Machine Learning

Logistic Regression

Dr. Shuang LIANG

Recall: Linear Regression

Model $y = b + wx_1$

Loss

$e = |y - \hat{y}|$ L is mean absolute error (**MAE**)

$e = (y - \hat{y})^2$ L is mean square error (**MSE**)

Optimization Gradient Descent

Regularization

L1 Regularization – Lasso

L2 Regularization – Ridge Regression

Recall: Gradient Descent

$$w^*, b^* = arg \min_{w,b} L$$

- (Randomly) Pick initial values w^0, b^0
- Compute

$$\boxed{\begin{array}{l} \frac{\partial L}{\partial w}|_{w=w^0,b=b^0} \\ \\ \frac{\partial L}{\partial b}|_{w=w^0,b=b^0} \end{array}}$$

$$w^1 \leftarrow w^0 - \eta \frac{\partial L}{\partial w}|_{w=w^0,b=b^0}$$

$$b^1 \leftarrow b^0 - \eta \frac{\partial L}{\partial b}|_{w=w^0,b=b^0}$$

- Update w and b interatively

Today’s Topics

- Type of classifiers
- Logistic Regression
- Logistic Regression vs Linear Regression
- Limitation of Logistic Regression

Today's Topics

- ***Type of classifiers***
- Logistic Regression
- Logistic Regression vs Linear Regression
- Limitation of Logistic Regression

Types of classifiers

- Instance based classifiers
  - Use observation directly (no models)
  - e.g. K nearest neighbors
- Generative
  - build a generative statistical model
  - e.g., Bayesian networks
- ***Discriminative***
  - ***directly estimate a decision rule/boundary***
  - ***e.g., decision tree, logistic regression***

Today’s Topics

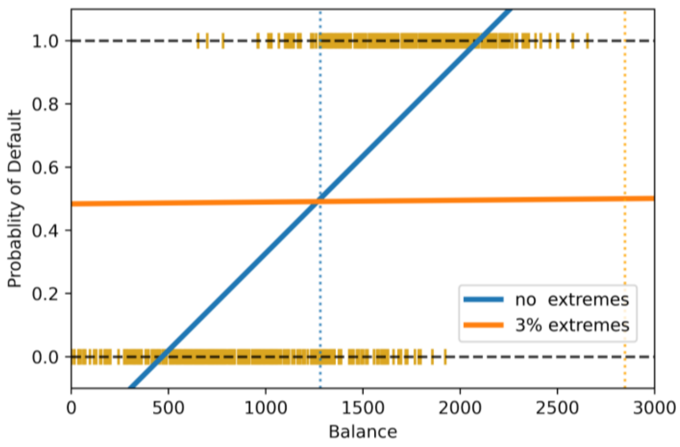
- Type of classifiers
- ***Logistic Regression***
- Logistic Regression vs Linear Regression
- Limitation of Logistic Regression

Motivation

- Rather than modeling the output *y* directly, we can **model the probability** that *x* belongs to a particular category.
- In the previous lecture, we used a linear regression model but

  -The predicted value is not in $[0,1]$

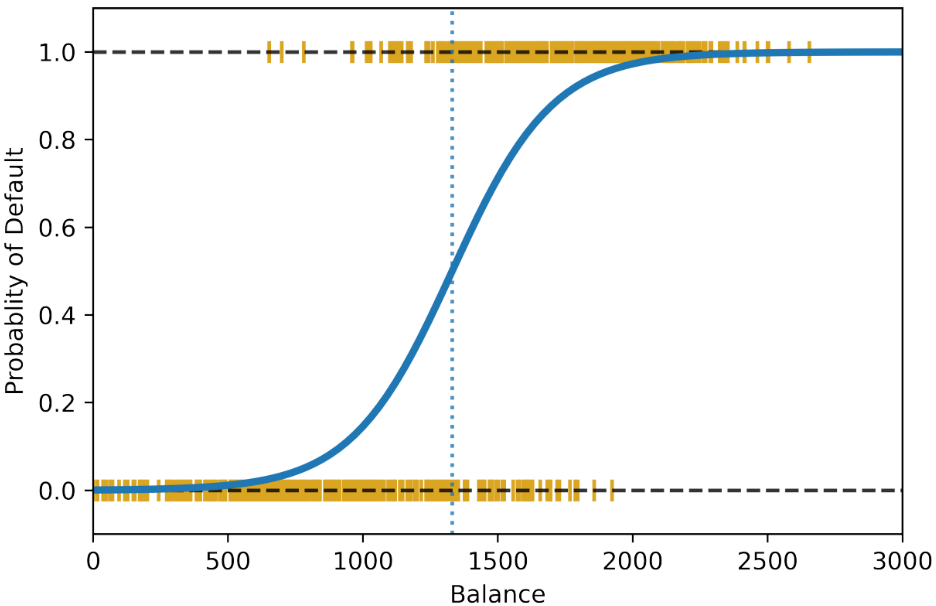
  -Very large or small values of the prediction contribute to the error even if they indicate we are very confident in the resulting classification



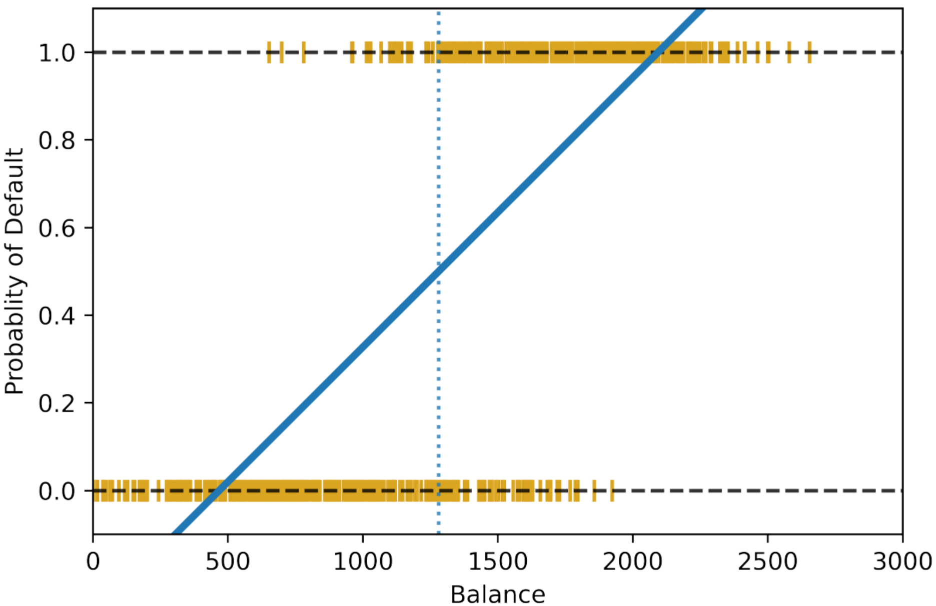
- **Solution**: map the prediction from $(-\infty, +\infty)$ to $[0,1]$

