} = w - \sum_{i=1}^m \alpha_i y_i x_i = 0 \quad \frac{\partial L(w, b, a, \varepsilon, \mu)}{\partial b} = \sum_{i=1}^m \alpha_i y_i = 0$$

$$\frac{\partial L(w, b, a, \varepsilon, \mu)}{\partial \varepsilon_i} = C - \alpha_i - \mu_i = 0$$

The slack variable  $\varepsilon$  can be introduced :

$$\min_{w,b} \frac{1}{2} \|w\|_2^2 + C \sum_i \varepsilon_i \quad \text{s.t.} \quad y_i(w^T x_i + b) \geq 1 - \varepsilon_i$$
$$\varepsilon_i \geq 0, i=1,2,\dots,m$$

Integrated into: (Where  $\alpha_i$  ,  $\varepsilon_i$  are Lagrangian multipliers)

$$L(w, b, a, \varepsilon, \mu) = \frac{1}{2} \|w\|^2 + C \sum_{i=1}^m \varepsilon_i + \sum_{i=1}^m \alpha_i (1 - \varepsilon_i - y_i(w^T x_i + b)) - \sum_{i=1}^m \mu_i \varepsilon_i$$

Let the partial derivative=0

then

$$w = \sum_{i=1}^m \alpha_i y_i x_i \quad \sum_{i=1}^m \alpha_i y_i = 0$$

$$C = \alpha_i + \mu_i$$

# 软间隔支持向量机 Soft Margin Support Vector Machine

The slack variable  $\varepsilon$  can be introduced :

$$\min_{w,b} \frac{1}{2} \|w\|_2^2 + C \sum_i \varepsilon_i \quad \text{s.t.} \quad y_i(w^T x_i + b) \geq 1 - \varepsilon_i$$

$$\varepsilon_i \geq 0, i=1,2,\dots,m$$

Integrated into: (Where  $\alpha_i$ ,  $\varepsilon_i$  are Lagrangian multipliers)

$$L(w, b, a, \varepsilon, \mu) = \frac{1}{2} \|w\|^2 + C \sum_{i=1}^m \varepsilon_i + \sum_{i=1}^m \alpha_i (1 - \varepsilon_i - y_i(w^T x_i + b)) - \sum_{i=1}^m \mu_i \varepsilon_i$$

Dual problem:

$$\max_a \sum_{i=1}^m \alpha_i - \sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j y_i y_j x_i^T x_j \quad \text{s.t.} \quad \sum_{i=1}^m \alpha_i y_i = 0, \quad C \geq \alpha_i \geq 0, i = 1, 2, \dots, m$$

Obtain the optima  $\alpha$  (SMO, Sequential Minimal Optimization) algorithm

The optimal solution can be obtained

$$f(x) = w^T x + b = \sum_{i=1}^m \alpha_i y_i x_i^T x + b$$

KKT Condition

$$\begin{cases} \alpha_i \geq 0, \mu_i \geq 0 \\ y_i f(x_i) - 1 + \varepsilon_i \geq 0 \\ \alpha_i (y_i f(x_i) - 1 + \varepsilon_i) = 0 \\ \varepsilon_i \geq 0, \mu_i \varepsilon_i = 0 \end{cases}$$



# 软间隔支持向量机 Soft Margin Support Vector Machine

对任意训练样本, 总有  $\alpha_i = 0$  或  $y_i f(x_i) = 1 - \varepsilon_i$

若  $\alpha_i = 0$ , 则该样本将不会在左式的求和中出现, 也就不会对  $f(x)$  有任何影响;

若  $\alpha_i > 0$ , 则必有  $y_i f(x_i) = 1 - \varepsilon_i$ , 即该样本是一个支持向量。

若  $\alpha_i < C$ , 则  $\mu_i > 0$ , 进而有  $\varepsilon_i = 0$ , 即该样本恰在最大间隔边界上;

若  $\alpha_i = C$ , 则有  $\mu_i = 0$ , 此时若  $\varepsilon_i \leq 1$ , 则该样本落在最大间隔内部; 若  $\varepsilon_i > 1$  则该样本被错误分类。

由此可看出软间隔支持向量机的最终模型仅与支持向量有关, 仍保持了稀疏性。

$$f(x) = w^T x + b = \sum_{i=1}^m \alpha_i y_i x_i^T x + b$$

$$+ b) \geq 1 - \varepsilon_i$$

$$i=1,2,\dots,m$$

$$(w^T x_i + b) - \sum_{i=1}^m \mu_i \varepsilon_i$$

$$C \geq \alpha_i \geq 0, i = 1, 2, \dots, m$$

KKT Condition

$$\begin{cases} \alpha_i \geq 0, \mu_i \geq 0 \\ y_i f(x_i) - 1 + \varepsilon_i \geq 0 \\ \alpha_i (y_i f(x_i) - 1 + \varepsilon_i) = 0 \\ \varepsilon_i \geq 0, \mu_i \varepsilon_i = 0 \end{cases}$$

# 软间隔支持向量机 Soft Margin Support Vector Machine

The slack variable  $\varepsilon$  can be introduced :

$$\min_{w,b} \frac{1}{2} \|w\|_2^2 + C \sum_i \varepsilon_i \quad \text{s.t.} \quad y_i(w^T x_i + b) \geq 1 - \varepsilon_i$$

Dual Problem:

$$\begin{aligned} \max_a \quad & \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j y_i y_j x_i^T x_j = \min_a \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j y_i y_j x_i^T x_j - \sum_{i=1}^m \alpha_i \\ \text{s.t.} \quad & \sum_{i=1}^m \alpha_i y_i = 0, C \geq \alpha_i \geq 0, i = 1, 2, \dots, m \end{aligned}$$

# 最优超平面求解

## Optimal hyperplane Solution

$$\begin{aligned}
 L(w, b, a) &= \frac{1}{2} \|w\|^2 + \sum_{i=1}^m \alpha_i (1 - y_i(w^T x_i + b)) \\
 &= \frac{1}{2} w^T w - \sum_{i=1}^m \alpha_i y_i w^T x_i - b \sum_{i=1}^m \alpha_i y_i + \sum_{i=1}^m \alpha_i \\
 &= \frac{1}{2} w^T \sum_{i=1}^m \alpha_i y_i x_i - \sum_{i=1}^m \alpha_i y_i w^T x_i + \sum_{i=1}^m \alpha_i \\
 &= \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i=1}^m \alpha_i y_i w^T x_i
 \end{aligned}$$

Dual problem:

$$\begin{aligned}
 \max_a \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j y_i y_j x_i^T x_j &= \min_a \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j y_i y_j x_i^T x_j - \sum_{i=1}^m \alpha_i \\
 \text{s.t. } \sum_{i=1}^m \alpha_i y_i &= 0, \alpha_i \geq 0, i = 1, 2, \dots, m
 \end{aligned}$$

KKT Condition

Obtain the optima  $\alpha$  (SMO, Sequential Minimal Optimization) algorithm

The optimal solution can be obtained

$$f(x) = w^T x + b = \sum_{i=1}^m \alpha_i y_i x_i^T x + b$$

$$\begin{cases} \alpha_i \geq 0, \\ y_i f(x_i) \geq 1, \\ \alpha_i (y_i f(x_i) - 1) = 0. \end{cases}$$

$y_i f(x_i) > 1 \implies \alpha_i = 0$   
 $\alpha_i > 0 \implies y_i f(x_i) = 1$

# 软间隔支持向量机 Soft Margin Support Vector Machine

The slack variable  $\varepsilon$  can be introduced :

$$\min_{w,b} \frac{1}{2} \|w\|_2^2 + C \sum_i \varepsilon_i \quad \text{s.t.} \quad y_i(w^T x_i + b) \geq 1 - \varepsilon_i$$

Dual Problem:

$$\begin{aligned} \max_a \quad & \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j y_i y_j x_i^T x_j = \min_a \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j y_i y_j x_i^T x_j - \sum_{i=1}^m \alpha_i \\ \text{s.t.} \quad & \sum_{i=1}^m \alpha_i y_i = 0, \quad C \geq \alpha_i \geq 0, i = 1, 2, \dots, m \end{aligned}$$

# 软间隔支持向量机 Soft Margin Support Vector Machine

The slack variable  $\varepsilon$  can be introduced :

$$\min_{w,b} \frac{1}{2} \|w\|_2^2 + C \sum_i \varepsilon_i \quad \text{s.t. } y_i(w^T x_i + b) \geq 1 - \varepsilon_i$$

在软间隔SVM中，引入正则化参数C控制了对分类错误的惩罚。

较小的C值会导致更大的间隔，容忍更多的分类错误，从而提高模型的容错性；

较大的C值会更强调正确分类，但可能导致对异常点更敏感。

$$\min_a \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j y_i y_j x_i^T x_j - \sum_{i=1}^m \alpha_i$$

$$C \geq \alpha_i \geq 0, i = 1, 2, \dots, m$$

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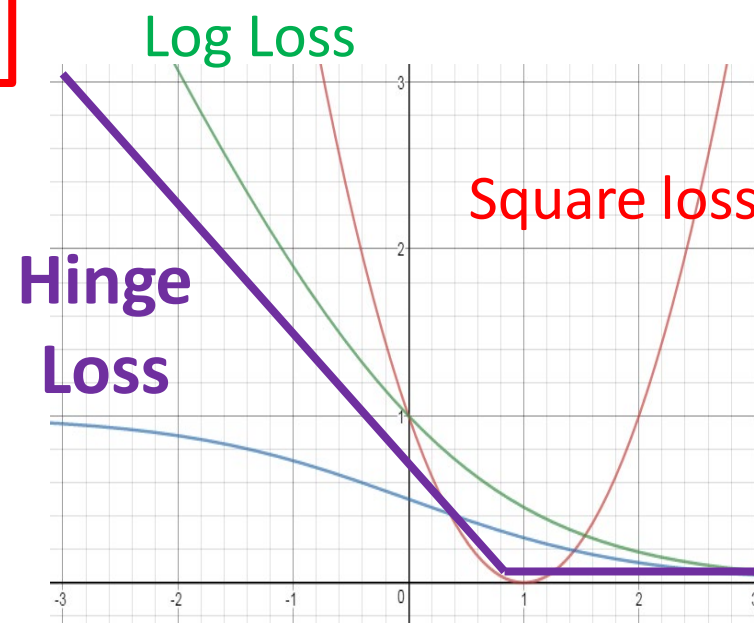


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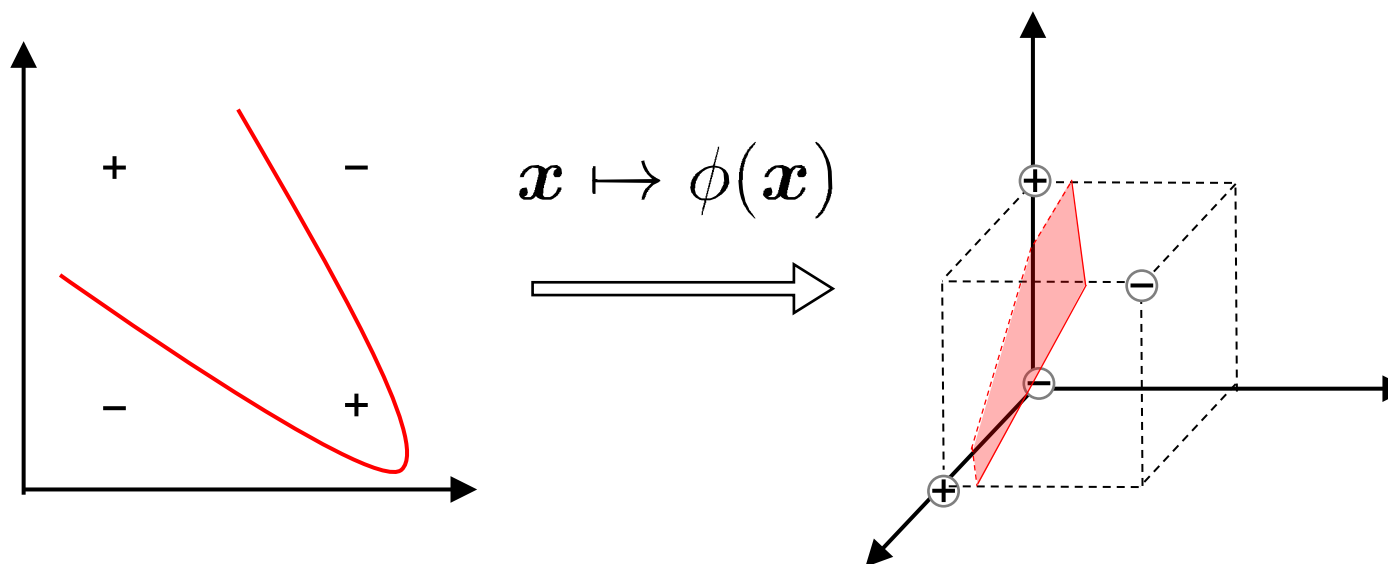
Hinge Loss function



# 线性不可分 linearly Inseparable Problem

-Q: What if there is no hyperplane that can correctly divide two types of samples?

