Artificial Intelligence (CS303)

Lecture 9: Linear Regression & Logistic Regression

Credit: Ansaf Salleb-Aouissi and “Artificial Intelligence, A Modern Approach” Stuart Russell and Peter Norvig. Third Edition. Pearson Education.

Supervised Learning 监督学习

Training data: “examples" x with “labels” y.

$$(x_1, y_1), \ldots, (x_n, y_n),\ x_i \in \mathbb{R}^d$$

- **Regression:** y is a real value, $y \in \mathbb{R}$.

  $f\colon \mathbb{R}^d \to \mathbb{R}$ (f is called a **regressor**) 回归器

- **Classification**: y is discrete. To simplify, $y \in \{-1, +1\}$

  $f\colon \mathbb{R}^d \to \{-1, +1\}$ (f is called a **binary classifier**)

Linear Regression 线性回归

Linear Regression: History

- A very popular technique.
- Rooted in Statistics.
- Method of Least Squares used as early as 1795 by Gauss.
- Re-invented in 1805 by Legendre.
- Frequently applied in **astronomy** to study the large scale of the universe.
- Still a very useful tool today.

Carl Friedrich Gauss

Linear Regression

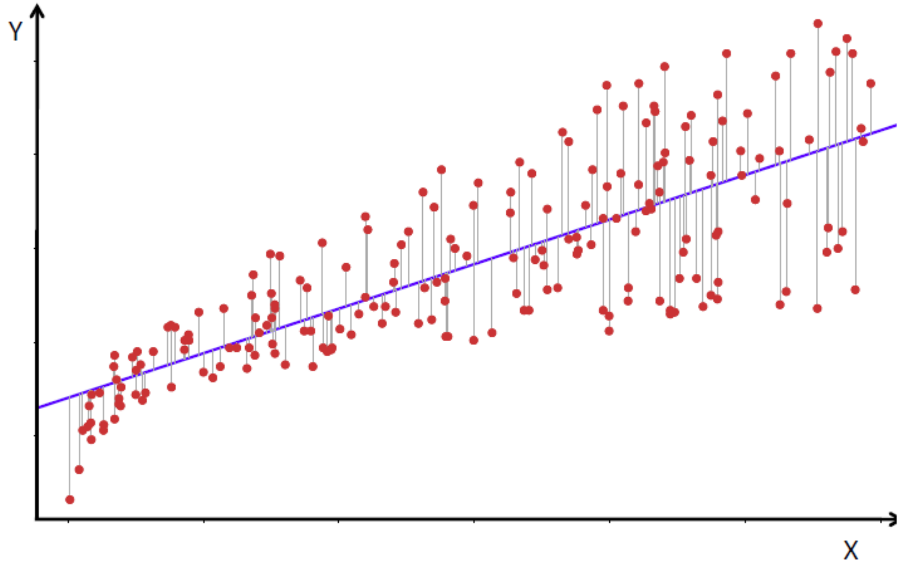
Given: Training data: $(x_1, y_1), \dots, (x_n, y_n)$, $x_i \in \mathbb{R}^d$ and $y \in \mathbb{R}$.

example $x_1 \rightarrow$	x_{11}	x_{12}	$\dots$	x_{1d}	$y_1 \leftarrow$ label
$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$
example $x_i \rightarrow$	x_{i1}	x_{i2}	$\dots$	x_{id}	$y_i \leftarrow$ label
$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$
example $x_n \rightarrow$	x_{n1}	x_{n2}	$\dots$	x_{nd}	$y_n \leftarrow$ label

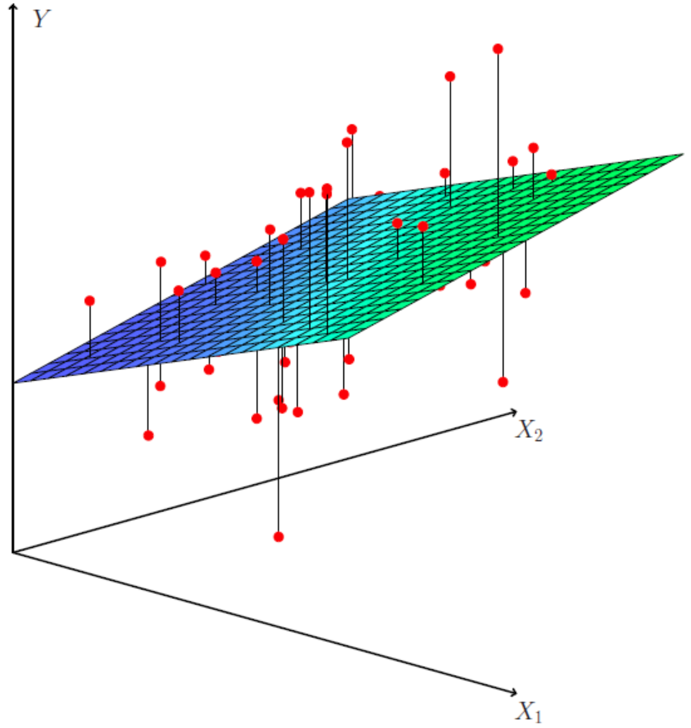
Task: Learn a regression function: $f\colon \mathbb{R}^d \rightarrow \mathbb{R}$, $\boxed{f(x) = y}$

Linear Regression: A regression model is said to be linear if it is represented by a linear function.