Motivation

- **Solution**: map the prediction from $(-\infty, +\infty)$ to $[0,1]$



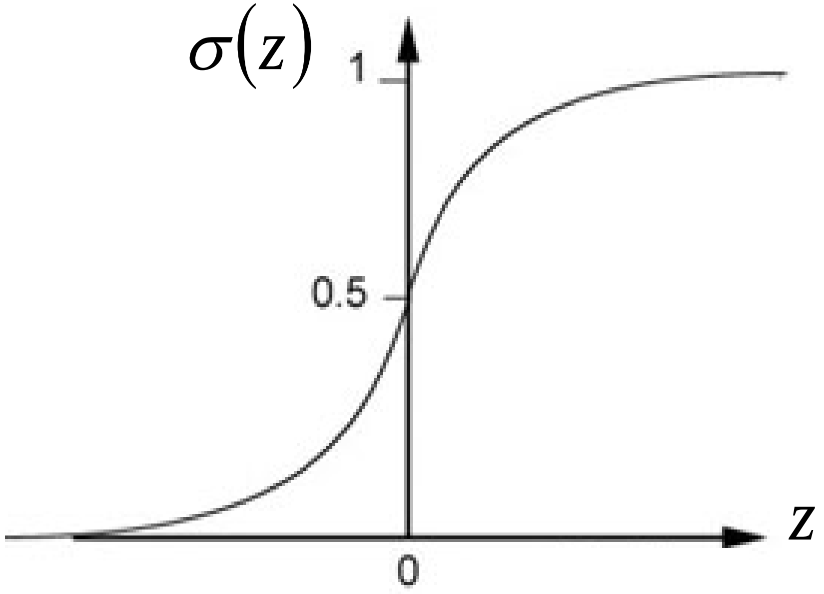
Logistic regression



Linear regression

The Logistic Function - Sigmoid

$$\sigma(z) = \frac{1}{1+e^{-z}}$$



Try to calculate two formulas:

- $1 - \sigma(z)$
- $\sigma'(z)$

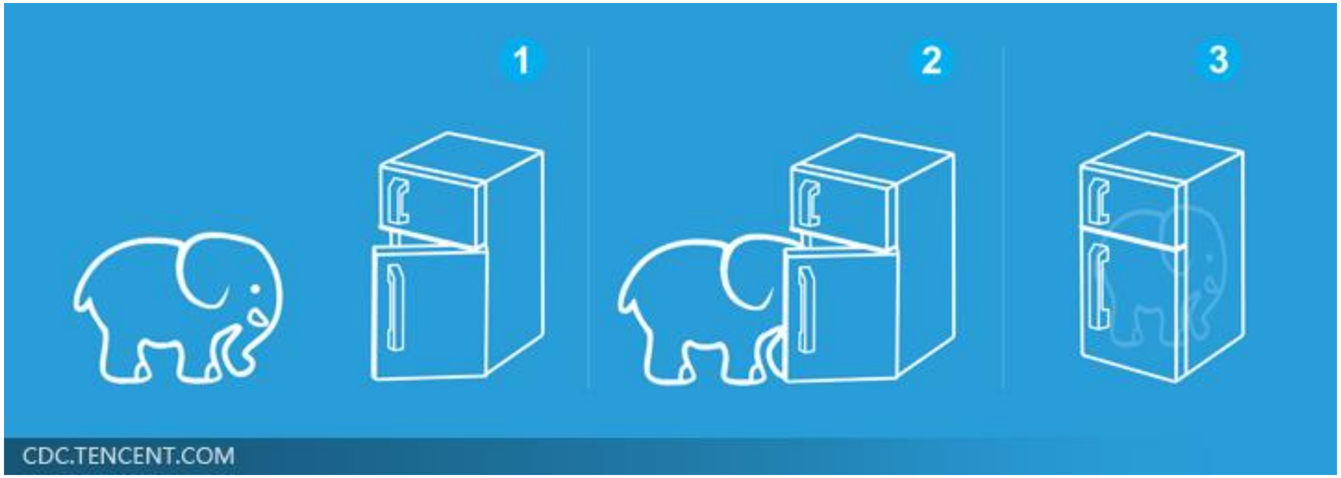
The Logistic Function - Sigmoid

- **Properties**

  - $1 - \sigma(z) = \frac{1+e^{-z}-1}{1+e^{-z}} = (1 + e^{z})^{-1} = \sigma(-z)$
  - $\sigma'(z) = -\frac{-e^{-z}}{(1+e^{-z})^2} = \frac{1}{(1+e^{-z})}\frac{1}{(1+e^{z})} = \sigma(z)(1 - \sigma(z))$

Recall: Typical process of ML

Step 1: function with unknown param → Step 2: define loss from training data → Step 3: optimization



Step1: Function Set

- **Label prediction**: quantize the probability
  - If $p(1|x) \geq 1/2$, you predict class 1
  - If $p(1|x) < 1/2$, you predict class 0

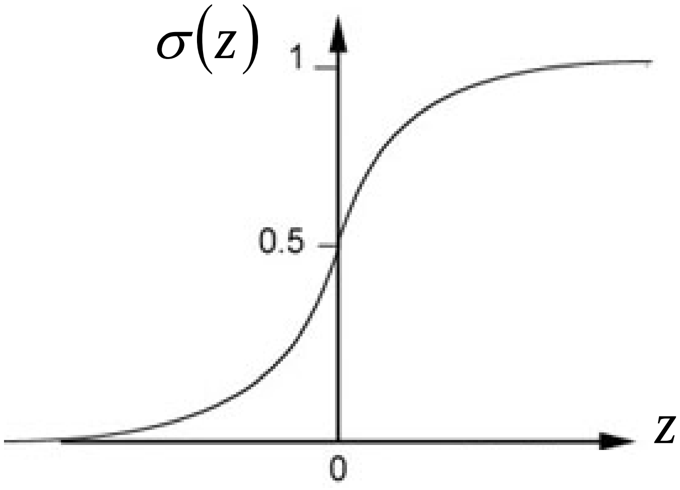
- Logistic regression models the probability that X belongs to a particular class using the logistic function

$$p(1|x) = P(Y = 1|X = x) = \sigma\left(\sum_i w_i x_i + b\right)$$

$$p(0|x) = P(Y = 0|X = x) = 1 - \sigma\left(\sum_i w_i x_i + b\right)$$

Step1: Function Set

- **Interpretation**
  - Very large $|\sum_i w_i x_i + b|$ corresponds to $p(1|x)$ very close to 0 or 1 (high confidence)
  - Small $|\sum_i w_i x_i + b|$ corresponds to $p(1|x)$ very close to 0.5 (low confidence)



	Logistic Regression	***Linear Regression***
Step 1:	$f_{w,b}(x) = \sigma\left(\sum_i w_i x_i + b\right)$ Output: between 0 and 1	$f_{w,b}(x) = \sum_i w_i x_i + b$ Output: any value
Step 2:		
Step 3:		

Step2: Goodness of a function

Training Data

x^1	x^2	x^3	……	x^N
C_1	C_1	C_2		C_1

Assume the data is generated based on $f_{w,b}(x) = P_{w,b}(C_1|x)$

Given a set of w and b, what is its probability of generating the data?