-A: The samples are mapped from the original space to a higher dimensional feature space, making the samples linearly separable in this feature space



# 最优超平面求解

## Optimal hyperplane Solution

$$\begin{aligned}
 L(w, b, a) &= \frac{1}{2} \|w\|^2 + \sum_{i=1}^m \alpha_i (1 - y_i (w^T x_i + b)) \\
 &= \frac{1}{2} w^T w - \sum_{i=1}^m \alpha_i y_i w^T x_i - b \sum_{i=1}^m \alpha_i y_i + \sum_{i=1}^m \alpha_i \\
 &= \frac{1}{2} w^T \sum_{i=1}^m \alpha_i y_i x_i - \sum_{i=1}^m \alpha_i y_i w^T x_i + \sum_{i=1}^m \alpha_i \\
 &= \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i=1}^m \alpha_i y_i w^T x_i
 \end{aligned}$$

Dual problem:

$$\begin{aligned}
 \max_a \sum_{i=1}^m \alpha_i - \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j y_i y_j x_i^T x_j &= \min_a \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j y_i y_j x_i^T x_j - \sum_{i=1}^m \alpha_i \\
 \text{s.t. } \sum_{i=1}^m \alpha_i y_i &= 0, \alpha_i \geq 0, i = 1, 2, \dots, m
 \end{aligned}$$

KKT Condition

Obtain the optima  $\alpha$  (SMO, Sequential Minimal Optimization) algorithm  
The optimal solution can be obtained

$$f(x) = w^T x + b = \sum_{i=1}^m \alpha_i y_i x_i^T x + b$$

$$\begin{cases} \alpha_i \geq 0, \\ y_i f(\mathbf{x}_i) \geq 1, \\ \alpha_i (y_i f(\mathbf{x}_i) - 1) = 0. \end{cases}$$

$y_i f(\mathbf{x}_i) > 1 \implies \alpha_i = 0$   
 $\alpha_i > 0 \implies y_i f(\mathbf{x}_i) = 1$

# 核支持向量机 Kernel SVM

sample  $\mathbf{x} \mapsto \phi(\mathbf{x})$ , then the hyperplane  $f(\mathbf{x}) = \mathbf{w}^\top \phi(\mathbf{x}) + b$

Original question:

$$\begin{aligned} \min_{\mathbf{w}, b} \quad & \frac{1}{2} \|\mathbf{w}\|^2 \\ \text{s.t.} \quad & y_i(\mathbf{w}^\top \phi(\mathbf{x}_i) + b) \geq 1, \quad i = 1, 2, \dots, m. \end{aligned}$$

Dual problem:

$$\begin{aligned} \min_{\alpha} \quad & \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j y_i y_j \phi(\mathbf{x}_i)^\top \phi(\mathbf{x}_j) - \sum_{i=1}^m \alpha_i \\ \text{s.t.} \quad & \sum_{i=1}^m \alpha_i y_i = 0, \quad \alpha_i \geq 0, \quad i = 1, 2, \dots, m. \end{aligned}$$

Optimal solution:

$$f(\mathbf{x}) = \mathbf{w}^\top \phi(\mathbf{x}) + b = \sum_{i=1}^m \alpha_i y_i \phi(\mathbf{x}_i)^\top \phi(\mathbf{x}) + b$$

# 核函数 Kernel Function

sample  $x \mapsto \phi(x)$ , then the hyperplane  $f(x) = \mathbf{w}^\top \phi(x) + b$

Original question:

Kernel Function

$$\begin{aligned} \min_{\mathbf{w}, b} \quad & \frac{1}{2} \|\mathbf{w}\|^2 \\ \text{s.t.} \quad & y_i(\mathbf{w}^\top \phi(\mathbf{x}_i) + b) \geq 1, \quad i = 1, 2, \dots, m. \end{aligned}$$

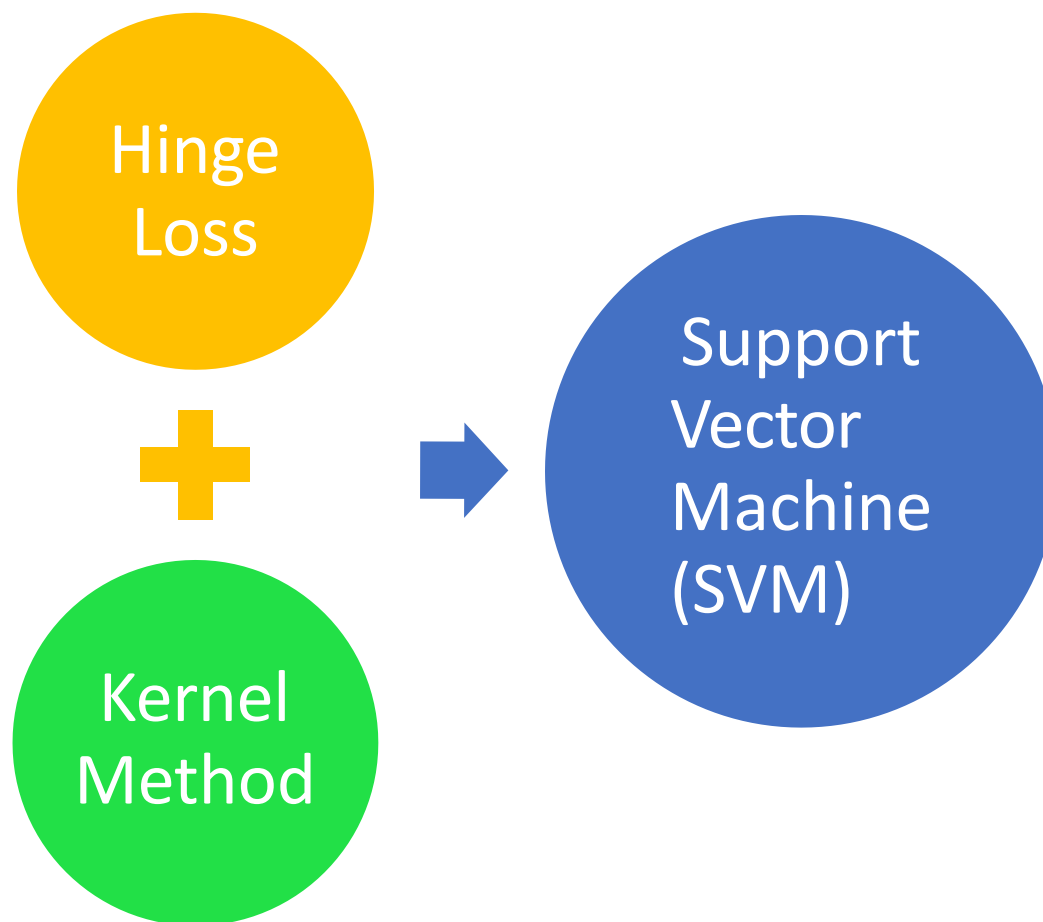
$$\kappa(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^\top \phi(\mathbf{x}_j)$$

Dual problem:

$$\begin{aligned} \min_{\alpha} \quad & \frac{1}{2} \sum_{i=1}^m \sum_{j=1}^m \alpha_i \alpha_j y_i y_j \phi(\mathbf{x}_i)^\top \phi(\mathbf{x}_j) - \sum_{i=1}^m \alpha_i \\ \text{s.t.} \quad & \sum_{i=1}^m \alpha_i y_i = 0, \quad \alpha_i \geq 0, \quad i = 1, 2, \dots, m. \end{aligned}$$

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# 监督学习

## Supervised Learning

- Given the training dataset of (data,label) pairs,

$$D = \{(x^{(i)}, y^{(i)})\}_{i=1,2,\dots,N}$$

let the machine learn a function from data to label

$$y^{(i)} \approx f_{\theta}(x^{(i)})$$

- Function set  $\{f_{\theta}(x^{(i)})\}$  is called hypothesis space
- Learning is referred to as updating the parameter  $\theta$  to make the prediction closed to the corresponding label

# 监督学习

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let the machine learn a function from data to label

$$y^{(i)} \approx f_{\theta}(x^{(i)})$$

- How to learn?

Update the parameter to make the prediction closed to the corresponding label

1. What is the learning objective?

2. How to update the parameters?



# 学习目标

## Learning Objective

- Minimize the total loss

$$\min_{\theta} \frac{1}{N} \sum_{i=1}^N L(y^{(i)}, f_{\theta}(x^{(i)}))$$

Loss function  $L(y^{(i)}, f_{\theta}(x^{(i)}))$  measures the error between the label and prediction for single sample.

We have used  
squared loss:

$$\frac{1}{2} (y^{(i)} - f_{\theta}(x^{(i)}))^2$$

Log loss:  $-y^{(i)} \log(f_{\theta}(x)) - (1 - y^{(i)}) \log(1 - f_{\theta}(x))$

# 线性回归

## Linear Regression

- Given the training dataset of (data,label) pairs,

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let the machine learn a function from data to label

$$y^{(i)} \approx f_{\theta}(x^{(i)})$$



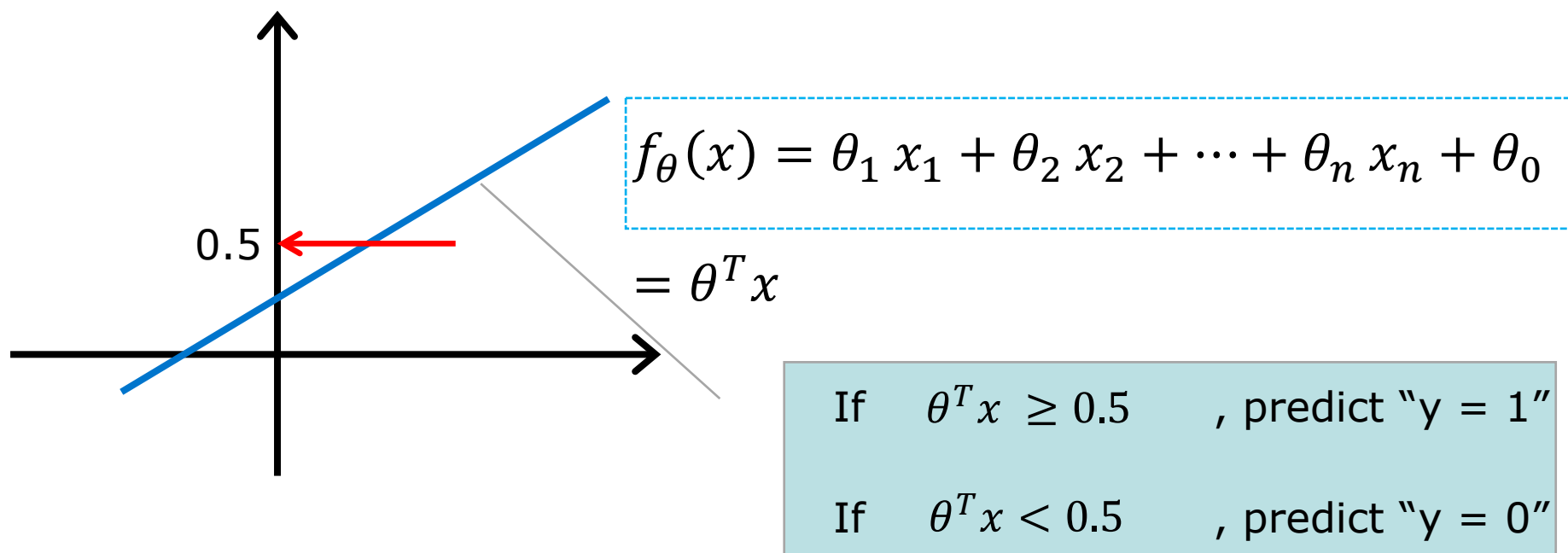
$$f_{\theta}(x) = \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_n x_n + \theta_0$$

- Function set  $\{f_{\theta}(x^{(i)})\}$  is called hypothesis space
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# 如何用于分类

## Classification task

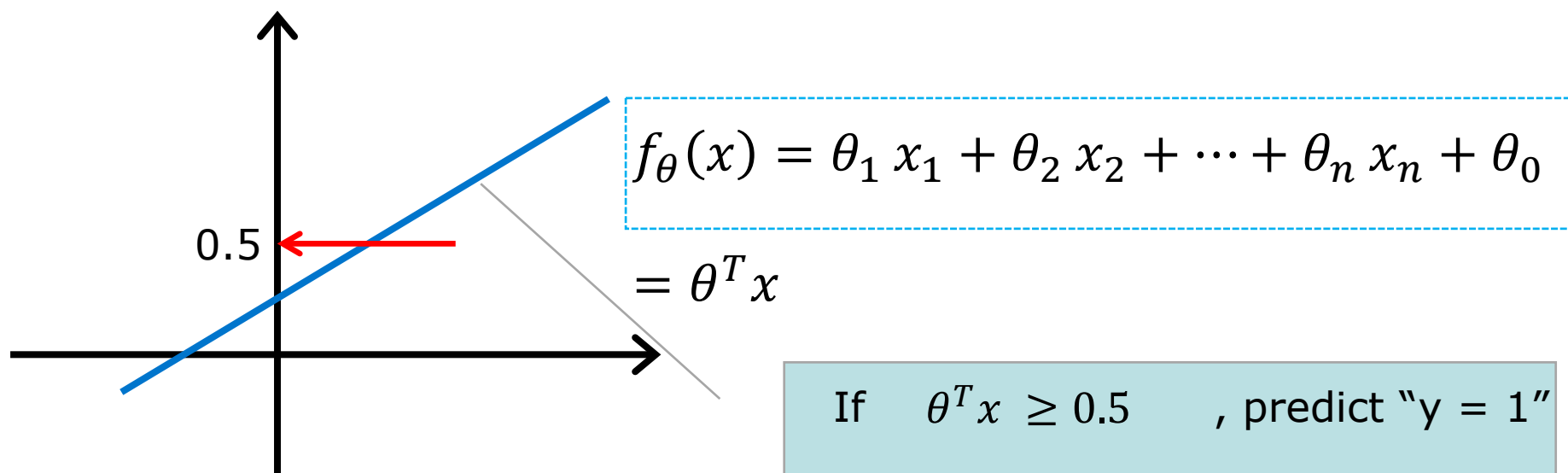
$y \in \{0, 1\}$  0: "Negative Class" (如, 坏瓜)  
1: "Positive Class" (如, 好瓜)



# 如何用于分类

## Classification task

$y \in \{0, 1\}$  0: "Negative Class" (如, 坏瓜)  
1: "Positive Class" (如, 好瓜)



If  $\theta^T x \geq 0.5$  , predict "y = 1"