Linear Regression



$d = 1$, line in $\mathbb{R}^2$



$d = 2$, hyperplane is $\mathbb{R}^3$

Linear Regression

Linear Regression Model:

$$f(x) = \beta_0 + \sum_{j=1}^{d} \beta_j x_j \quad \text{with} \quad \beta_j \in \mathbb{R}, \quad j \in \{1, \ldots, d\}$$

β 's are called parameters or coefficients or weights.

Learning the linear model → learning the β 's

Estimation with Least squares:

Use least square loss: $\ell oss(y_i, f(x_i)) = (y_i - f(x_i))^2$

We want to minimize the loss over all examples, that is minimize the *risk or cost function R*:

$$R = \frac{1}{2n} \sum_{i=1}^{n} (y_i - f(x_i))^2$$

Linear Regression

A simple case with one feature ($d = 1$): $f(x) = \beta_0 + \beta_1 x$

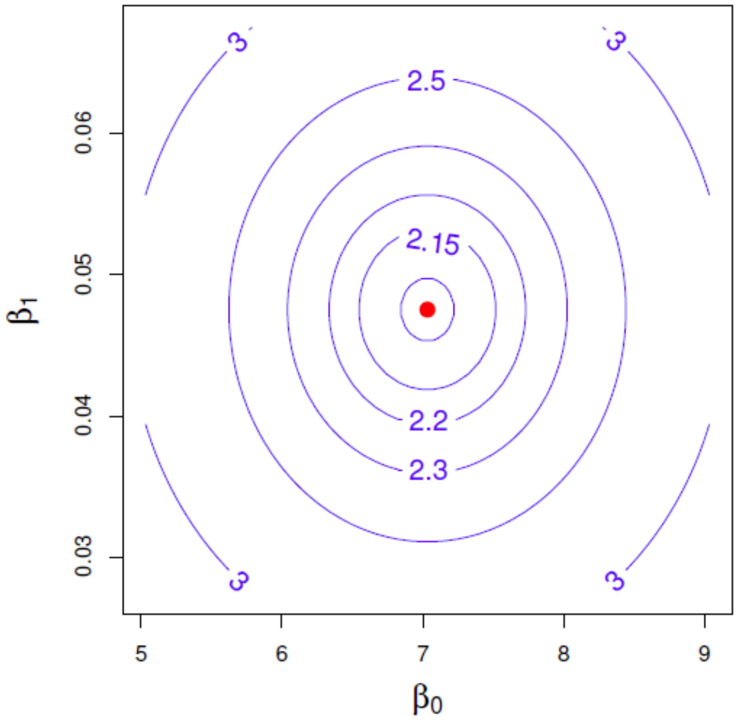
We want to minimize: $R = \frac{1}{2n} \sum_{i=1}^{n} (y_i - f(x_i))^2$

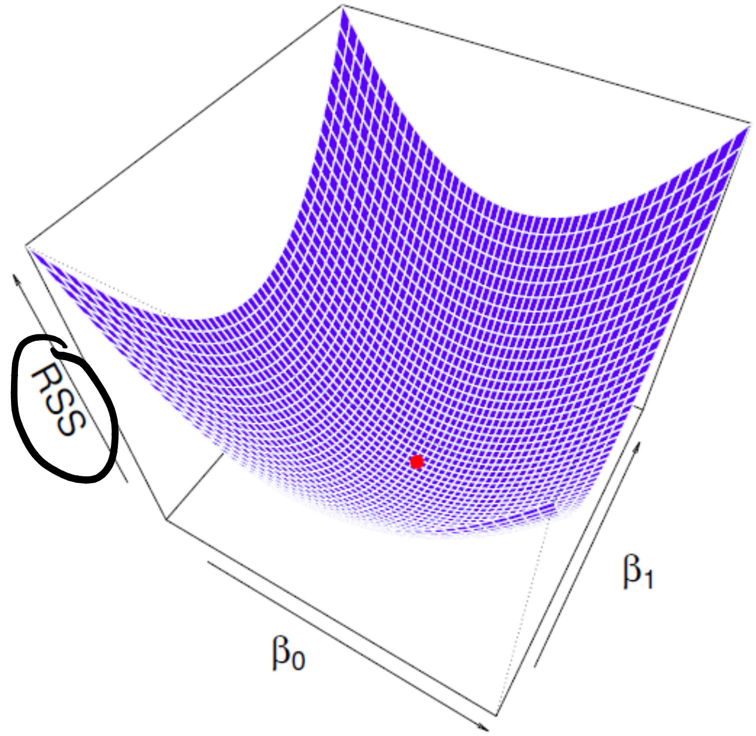
$$R(\beta) = \frac{1}{2n} \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2$$