$$L(w,b) = f_{w,b}(x^1) f_{w,b}(x^2) \left(1 - f_{w,b}(x^3)\right) \cdots f_{w,b}(x^N)$$

The most likely w* and b* is the one with the largest $L(w,b)$.

$$w^*, b^* = arg \max_{w,b} L(w,b)$$

$$\boxed{\begin{matrix} x^1 & x^2 & x^3 & \\ C_1 & C_1 & C_2 & \cdots\cdots \end{matrix}} \Rightarrow \boxed{\begin{matrix} x^1 & x^2 & x^3 & \\ \hat{y}^1 = 1 & \hat{y}^2 = 1 & \hat{y}^3 = 0 & \cdots\cdots \end{matrix}}$$

$\hat{y}^n$: 1 for class 1, 0 for class 2

$$L(w,b) = f_{w,b}(x^1) f_{w,b}(x^2) \left(1 - f_{w,b}(x^3)\right) \cdots$$

$$\boxed{w^*, b^* = arg \max_{w,b} L(w,b)} = \boxed{w^*, b^* = arg \min_{w,b} -lnL(w,b)}$$

$$-lnL(w,b)$$

$$= -lnf_{w,b}(x^1) \Rightarrow -\left[\boxed{1}\, lnf(x^1) + \cancel{\boxed{0}\, ln\left(1 - f(x^1)\right)}\right]$$

$$-lnf_{w,b}(x^2) \Rightarrow -\left[\boxed{1}\, lnf(x^2) + \cancel{\boxed{0}\, ln\left(1 - f(x^2)\right)}\right]$$

$$-ln\left(1 - f_{w,b}(x^3)\right) \Rightarrow -\left[\cancel{\boxed{0}\, lnf(x^3)} + \boxed{1}\, ln\left(1 - f(x^3)\right)\right]$$

$$\vdots$$

Step2: Goodness of a function

$$L(w,b) = f_{w,b}(x^1) f_{w,b}(x^2) \left(1 - f_{w,b}(x^3)\right) \cdots f_{w,b}(x^N)$$

$$-lnL(w,b) = -\left[ln f_{w,b}(x^1) + ln f_{w,b}(x^2) + ln\left(1 - f_{w,b}(x^3)\right)\right] \cdots$$

$\hat{y}^n$: 1 for class 1, 0 for class 2

$$= \sum_n \underline{-\left[\hat{y}^n ln f_{w,b}(x^n) + (1-\hat{y}^n) ln\left(1 - f_{w,b}(x^n)\right)\right]}$$

Cross entropy between two Bernoulli distribution

$$H(p,q) = -\sum_x p(x) ln\big(q(x)\big)$$

Distribution p:

$p(x=1) = \hat{y}^n$

$p(x=0) = 1 - \hat{y}^n$

cross entropy

Distribution q:

$q(x=1) = f(x^n)$

$q(x=0) = 1 - f(x^n)$

Step2: Goodness of a function

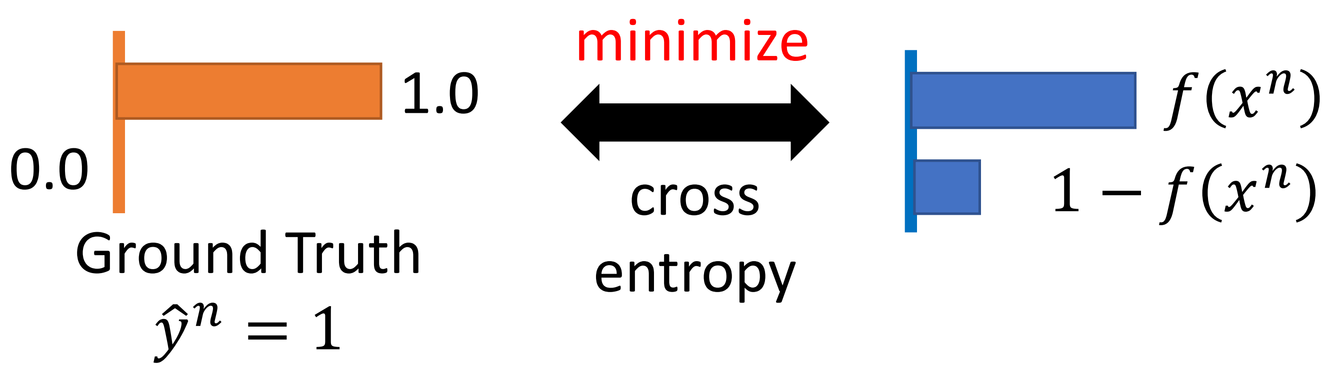
$$L(w,b) = f_{w,b}(x^1) f_{w,b}(x^2) \left(1 - f_{w,b}(x^3)\right) \cdots f_{w,b}(x^N)$$

$$-lnL(w,b) = -\left[ln f_{w,b}(x^1) + ln f_{w,b}(x^2) + ln\left(1 - f_{w,b}(x^3)\right)\right] \cdots$$

$\hat{y}^n$: 1 for class 1, 0 for class 2

$$= \sum_n \underline{-\left[\hat{y}^n ln f_{w,b}(x^n) + (1-\hat{y}^n) ln\left(1 - f_{w,b}(x^n)\right)\right]}$$

Cross entropy between two Bernoulli distribution



	Logistic Regression	Linear Regression
Step 1:	$f_{w,b}(x) = \sigma\left(\sum_i w_i x_i + b\right)$ Output: between 0 and 1	$f_{w,b}(x) = \sum_i w_i x_i + b$ Output: any value
Step 2:	Training data: $(x^n, \hat{y}^n)$ $\boxed{\hat{y}^n\text{: 1 for class 1, 0 for class 2}}$ $L(f) = \sum_n l(f(x^n), \hat{y}^n)$	Training data: $(x^n, \hat{y}^n)$ $\hat{y}^n$: a real number $L(f) = \frac{1}{2}\sum_n \left(f(x^n) - \hat{y}^n\right)^2$

Cross entropy:

$$l(f(x^n), \hat{y}^n) = -\left[\hat{y}^n ln f(x^n) + (1 - \hat{y}^n) ln\left(1 - f(x^n)\right)\right]$$