If  $\theta^T x < 0.5$  , predict "y = 0"

$$g(x) = \begin{cases} 1 & f(x) \geq 0 \\ 0 & f(x) < 0 \end{cases}$$

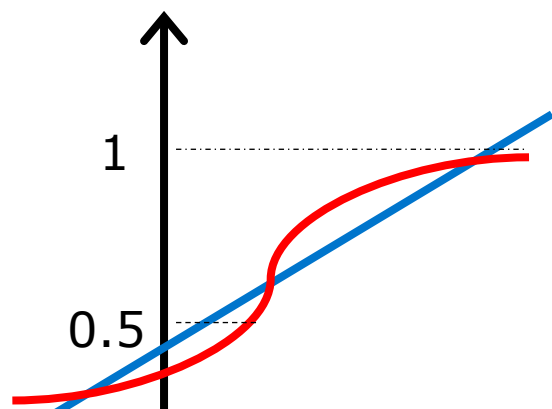
# 逻辑斯蒂回归

## Logistic regression

$y \in \{0, 1\}$

0: "Negative Class" (如, 坏瓜)

1: "Positive Class" (如, 好瓜)



$$P(y = 1/x) = \frac{1}{1 + e^{-\theta^T x}}$$

$$P(y = 0/x) = \frac{e^{-\theta^T x}}{1 + e^{-\theta^T x}}$$

$$f_{\theta}(x) = \frac{1}{1 + e^{-\theta^T x}}$$

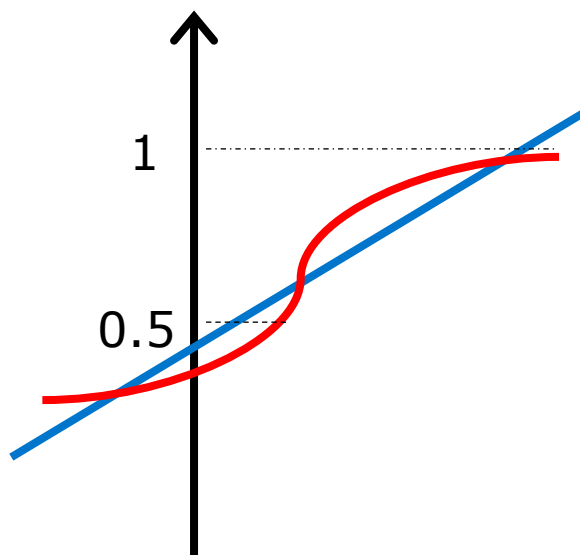
= estimated probability  
that  $y = 1$ ,  
given  $x$ , parameterized by  $\theta$

= estimated probability  
that  $y = 0$ ,  
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## Logistic regression

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= estimated probability  
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= estimated probability  
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Logistic regression

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$$y^{(i)} \approx f_{\theta}(x^{(i)}) \quad \rightarrow \quad f_{\theta}(x) = \frac{1}{1 + e^{-\theta^T x}}$$
$$g(x) = \begin{cases} 1 & f(x) \geq 0 \\ 0 & f(x) < 0 \end{cases}$$

Cross-entropy loss:

$$-y^{(i)} \log(f_{\theta}(x)) - (1 - y^{(i)}) \log(1 - f_{\theta}(x))$$

# 二分类 Binary Classification

- Step 1: Function (Model)

$$g(x) = \begin{cases} 1 & f(x) \geq 0 \\ 0 & f(x) < 0 \end{cases}$$



# 二分类 Binary Classification

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$$C(f) = \sum_n \delta(g(x^{(i)}) \neq y^{(i)})$$

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The number of times  
get incorrect results  
on training data.

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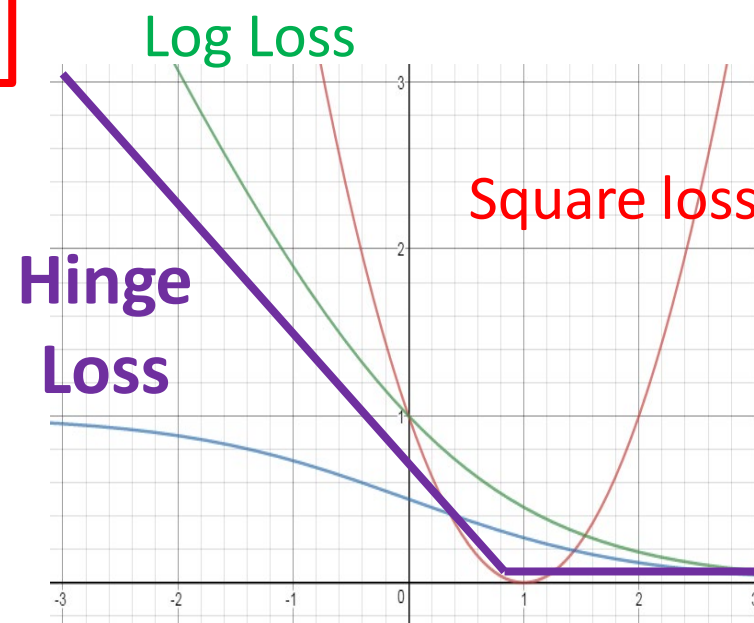
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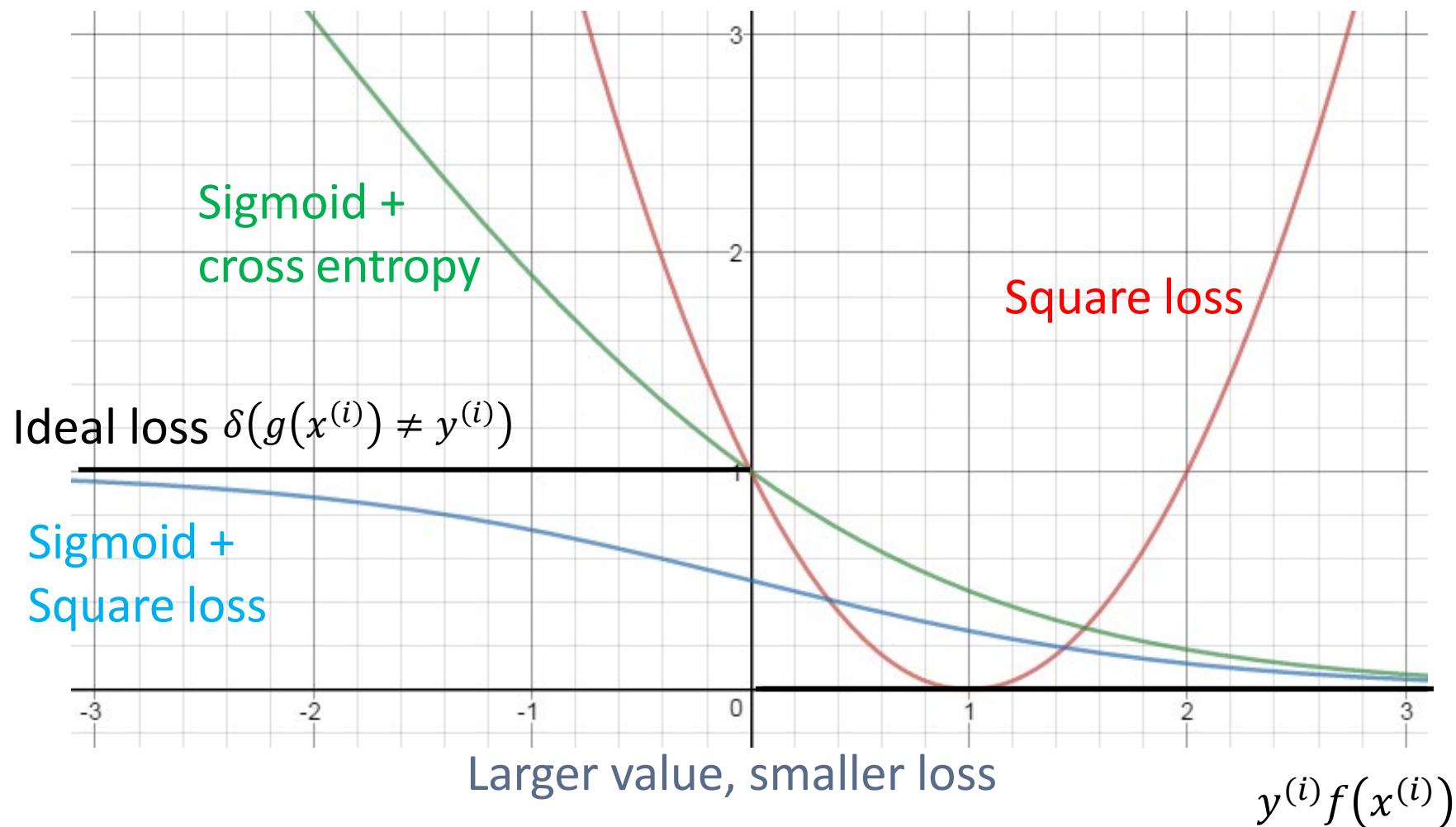
$$\varepsilon^i = \max(0, 1 - y^{(i)} f(x^{(i)}))$$

Hinge Loss function



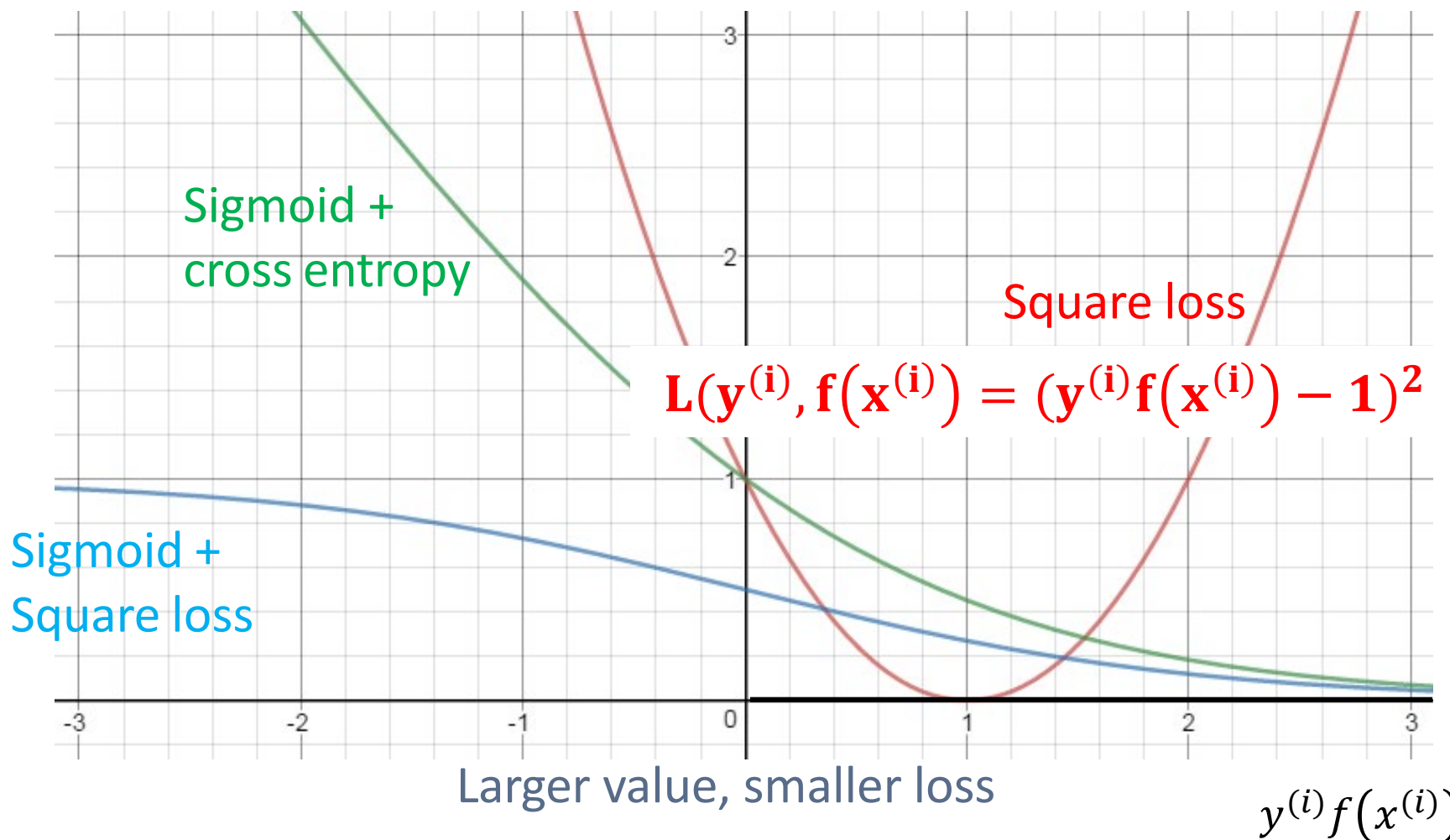


# 损失函数 Loss function

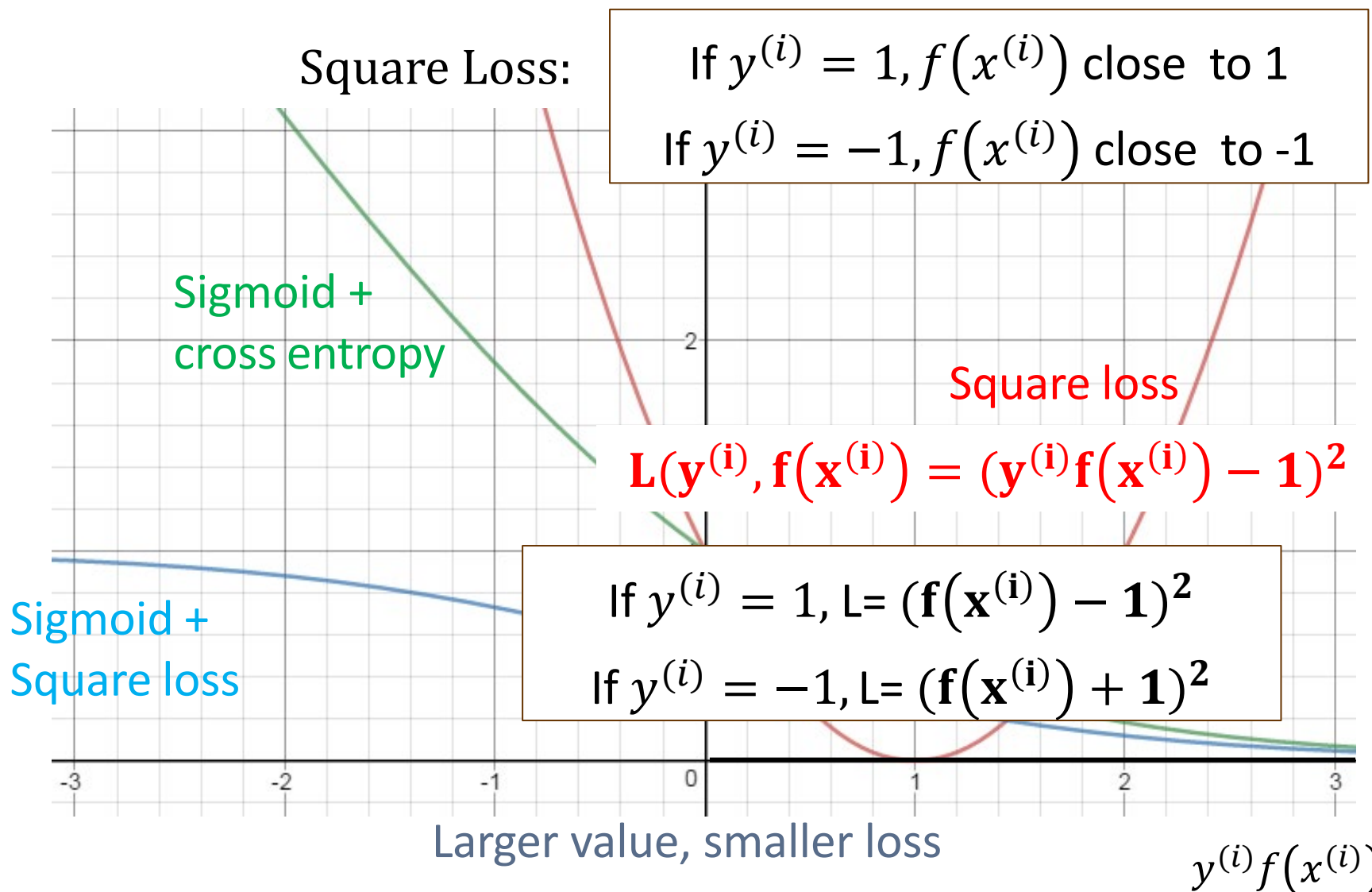


# 损失函数 Loss function

Square Loss:

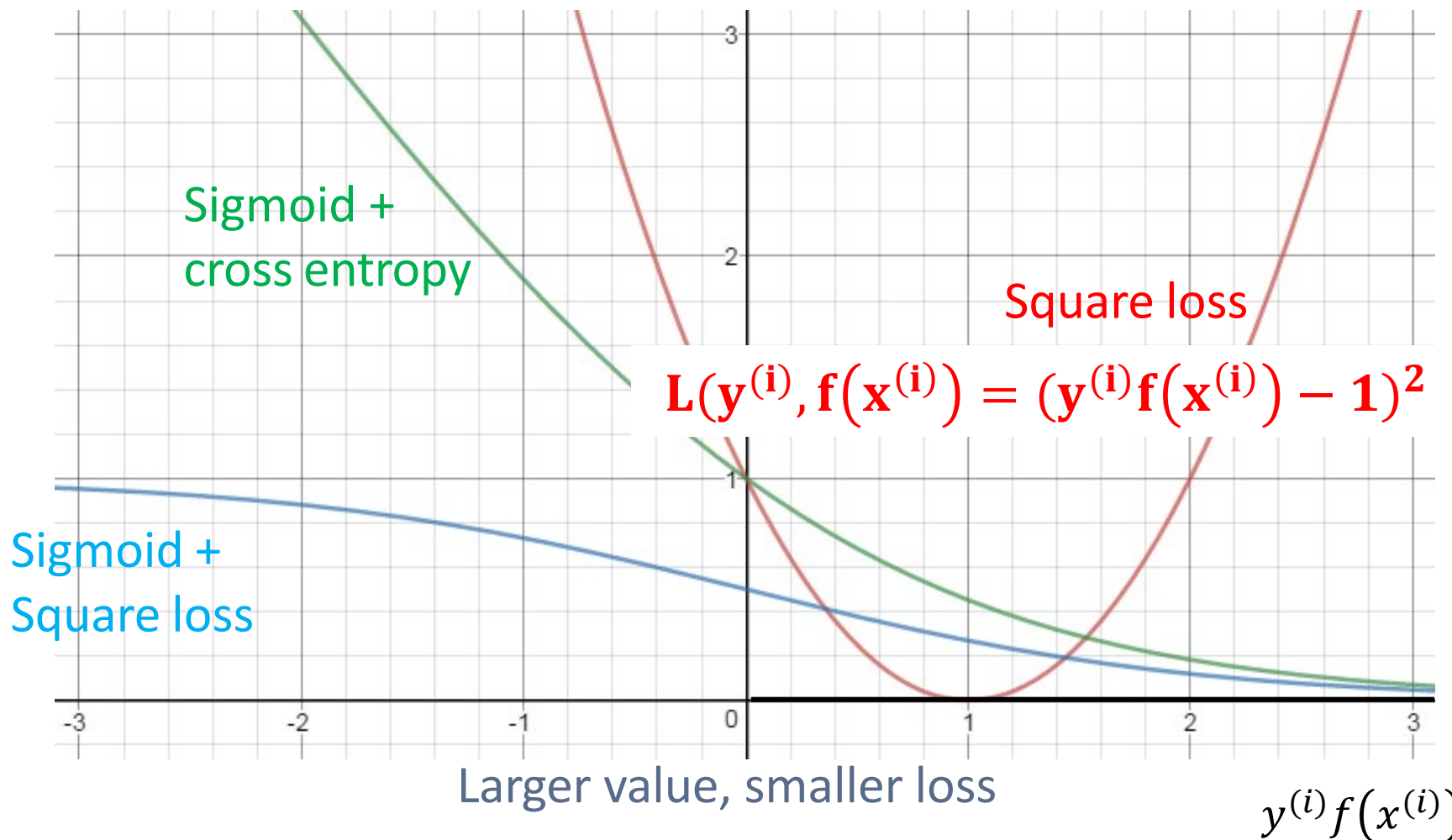


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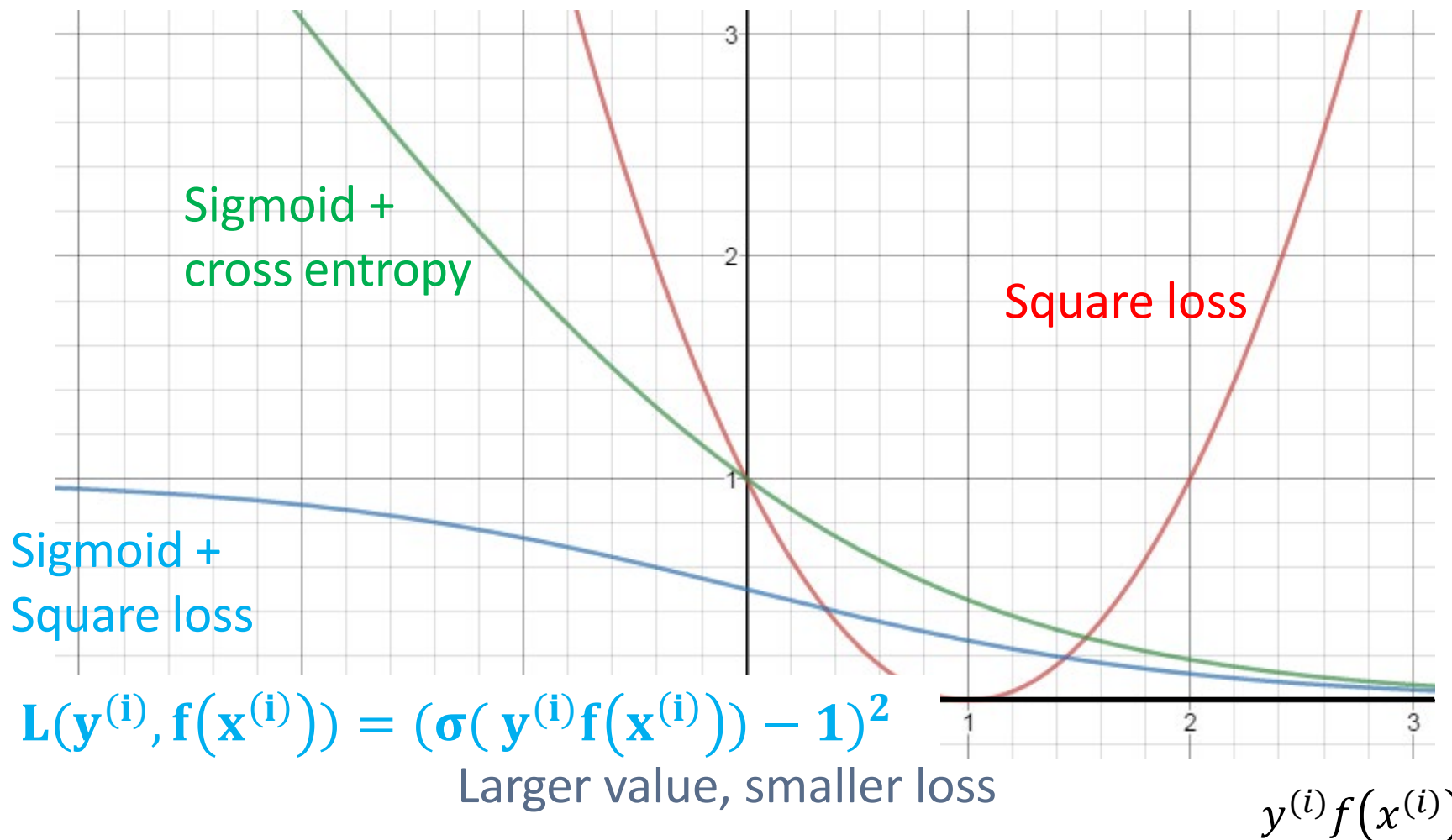
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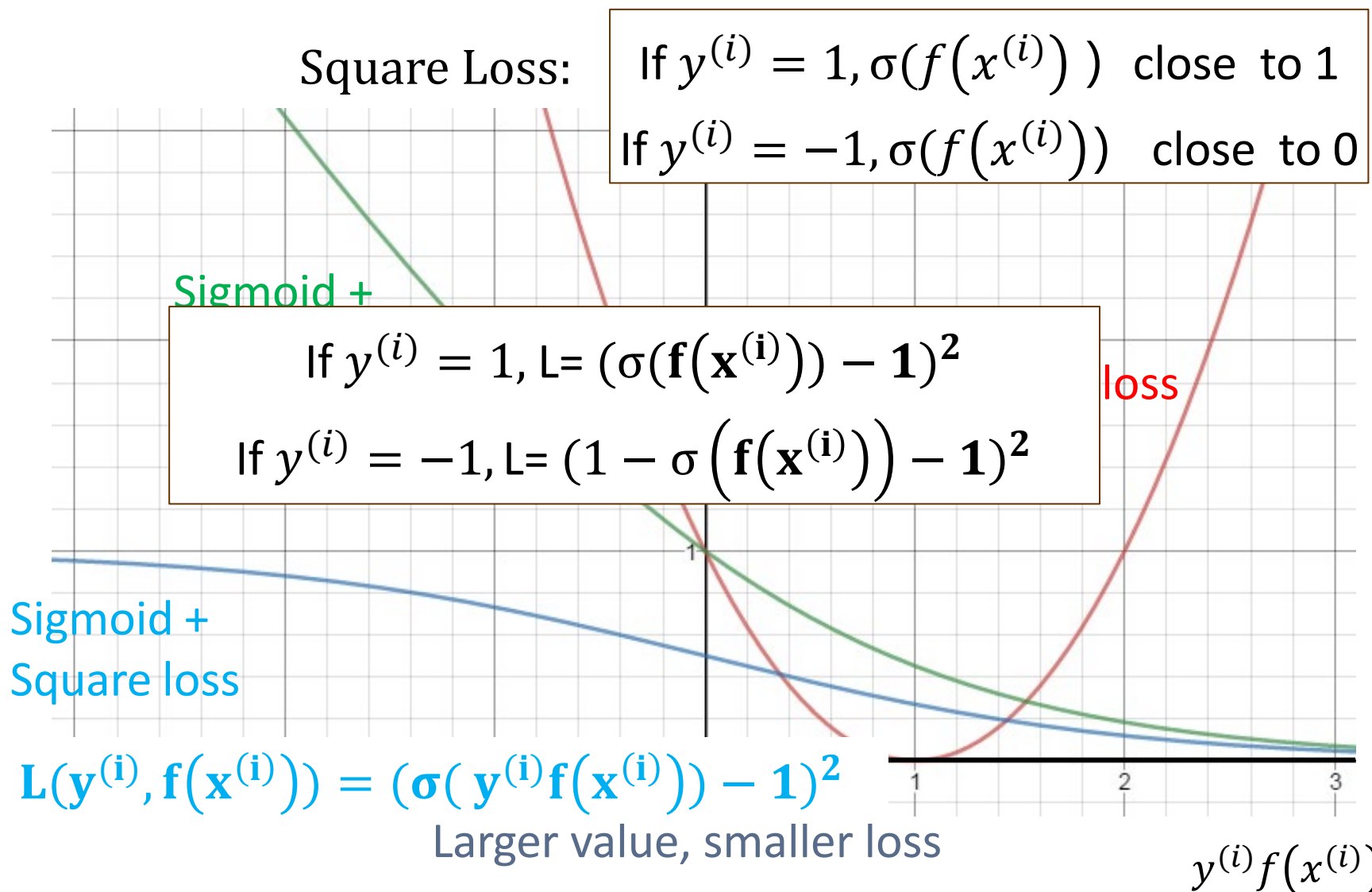