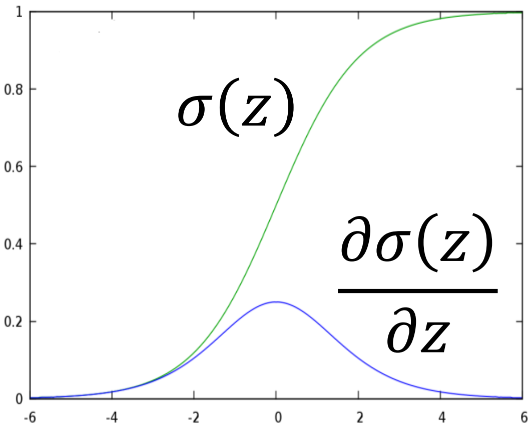
Step3: Find the best function

- Loss: Cross-Entropy $\left(1 - f_{w,b}(x^n)\right) x_i^n$

$$\frac{-lnL(w,b)}{\partial w_i} = \sum_n -\left[\hat{y}^n \boxed{\frac{ln f_{w,b}(x^n)}{\partial w_i}} + (1-\hat{y}^n)\frac{ln\left(1 - f_{w,b}(x^n)\right)}{\partial w_i}\right]$$

$$\frac{\partial ln f_{w,b}(x)}{\partial w_i} = \frac{\partial ln f_{w,b}(x)}{\partial z}\frac{\partial z}{\partial w_i} \qquad \frac{\partial z}{\partial w_i} = x_i$$

$$\frac{\partial ln\sigma(z)}{\partial z} = \frac{1}{\sigma(z)}\frac{\partial \sigma(z)}{\partial z} = \frac{1}{\cancel{\sigma(z)}}\cancel{\sigma(z)}\left(1 - \sigma(z)\right)$$



$$f_{w,b}(x) = \sigma(z)$$
$$= 1/1 + exp(-z)$$

$$z = w \cdot x + b = \sum_i w_i x_i + b$$

Step3: Find the best function

- Loss: Cross-Entropy

$$\left(1-f_{w,b}(x^n)\right)x_i^n \qquad\qquad -f_{w,b}(x^n)x_i^n$$

$$\frac{-lnL(w,b)}{\partial w_i} = \sum_n -\left[\hat{y}^n \boxed{\frac{lnf_{w,b}(x^n)}{\partial w_i}} + (1-\hat{y}^n) \boxed{\frac{ln\left(1-f_{w,b}(x^n)\right)}{\partial w_i}}\right]$$

$$\frac{\partial ln\left(1-f_{w,b}(x)\right)}{\partial w_i} = \frac{\partial ln\left(1-f_{w,b}(x)\right)}{\partial z}\frac{\partial z}{\partial w_i} \qquad \frac{\partial z}{\partial w_i} = x_i$$

$$\frac{\partial ln\left(1-\sigma(z)\right)}{\partial z} = -\frac{1}{1-\sigma(z)}\frac{\partial \sigma(z)}{\partial z} = -\frac{1}{\cancel{1-\sigma(z)}}\sigma(z)\cancel{\left(1-\sigma(z)\right)}$$

$$f_{w,b}(x) = \sigma(z)$$

$$= 1/1 + exp(-z)$$

$$z = w \cdot x + b = \sum_i w_i x_i + b$$

Step3: Find the best function

- Loss: Cross-Entropy

$$\frac{-lnL(w,b)}{\partial w_i} = \sum_n -\left[\hat{y}^n \underbrace{\boxed{\frac{ln f_{w,b}(x^n)}{\partial w_i}}}_{\left(1-f_{w,b}(x^n)\right)x_i^n} + (1-\hat{y}^n) \underbrace{\boxed{\frac{ln\left(1-f_{w,b}(x^n)\right)}{\partial w_i}}}_{-f_{w,b}(x^n)x_i^n}\right]$$

$$= \sum_n -\left[\hat{y}^n \left(1-f_{w,b}(x^n)\right)x_i^n - (1-\hat{y}^n) f_{w,b}(x^n)x_i^n\right]$$

$$= \sum_n -\left[\hat{y}^n \cancel{-\hat{y}^n f_{w,b}(x^n)} - f_{w,b}(x^n) \cancel{+\hat{y}^n f_{w,b}(x^n)}\right] x_i^n$$

$$= \sum_n -\left(\hat{y}^n - f_{w,b}(x^n)\right)x_i^n$$

Larger difference, larger update

$$w_i \leftarrow w_i - \eta \sum_n -\left(\hat{y}^n - f_{w,b}(x^n)\right)x_i^n$$

	Logistic Regression	Linear Regression
Step 1:	$f_{w,b}(x) = \sigma\left(\sum_i w_i x_i + b\right)$ Output: between 0 and 1	$f_{w,b}(x) = \sum_i w_i x_i + b$ Output: any value
Step 2:	Training data: $(x^n, \hat{y}^n)$ $\boxed{\hat{y}^n\text{: 1 for class 1, 0 for class 2}}$ $L(f) = \sum_n l(f(x^n), \hat{y}^n)$	Training data: $(x^n, \hat{y}^n)$ $\hat{y}^n$: a real number $L(f) = \frac{1}{2}\sum_n (f(x^n) - \hat{y}^n)^2$

Step 3:

Logistic regression: $w_i \leftarrow w_i - \eta \sum_n -\left(\underline{\hat{y}^n - f_{w,b}(x^n)}\right) x_i^n$

Linear regression: $w_i \leftarrow w_i - \eta \sum_n -\left(\underline{\hat{y}^n - f_{w,b}(x^n)}\right) x_i^n$

Step3: Find the best function

- Loss: Square Error

Step 1: $f_{w,b}(x) = \sigma\left(\sum_i w_i x_i + b\right)$

Step 2: Training data: $(x^n, \hat{y}^n)$, $\hat{y}^n$: 1 for class 1, 0 for class 2

$$L(f) = \frac{1}{2}\sum_n \left(f_{w,b}(x^n) - \hat{y}^n\right)^2$$

Step 3:

$$\frac{\partial\, (f_{w,b}(x) - \hat{y})^2}{\partial w_i} = 2\left(f_{w,b}(x) - \hat{y}\right) \frac{\partial f_{w,b}(x)}{\partial z} \frac{\partial z}{\partial w_i}$$

$$= 2\left(f_{w,b}(x) - \hat{y}\right) f_{w,b}(x)\left(1 - f_{w,b}(x)\right) x_i$$

$\hat{y}^n = 1$

If $f_{w,b}(x^n) = 1$ (close to target) $\Rightarrow$ $\partial L / \partial w_i = 0$

If $f_{w,b}(x^n) = 0$ (far from target) $\Rightarrow$ $\partial L / \partial w_i = 0$

Step3: Find the best function

- Loss: Square Error

Step 1: $f_{w,b}(x) = \sigma\left(\sum_i w_i x_i + b\right)$

Step 2: Training data: $(x^n, \hat{y}^n)$, $\hat{y}^n$: 1 for class 1, 0 for class 2

$$L(f) = \frac{1}{2}\sum_n \left(f_{w,b}(x^n) - \hat{y}^n\right)^2$$

Step 3:

$$\frac{\partial\,(f_{w,b}(x) - \hat{y})^2}{\partial w_i} = 2\left(f_{w,b}(x) - \hat{y}\right)\frac{\partial f_{w,b}(x)}{\partial z}\frac{\partial z}{\partial w_i}$$

$$= 2\left(f_{w,b}(x) - \hat{y}\right) f_{w,b}(x)\left(1 - f_{w,b}(x)\right) x_i$$

$\hat{y}^n = 0$

If $f_{w,b}(x^n) = 1$ (far from target) $\Rightarrow$ $\partial L / \partial w_i = 0$

If $f_{w,b}(x^n) = 0$ (close to target) $\Rightarrow$ $\partial L / \partial w_i = 0$

Step3: Find the best function

- Based on Gradient Descent Method

Loss: Cross-Entropy

Larger difference, larger update

$$w_i \leftarrow w_i - \eta \sum_n -\underline{\left(\hat{y}^n - f_{w,b}(x^n)\right)} x_i^n$$