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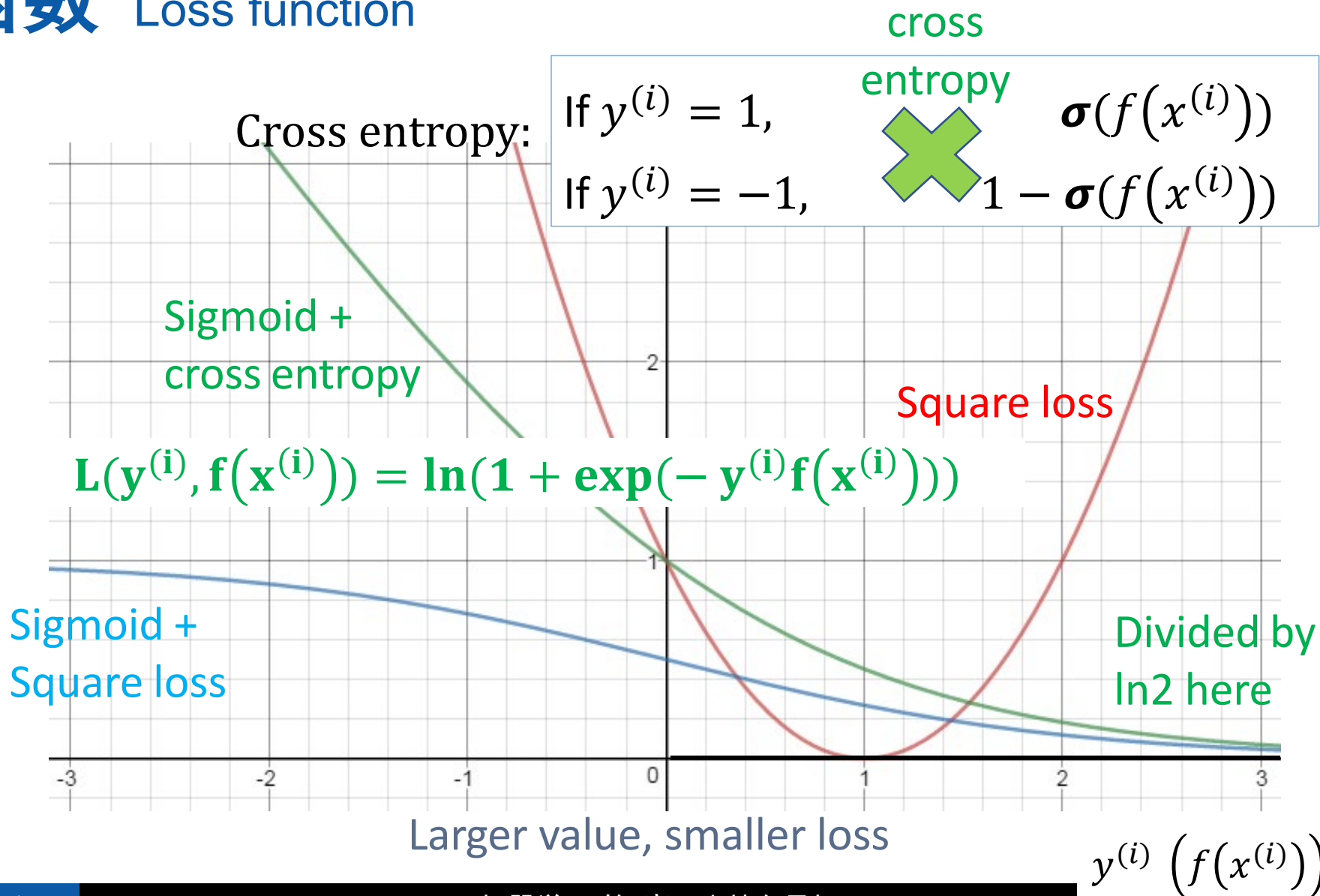
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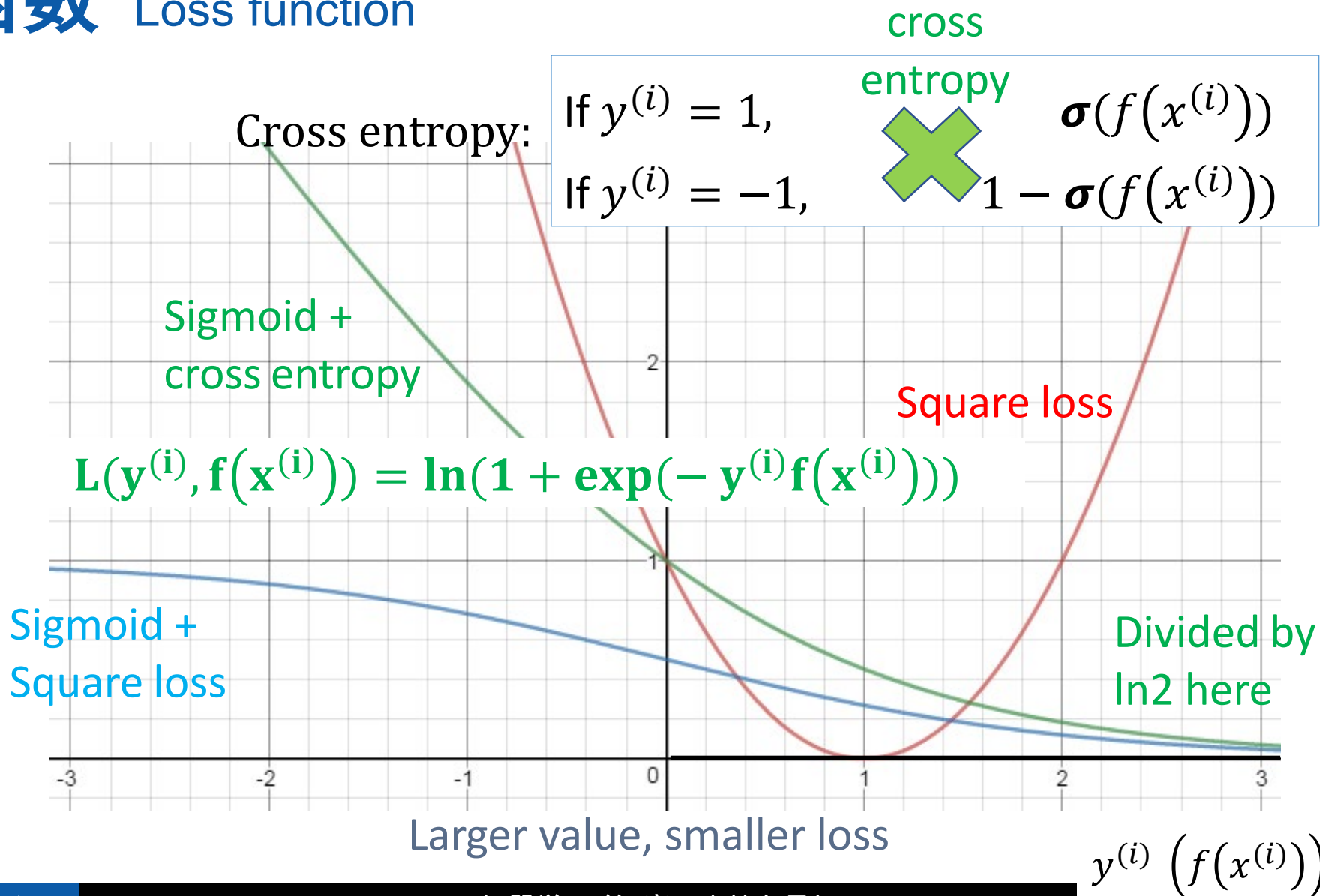
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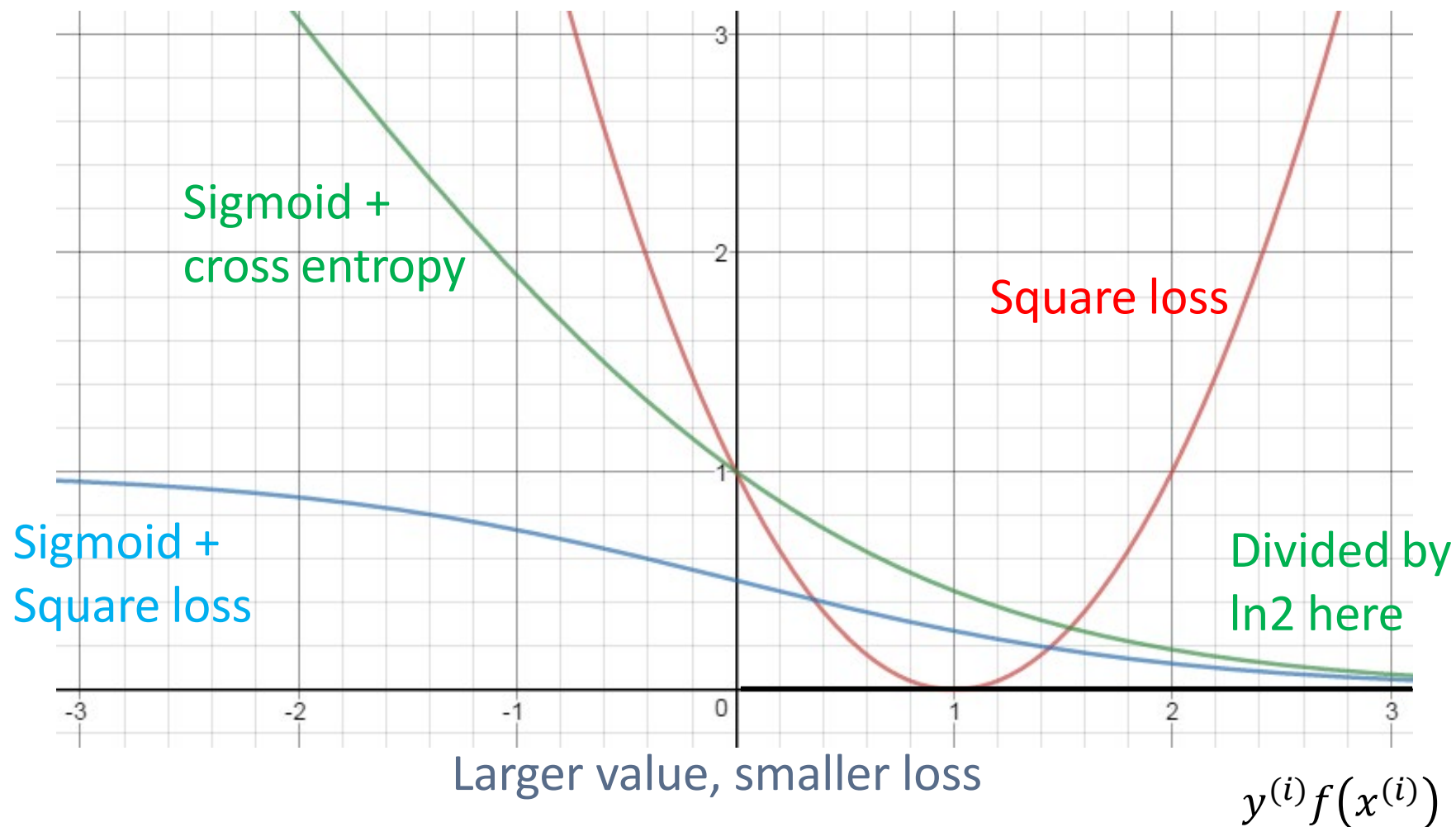


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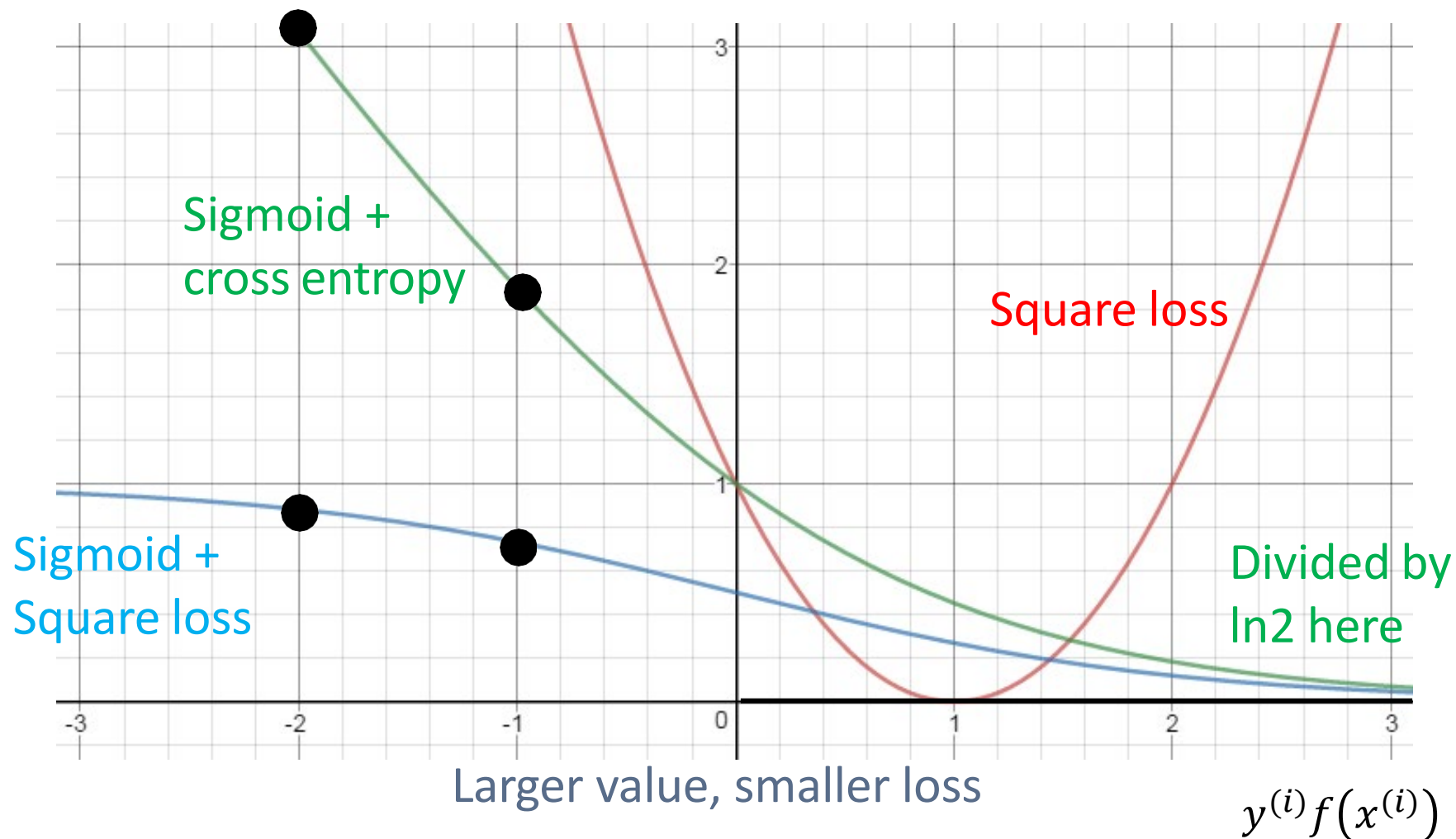




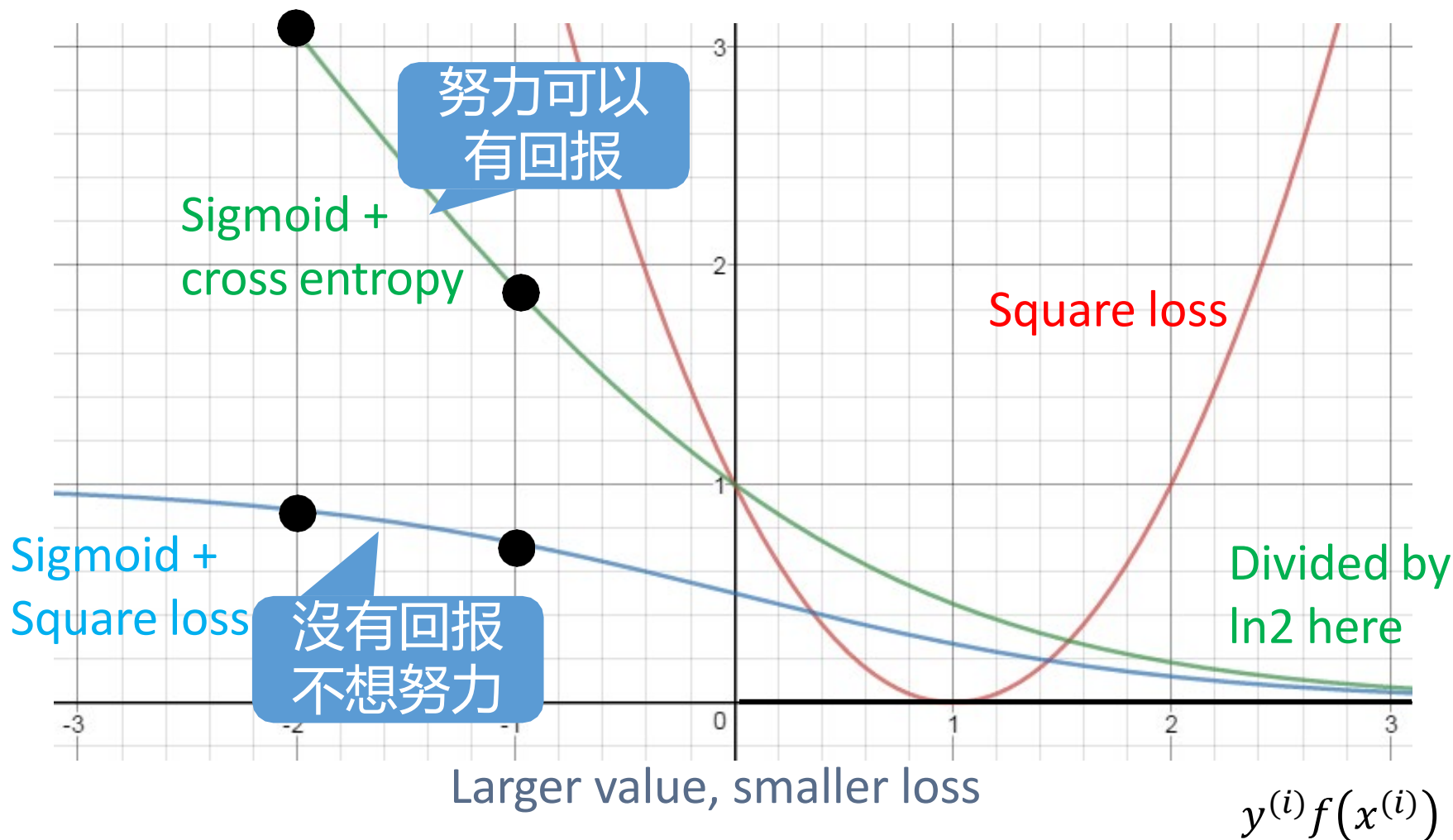
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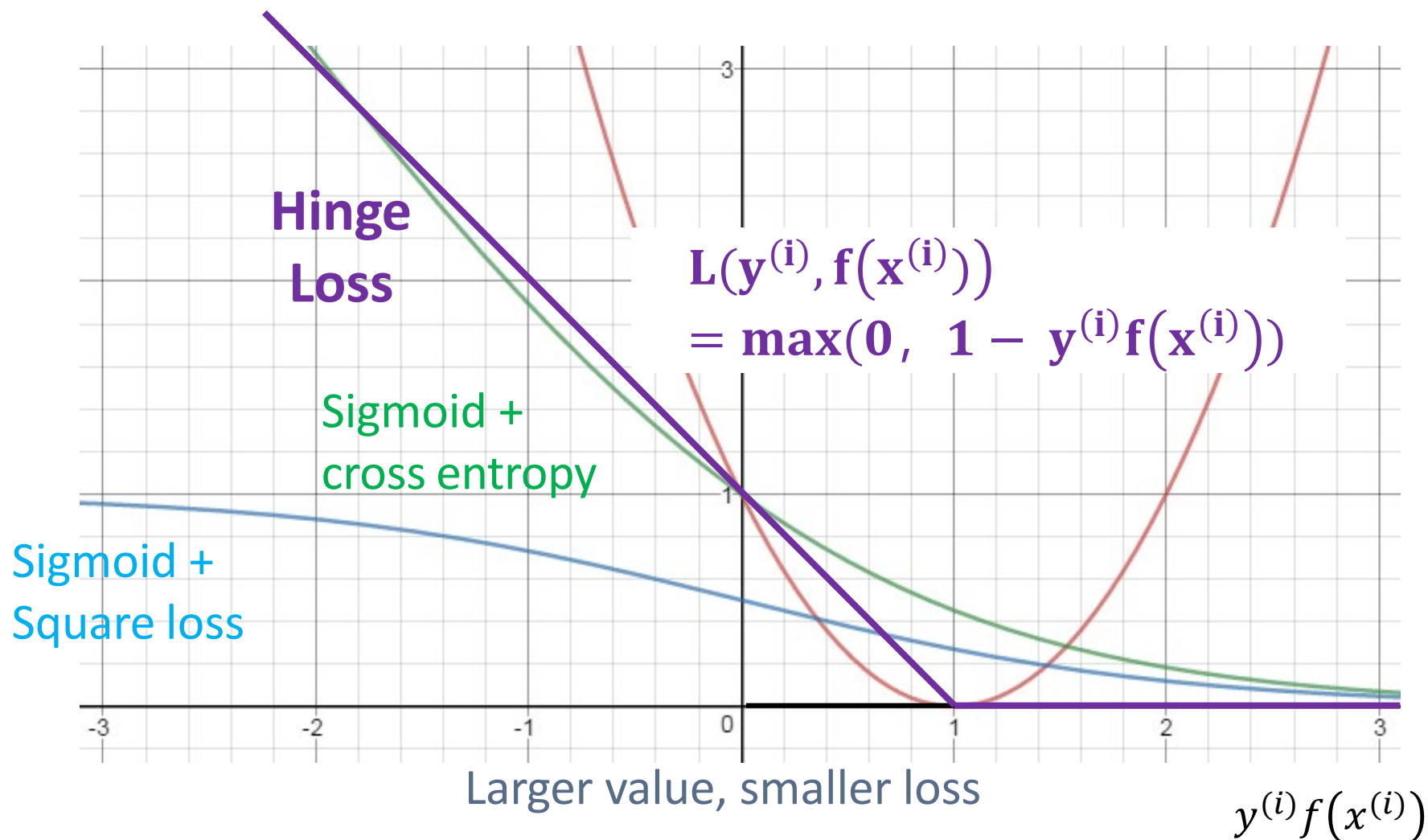
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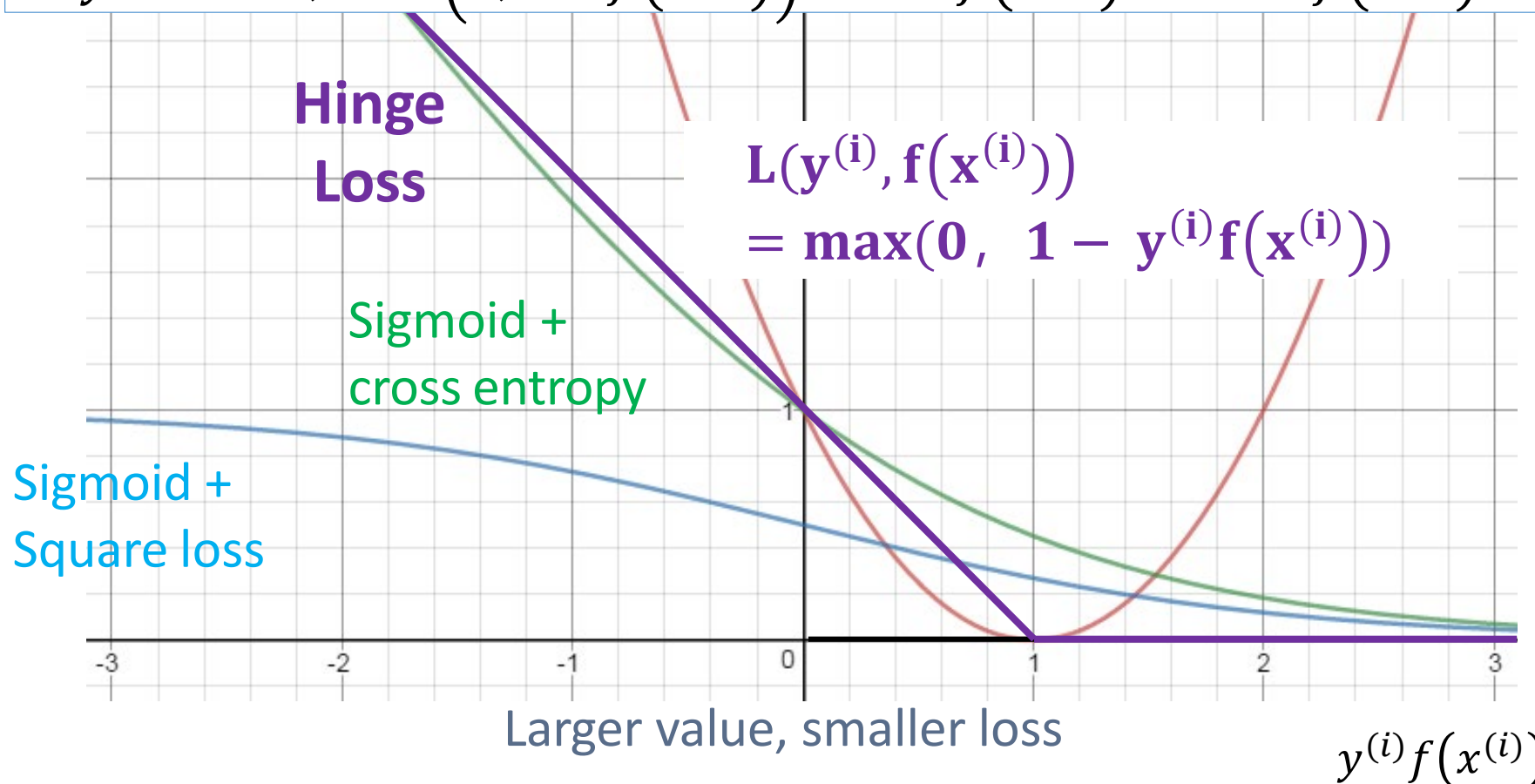
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# 损失函数 Loss function

$$\text{If } y^{(i)} = 1, \max(0, 1 - f(x^{(i)})) \quad 1 - f(x^{(i)}) < 0 \quad f(x^{(i)}) > 1$$