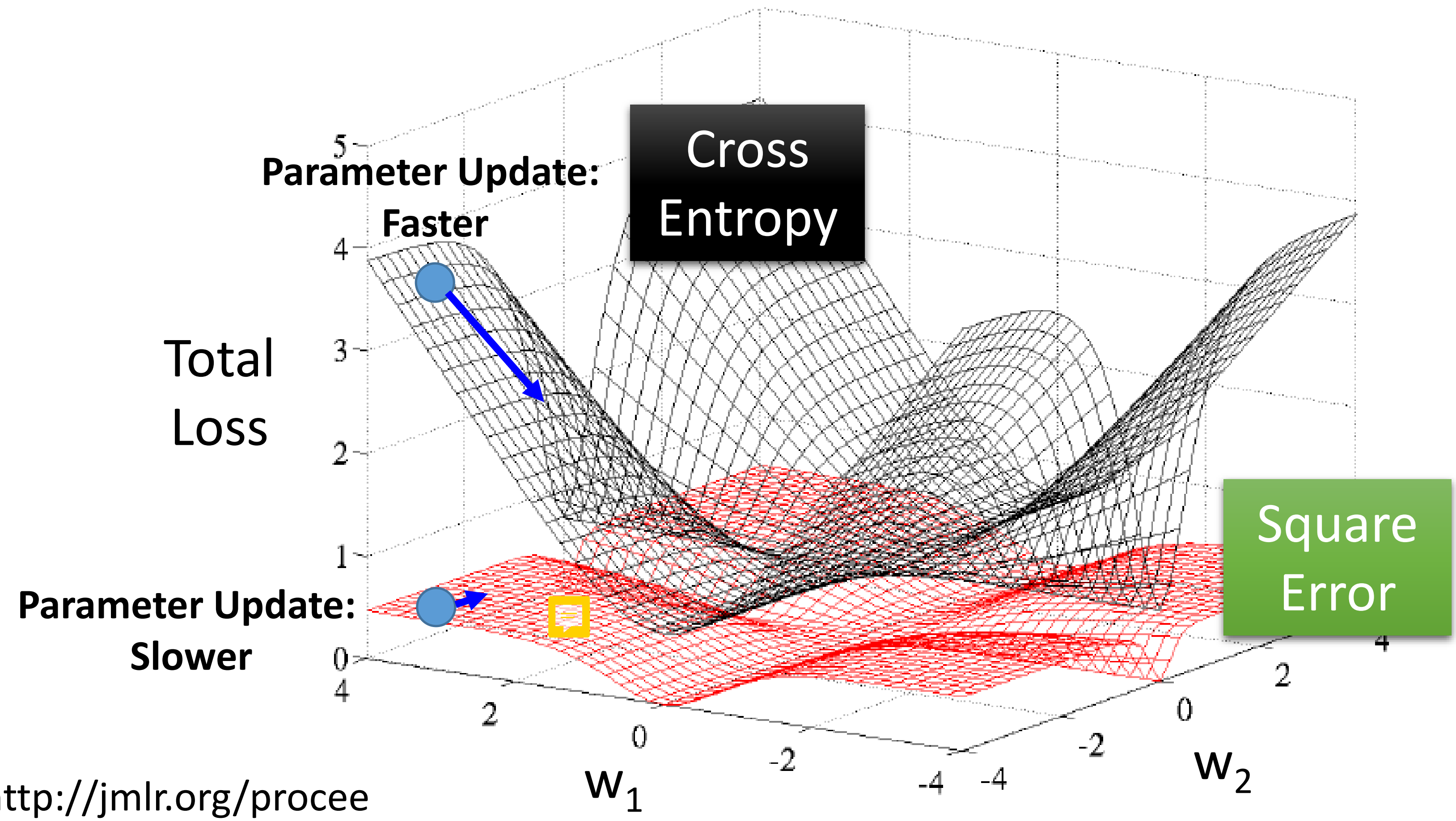
Loss: Square Error

$$L(f) = \frac{1}{2}\sum_n \left(f_{w,b}(x^n) - \hat{y}^n\right)^2$$

$$\frac{\partial\, (f_{w,b}(x) - \hat{y})^2}{\partial w_i}$$

$$= 2\left(f_{w,b}(x) - \hat{y}\right) f_{w,b}(x)\left(1 - f_{w,b}(x)\right) x_i$$

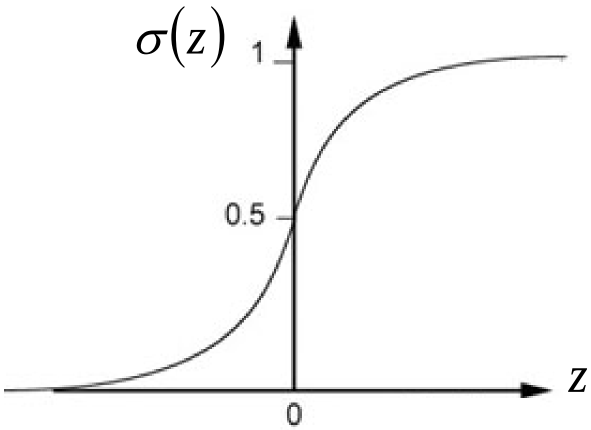
Cross Entropy v.s. Square Error



http://jmlr.org/proceedings/papers/v9/glorot10a/glorot10a.pdf

Logistic Regression

- **Summary**
  - Function set



$$f_{w,b}(x) = \sigma\left(\sum_i w_i x_i + b\right)$$

Output: between 0 and 1

  - Loss: Cross Entropy

$$= \sum_n -\left[\hat{y}^n ln f_{w,b}(x^n) + (1-\hat{y}^n) ln\left(1 - f_{w,b}(x^n)\right)\right]$$

  - Optimization: Gradient Descent

$$w_i \leftarrow w_i - \eta \sum_n -\left(\hat{y}^n - f_{w,b}(x^n)\right) x_i^n$$

Today’s Topics

- Type of classifiers
- Logistic Regression
- ***Logistic Regression vs Linear Regression***
- Limitation of Logistic Regression

	Logistic Regression	***Linear Regression***
Step 1:	$f_{w,b}(x) = \sigma\left(\sum_i w_i x_i + b\right)$ Output: between 0 and 1	$f_{w,b}(x) = \sum_i w_i x_i + b$ Output: any value
Step 2:	Training data: $(x^n, \hat{y}^n)$ $\boxed{\hat{y}^n\text{: 1 for class 1, 0 for class 2}}$ $L(f) = \sum_n l(f(x^n), \hat{y}^n)$	Training data: $(x^n, \hat{y}^n)$ $\hat{y}^n$: a real number $L(f) = \frac{1}{2}\sum_n (f(x^n) - \hat{y}^n)^2$