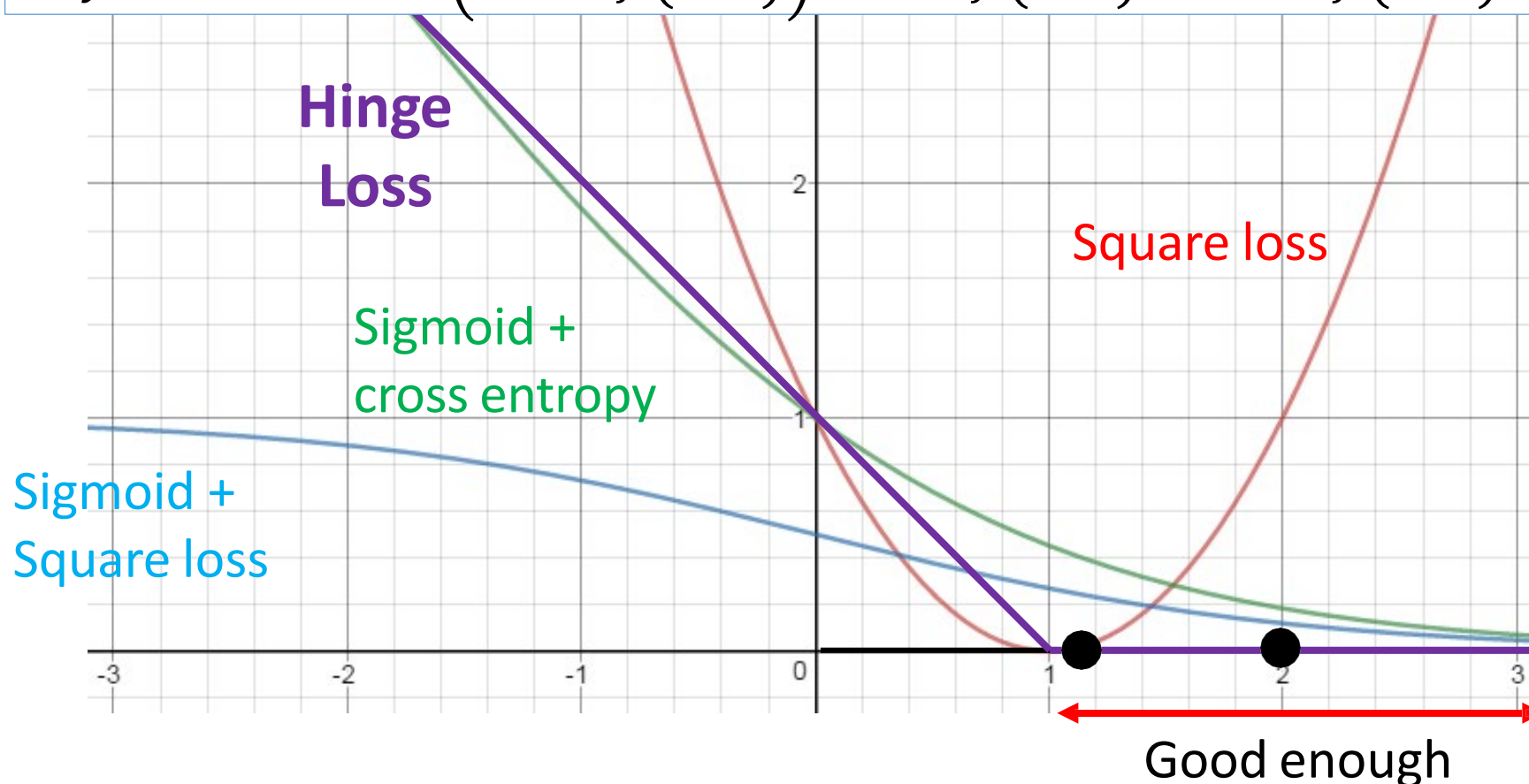
$$\text{If } y^{(i)} = -1, \max(0, 1 + f(x^{(i)})) \quad 1 + f(x^{(i)}) < 0 \quad f(x^{(i)}) < -1$$



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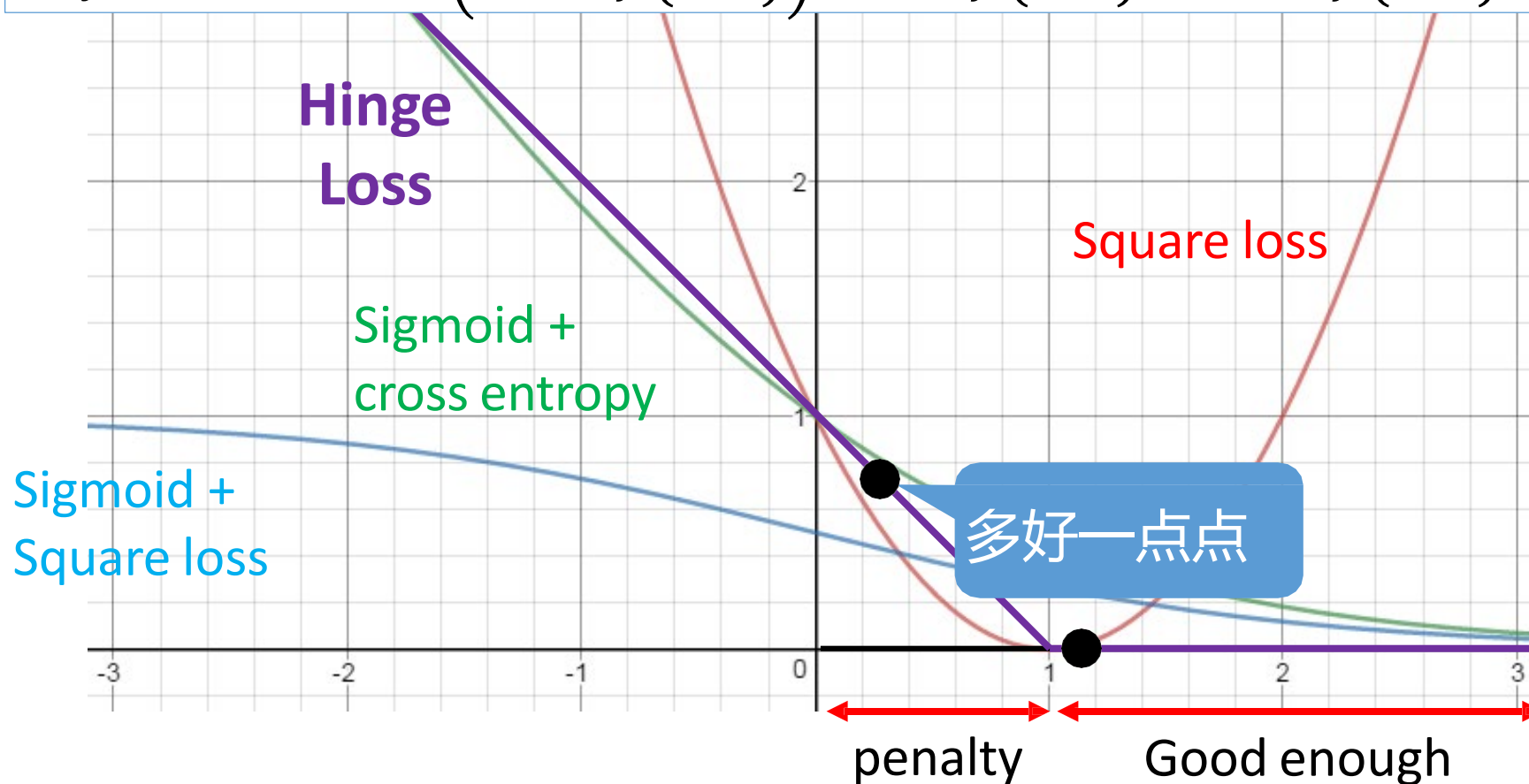
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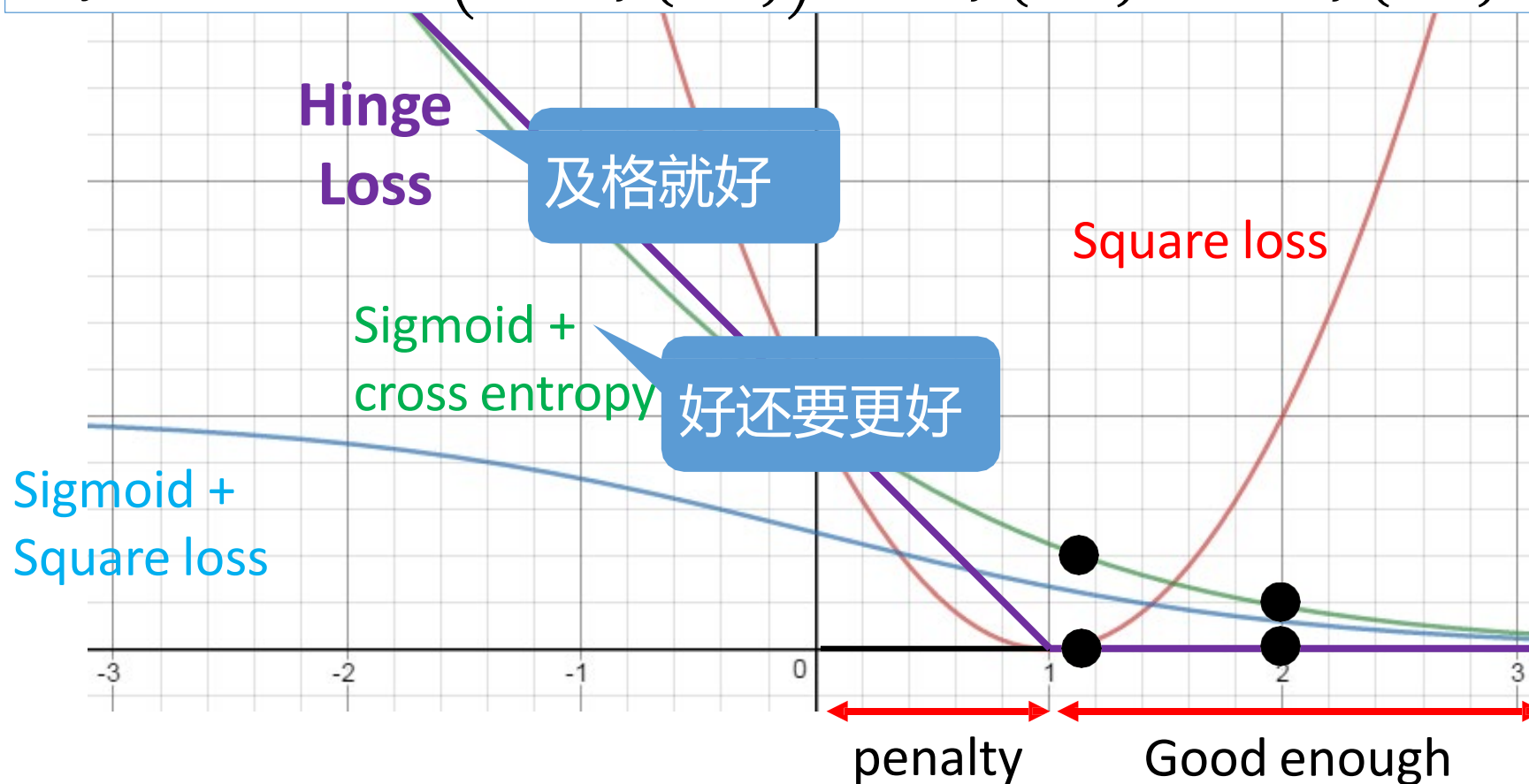
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$$f(x) = \sum_j w_j x_j + b$$

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$$C(f) = \sum_n L(f(x^{(i)}), y^{(i)})$$

# 线性SVM Linear SVM

- Step 1: Function (Model)

$$f(x) = \sum_j w_j x_j + b = \overset{\text{New } w}{\begin{bmatrix} w \\ b \end{bmatrix}} \cdot \underset{\text{New } x}{\begin{bmatrix} x \\ 1 \end{bmatrix}} = w^T x$$

- Step 2: Cost function  $= \sum_i L(f(x^{(i)}), y^{(i)}) + \lambda \|w\|_2$

$$L(y^{(i)}, f(x^{(i)})) = \max(0, 1 - y^{(i)} f(x^{(i)}))$$

Hinge loss

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convex

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Ignore regularization for simplicity

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$$f(x^n) = w^T \cdot x^n$$

$x_j^i$




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$$\boxed{w_j \leftarrow w_j - \eta \sum_i c^n(W) x_j^i}$$

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Minimizing total loss function L:

$$\min \sum_i (\max(0, 1 - y^{(i)} f(x^{(i)}))) + \lambda \|w\|_2$$

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$$y^{(i)} (w^T x_j + b) \geq 1 - \varepsilon^i$$



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$$s. t. y^{(i)}(w^T x_j + b) \geq 1 - \varepsilon^i$$

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$$\min \frac{1}{2} \|w\|_2 + C \sum_i \varepsilon^i$$

$$s. t. y^{(i)}(w^T x_j + b) \geq 1 - \varepsilon^i$$

# 支持向量

Support vectors

$$w^{(*)} = \sum_n a_n^* x^n$$

$a^{(*)}$  may be sparse



Linear combination of data points


$x^{(i)}$  with non-zero  $a^{(*)}$  are  
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Hinge loss:  
usually zero

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If  $w$  initialized as 0

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If  $w$  initialized as 0

c.f. for logistic regression,  
it is always non-zero

$$c^n(w) = \frac{\partial L(y^{(i)} f(x^{(i)}))}{\partial f(x^{(i)})}$$

Hinge loss:  
usually zero



# 逻辑斯蒂回归求解

Logistic regression solution

$$J(\theta) = \frac{1}{N} \sum_{i=1}^N \left[ -y^{(i)} \log \left( f_{\theta}(x^{(i)}) \right) - (1 - y^{(i)}) \log \left( 1 - f_{\theta}(x^{(i)}) \right) \right]$$

Want  $\{ \min_{\theta} J(\theta) \}$  :

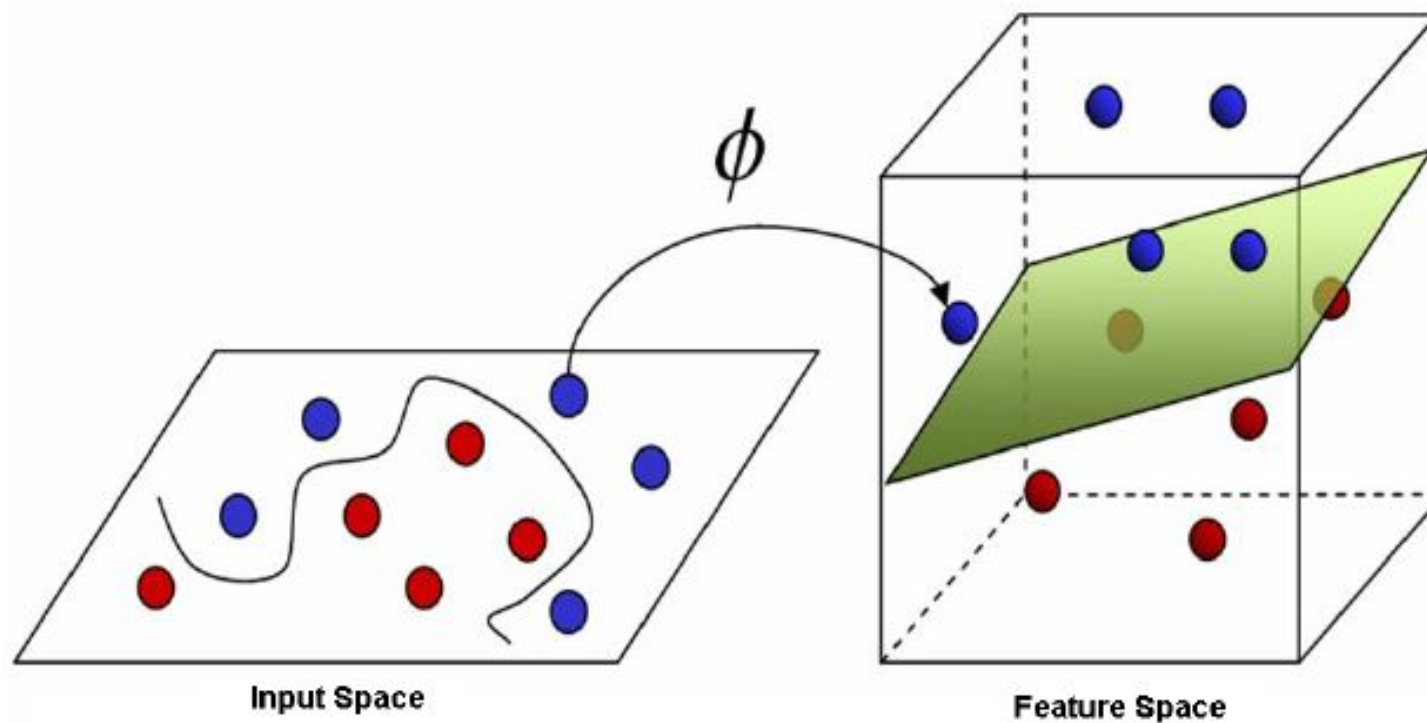
Repeat

$$\theta_j := \theta_j - a \frac{1}{N} \sum_{i=1}^N (f_{\theta}(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

(simultaneously update all  $\theta_j$  )  
}

Algorithm looks identical to linear regression!