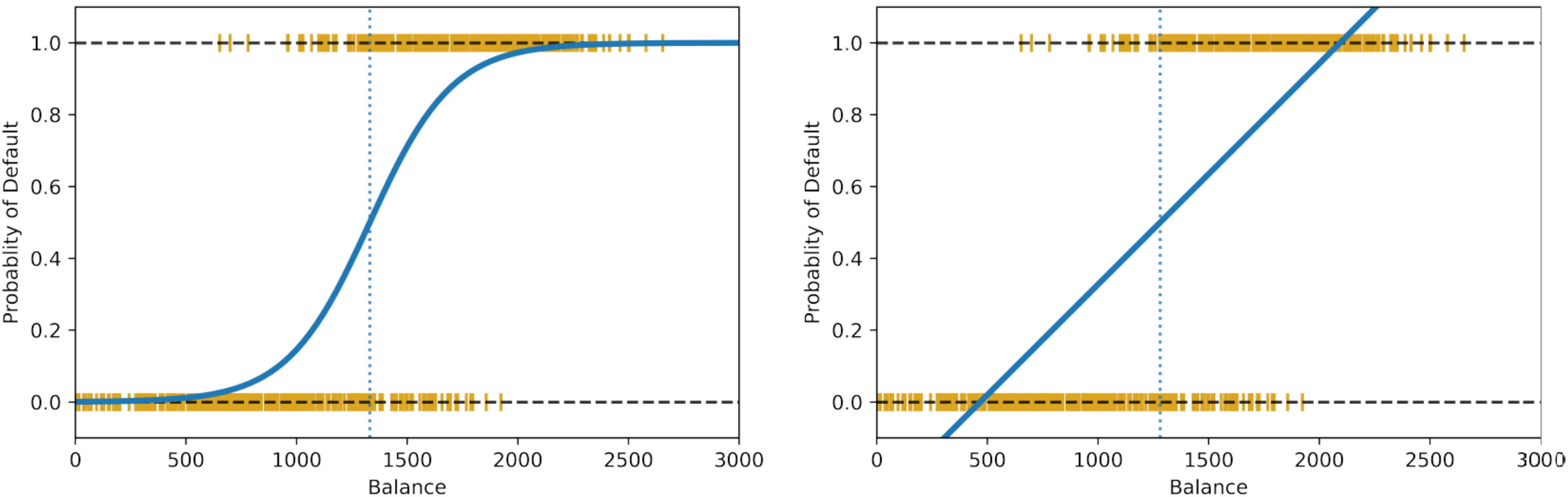
Step 3:

Logistic regression: $w_i \leftarrow w_i - \eta \sum_n -\left(\underline{\hat{y}^n - f_{w,b}(x^n)}\right) x_i^n$

Linear regression: $w_i \leftarrow w_i - \eta \sum_n -\left(\underline{\hat{y}^n - f_{w,b}(x^n)}\right) x_i^n$

Logistic Regression v.s. Linear Regression

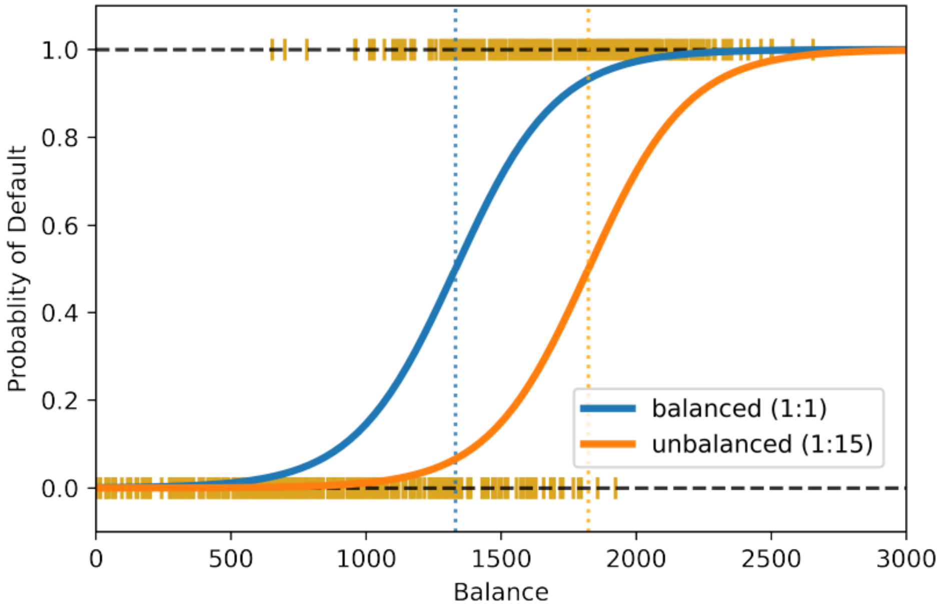
- **From Data**
- Comparison of logistic and linear regression for **balanced** data



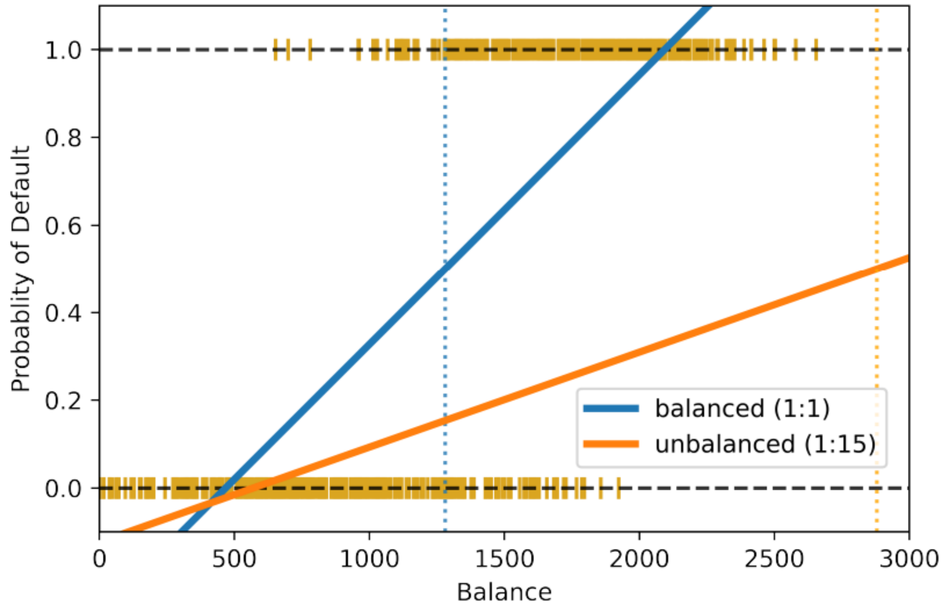
Logistic regression **Linear regression**

Logistic Regression v.s. Linear Regression

- **From Data**
- Comparison of logistic and linear regression for **unbalanced** data



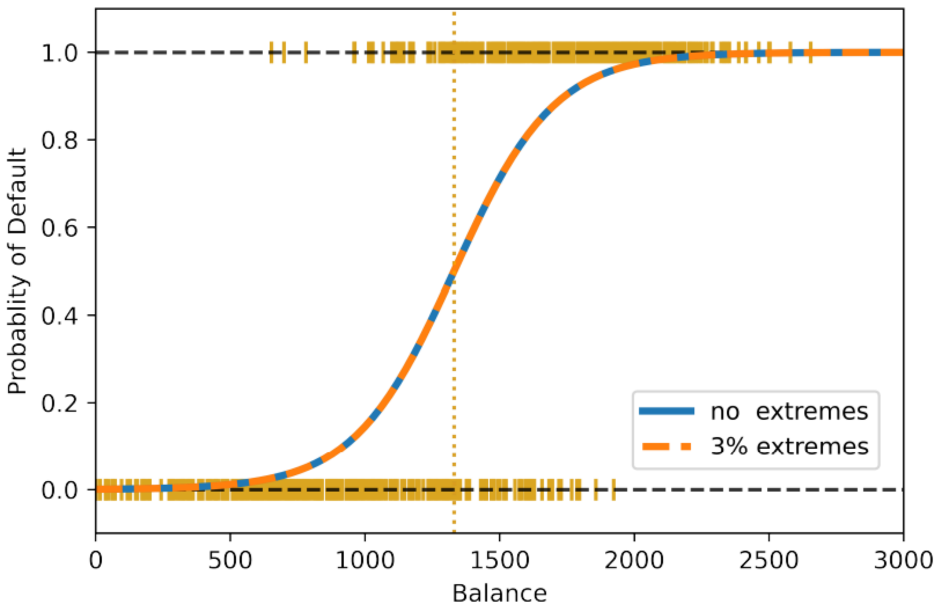
Logistic regression



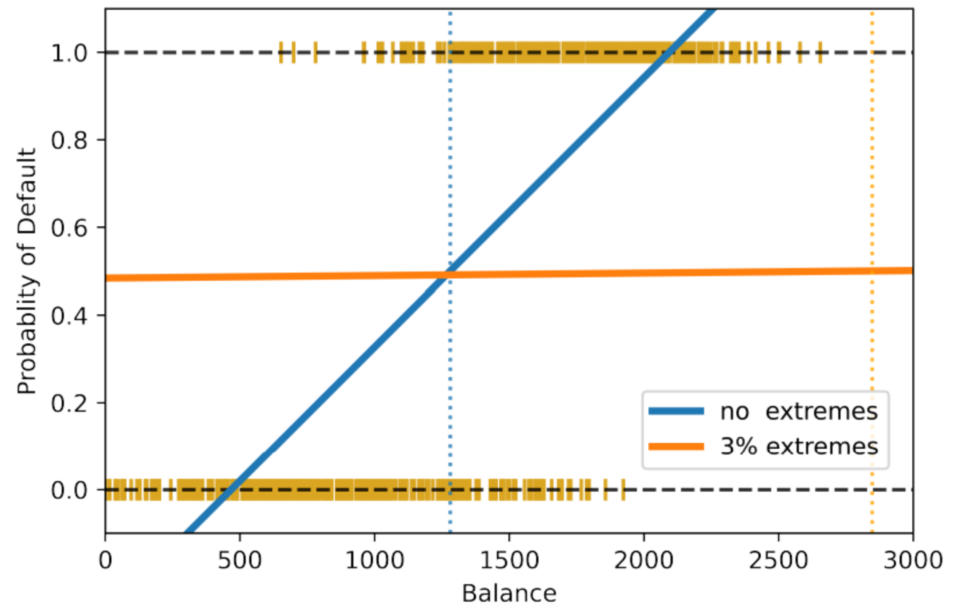
Linear regression

Logistic Regression v.s. Linear Regression

- **From Data**
  - Comparison of logistic and linear regression for data with **extreme values**



Logistic regression



Linear regression

Today's Topics

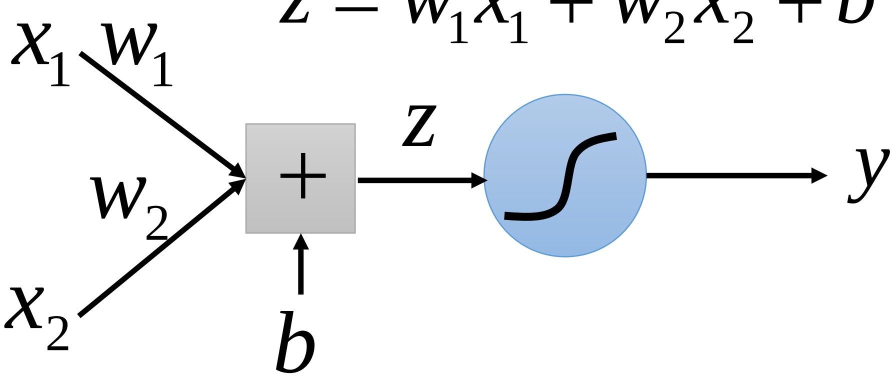
- Type of classifiers
- Logistic Regression
- Logistic Regression vs Linear Regression
- ***Limitation of Logistic Regression***

Limitation of Logistic Regression

- Logistic Regression has some advantages
  - No prior assumptions about data distribution
  - Useful for tasks that require probabilities to make decision
  - Sigmoid is a derivable convex function of any order, and it is easy to find the optimal solution
- But there are situations where logistic regression is powerless

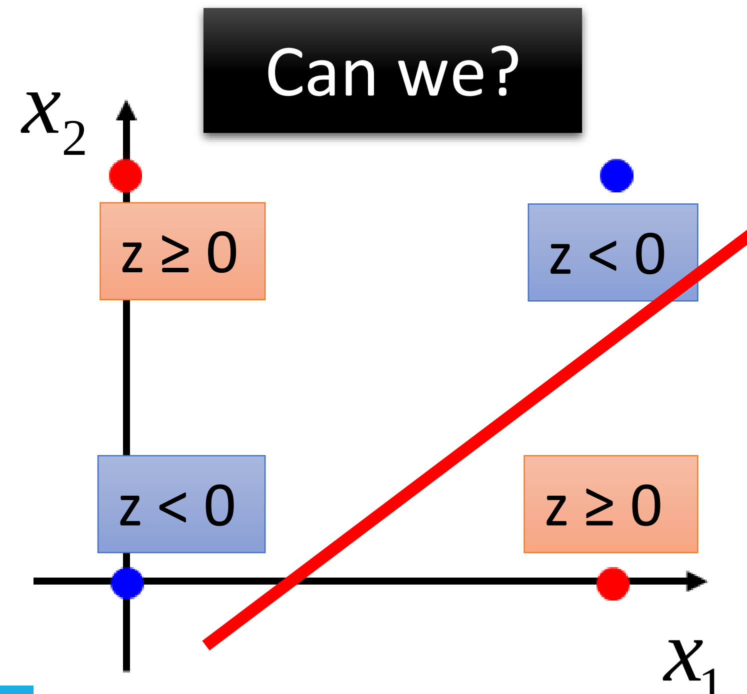
Limitation of Logistic Regression

$$z = w_1 x_1 + w_2 x_2 + b$$



$$\begin{cases} Class1 & y \geq 0.5 \quad (z \geq 0) \\ Class2 & y < 0.5 \quad (z < 0) \end{cases}$$