# 核技巧 Kernel Trick



# 核技巧 Kernel Trick

$$w = \sum_n a_n x^n = Xa$$

$$X = \begin{bmatrix} x^1 & x^2 & \dots & x^N \end{bmatrix} \quad \alpha = \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_N \end{bmatrix}$$

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$$w = \sum_n a_n x^n = Xa$$
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Step 1:  $f(x) = w^T x$

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$$w = \sum_n a_n x^n = Xa \quad X = \begin{bmatrix} x^1 & x^2 & \dots & x^N \end{bmatrix} \quad \alpha = \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_N \end{bmatrix}$$

$$\text{Step 1: } f(x) = w^T x \quad \xrightarrow{w = X\alpha} \quad f(x) = \alpha^T X^T x$$

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$$w = \sum_n a_n x^n = Xa$$

$$X = \begin{bmatrix} x^1 & x^2 & \dots & x^N \end{bmatrix}$$

$$a = \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_N \end{bmatrix}$$

Step 1:  $f(x) = w^T x \xrightarrow{w = Xa} f(x) = a^T X^T x$

Diagram illustrating the kernel trick:

- The vector  $a = [\alpha_1 \dots \alpha_N]$  is shown.
- The matrix  $X^T$  is shown as a column of inner products:  $\begin{bmatrix} x^1 \cdot x \\ x^2 \cdot x \\ \vdots \\ x^N \cdot x \end{bmatrix}$ .
- The input  $x$  is shown as a green box.
- The inner products are calculated as  $x^1 \cdot x, x^2 \cdot x, \dots, x^N \cdot x$ .

$$f(x) = \sum_n a_n (x^n \cdot x)$$

$$= \sum_n a_n K(x^n, x)$$

# 核技巧 Kernel Trick

Step 1:  $f(x) = \sum_n a_n K(x^n \cdot x)$  Find  $a_1^*, a_2^*, \dots, a_n^*$ ,

Step 2, 3: Find  $a_1^*, \dots, a_n^*, \dots, a_N^*$  , minimizing loss function L

$$\begin{aligned} L(f) &= \sum_i L(f(x^{(i)}), y^{(i)}) \\ &= \sum_i L\left(\sum_n a_n K(x^n \cdot x), y^{(i)}\right) \end{aligned}$$

We only need to know the inner product between a pair of vectors  $x$  and  $z$

Kernel Trick

# 常用核函数

## Kernel Function

- Liner kernel

$$K(x, z) = x^T z$$

- Polynomial kernel

$$K(x, z) = (x^T z)^d$$

- Gaussian kernel / Radial Basis Function Kernel

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

- Sigmoid kernel

$$K(x, z) = \tanh(\beta x^T z + \theta)$$



# RBF核 Radial Basis Function Kernel

$$K(x, z) = \exp\left(-\frac{1}{2}\|x - z\|_2\right) = \phi(x) \cdot \phi(z)?$$

$$= \exp\left(-\frac{1}{2}\|x\|_2 - \frac{1}{2}\|z\|_2 + x \cdot z\right)$$

$\phi(*)$  has inf dim!!!

$$= \exp\left(-\frac{1}{2}\|x\|_2\right) \exp\left(-\frac{1}{2}\|z\|_2\right) \exp(x \cdot z) = C_x C_z \exp(x \cdot z)$$

$$= C_x C_z \sum_{i=0}^{\infty} \frac{(x \cdot z)^i}{i!} = C_x C_z + C_x C_z (x \cdot z) + C_x C_z \frac{1}{2} (x \cdot z)^2 \dots$$

$$[C_x] \cdot [C_z] \quad \begin{bmatrix} C_x x_1 \\ C_x x_2 \\ \vdots \end{bmatrix} \cdot \begin{bmatrix} C_z z_1 \\ C_z z_2 \\ \vdots \end{bmatrix} \quad \frac{1}{\sqrt{2}} \begin{bmatrix} C_x x_1^2 \\ \vdots \\ \sqrt{2} C_x x_1 x_2 \\ \vdots \end{bmatrix} \cdot \frac{1}{\sqrt{2}} \begin{bmatrix} C_z z_1^2 \\ \vdots \\ \sqrt{2} C_z z_1 z_2 \\ \vdots \end{bmatrix}$$

# Sigmoid核 Sigmoid Kernel

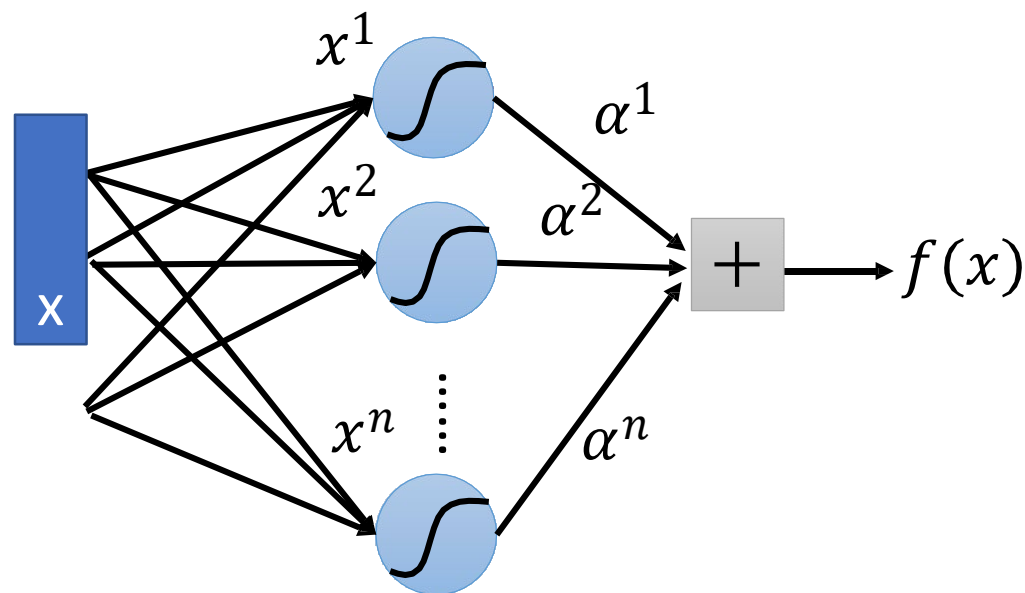
$$K(x, z) = \tanh(x \cdot z)$$

- When using sigmoid kernel, we have a 1 hidden layer network.

$$f(x) = \sum_n a_n K(x^n, x) = \sum_n a_n \tanh(x^n \cdot x)$$

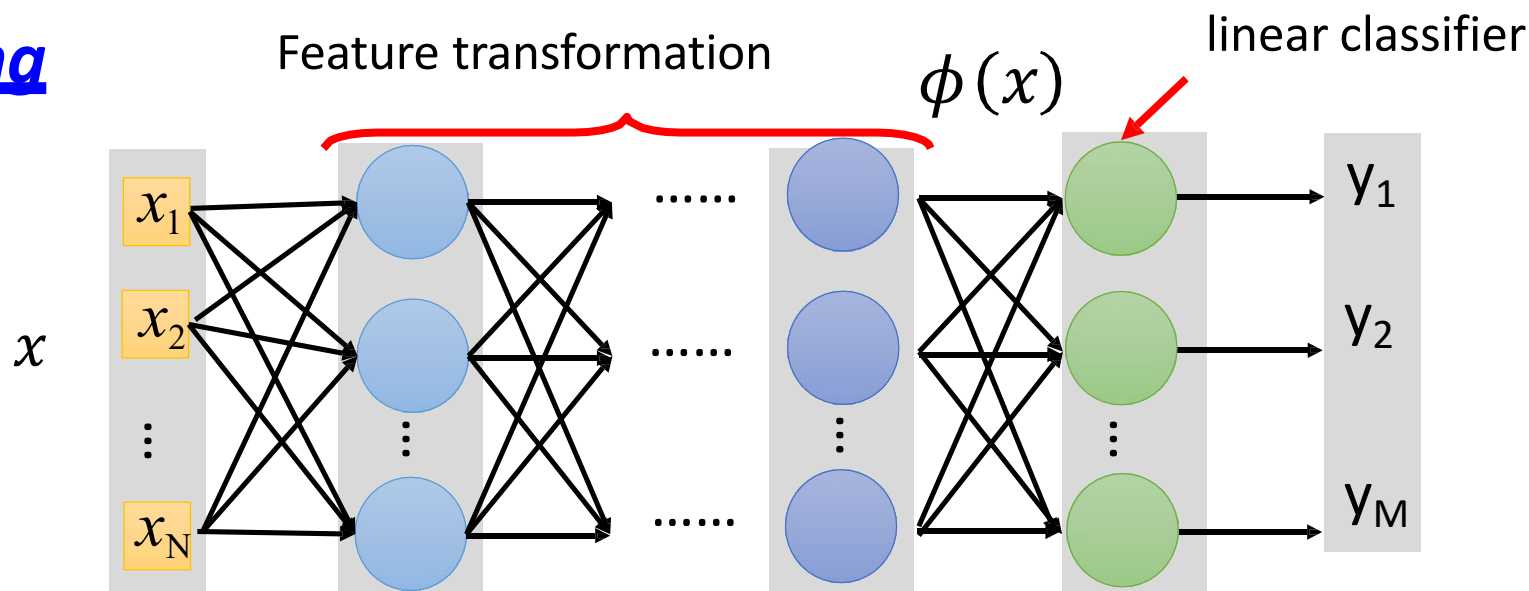
The weight of each neuron is a data point

The number of support vectors is the number of neurons.



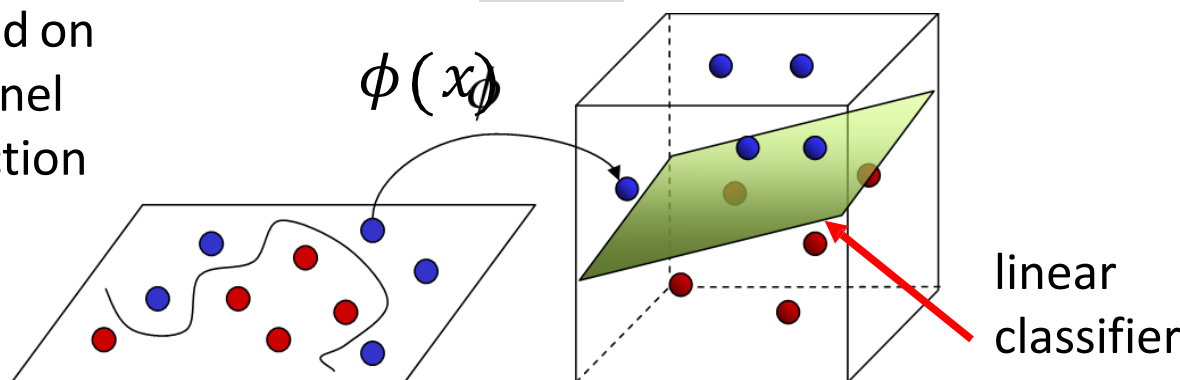
# 深度学习和支持向量机 Deep learning VS SVM

## Deep Learning



## SVM

Based on  
kernel  
function



Multiple Kernel learning  
[Alpaydin, Chapter 13.8]

Input Space

Feature Space

# SVM 软件包

- LIBSVM  
<http://www.csie.ntu.edu.tw/~cjlin/libsvm/>
- LIBLINEAR  
<http://www.csie.ntu.edu.tw/~cjlin/liblinear/>
- SVM<sup>light</sup>、SVM<sup>perf</sup>、SVM<sup>struct</sup>  
[http://svmlight.joachims.org/svm\\_struct.html](http://svmlight.joachims.org/svm_struct.html)
- Pegasos  
<http://www.cs.huji.ac.il/~shais/code/index.html>
- Demo
- [Support Vector Machine \(dash.gallery\)](#)

# SVM 方法

## SVM related methods

- Support Vector Regression (SVR)
  - [Bishop chapter 7.1.4]
- Ranking SVM
  - [Alpaydin, Chapter 13.11]
- One-class SVM
  - [Alpaydin, Chapter 13.11]
- [Support Vector Machine \(dash.gallery\)](#)