Input Feature		Label
x_1	x_2	
0	0	Class 2
0	1	Class 1
1	0	Class 1
1	1	Class 2



Limitation of Logistic Regression

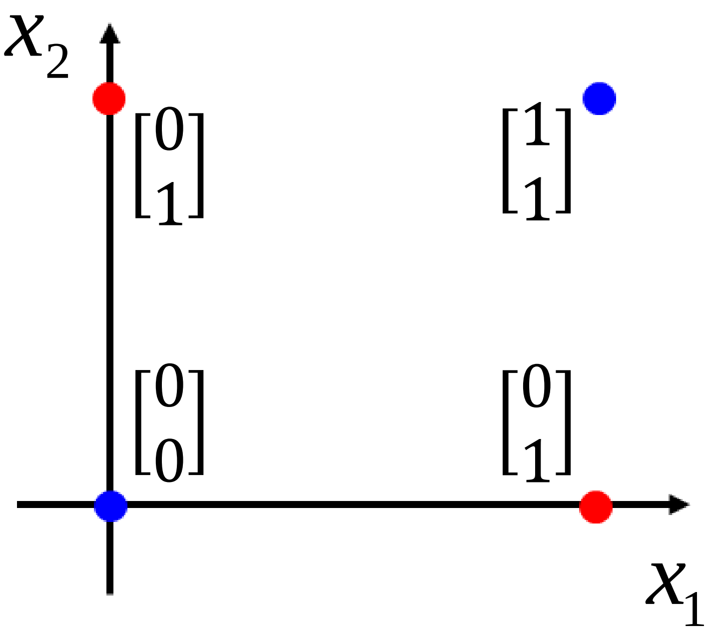
- ***Feature transformation***

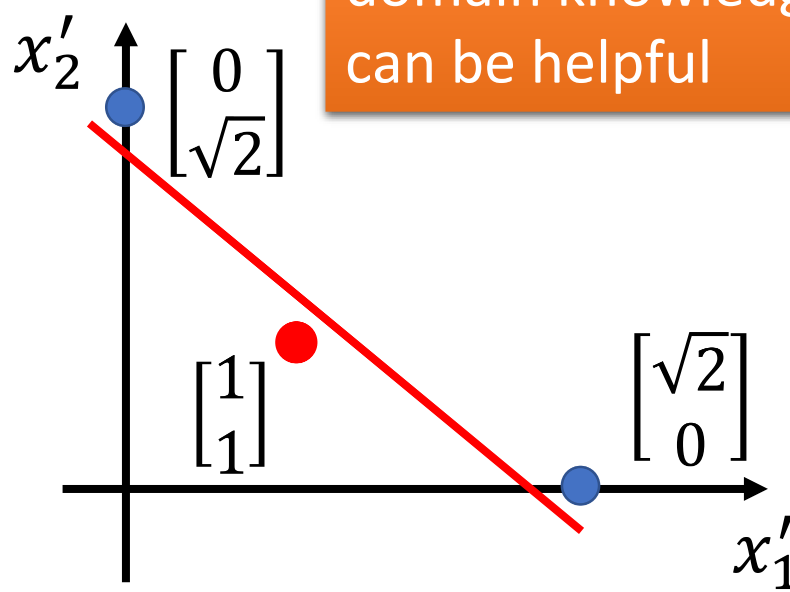
x_1': distance to $\begin{bmatrix}0\\0\end{bmatrix}$

x_2': distance to $\begin{bmatrix}1\\1\end{bmatrix}$

$\begin{bmatrix}x_1\\x_2\end{bmatrix} \longrightarrow \begin{bmatrix}x_1'\\x_2'\end{bmatrix}$

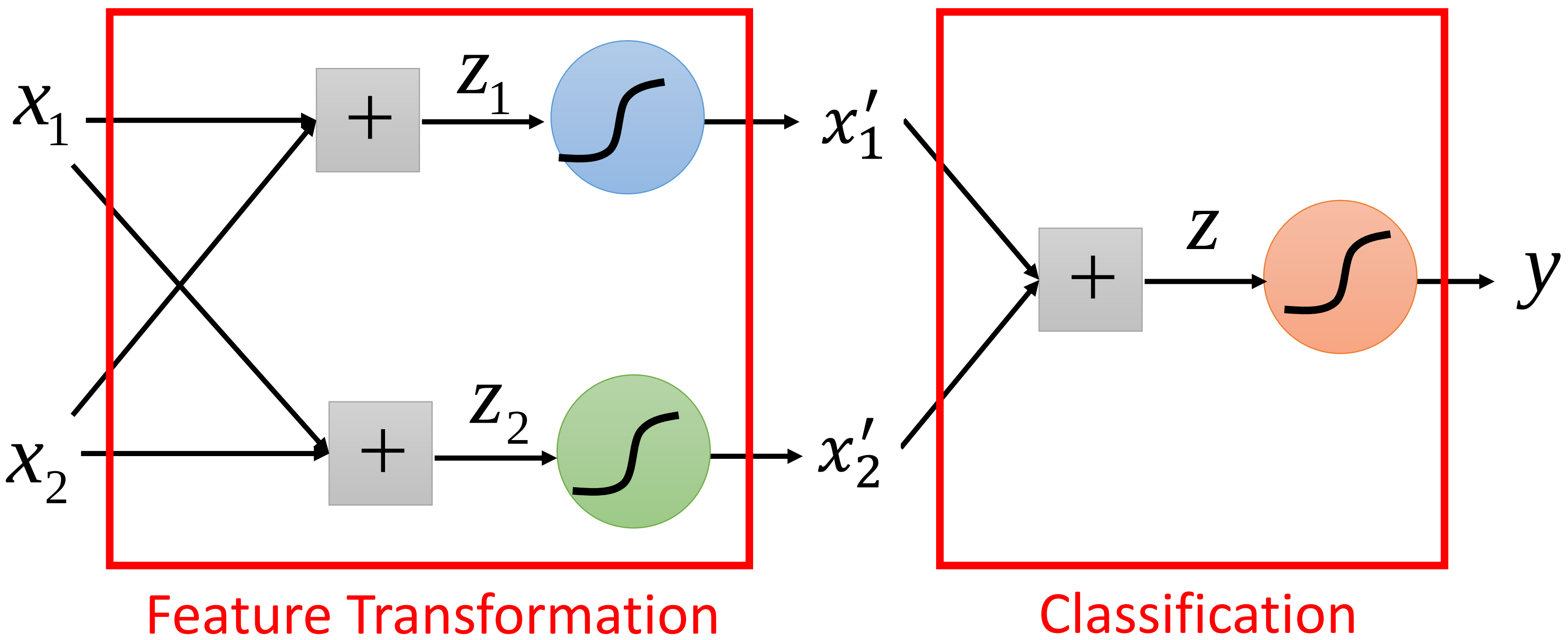
Not always easy ….. domain knowledge can be helpful





Limitation of Logistic Regression

- Cascading logistic regression models



All the parameters of the logistic regressions are jointly learned.

(ignore bias in this figure)

Summary

- **Logistic Regression**
  - Motivation
  - Sigmoid
  - model, loss, optimization
  - Difference with Linear Regression
  - Limitation

Some questions…

- Usually we call logistic regression “逻辑回归”. Is this a reasonable name?
- Can you learn more about the structure?