Find β_0 and β_1 that minimize:

$$R(\beta) = \frac{1}{2n} \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2$$

Linear Regression





Linear Regression

Find β_0 and β_1 that minimize: $argmin_\beta(\frac{1}{2n}\sum_{i=1}^{n}(y_i-\beta_0-\beta_1 x_i)^2)$

Minimize: $R(\beta_0, \beta_1)$, that is: $\frac{\partial R}{\partial \beta_0} = 0$ $\quad \frac{\partial R}{\partial \beta_1} = 0$

$$\frac{\partial R}{\partial \beta_0} = 2 \times \frac{1}{2n}\sum_{i=1}^{n}(y_i-\beta_0-\beta_1 x_i) \times \frac{\partial}{\partial \beta_0}(y_i-\beta_0-\beta_1 x_i)$$

$$\frac{\partial R}{\partial \beta_0} = \frac{1}{n}\sum_{i=1}^{n}(y_i-\beta_0-\beta_1 x_i) \times (-1) = 0$$

$$\beta_0 = \frac{1}{n}\sum_{i=1}^{n} y_i - \beta_1 \frac{1}{n}\sum_{i=1}^{n} x_i$$

Linear Regression

$$\frac{\partial R}{\partial \beta_1} = 2 \times \frac{1}{2n} \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i) \times \frac{\partial}{\partial \beta_1}(y_i - \beta_0 - \beta_1 x_i)$$

$$\frac{\partial R}{\partial \beta_1} = \cancel{\frac{1}{n}} \sum_{i=1}^{n} -(y_i + \beta_0 + \beta_1 x_i) \times (+x_i) = 0$$

$$\beta_1 \sum_{i=1}^{n} {x_i}^2 = \sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} \beta_0 x_i$$

Plugging β_0 and β_1:

$$\beta_1 = \frac{\sum_{i=1}^{n} y_i x_i - \frac{1}{n} \sum_{i=1}^{n} y_i \sum_{i=1}^{n} x_i}{\sum_{i=1}^{n} x_i^2 - \frac{1}{n} \sum_{i=1}^{n} x_i \sum x_i}$$

Linear Regression

$x = (x_1, x_2, x_3 \cdots x_d)$

With more than one feature:

$$f(x) = \beta_0 + \sum_{j=1}^{d} \beta_j x_j$$

Find the β_j that minimize:

$$R = \frac{1}{2n} \sum_{i=1}^{n} (y_i - \beta_0 - \sum_{j=1}^{d} \beta_j x_{ij}))^2$$

Let's write it more elegantly with matrices!

Matrix representation

Let X be an $n \times (d+1)$ matrix where each row starts with a 1 followed by a feature vector.

Let y be the label vector of the training set.

Let β be the vector of weights (that we want to estimate!).

$$X := \begin{pmatrix} 1 & x_{11} & \cdots & x_{1j} & \cdots & x_{1d} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{i1} & \cdots & x_{ij} & \cdots & x_{id} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & \cdots & x_{nj} & \cdots & x_{nd} \end{pmatrix} \qquad y := \begin{pmatrix} y_1 \\ \vdots \\ y_i \\ \vdots \\ y_n \end{pmatrix} \qquad \beta := \begin{pmatrix} \beta_0 \\ \vdots \\ \beta_j \\ \vdots \\ \beta_d \end{pmatrix}$$

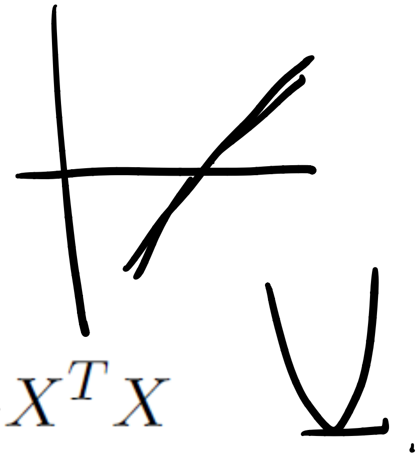
Normal Equation

We want to find $(d+1)$ β's that minimize R. We write R:

$$R(\beta) = \frac{1}{2n}||(y - X\beta)||^2$$

$$R(\beta) = \frac{1}{2n}(y - X\beta)^T(y - X\beta)$$

$$\frac{\partial R}{\partial \beta} = -\frac{1}{n}X^T(y - X\beta)$$



We have that: $\frac{\partial^2 R}{\partial \beta} = +\frac{1}{n}X^T X$

is positive definite which ensures that β is a minimum. We solve:

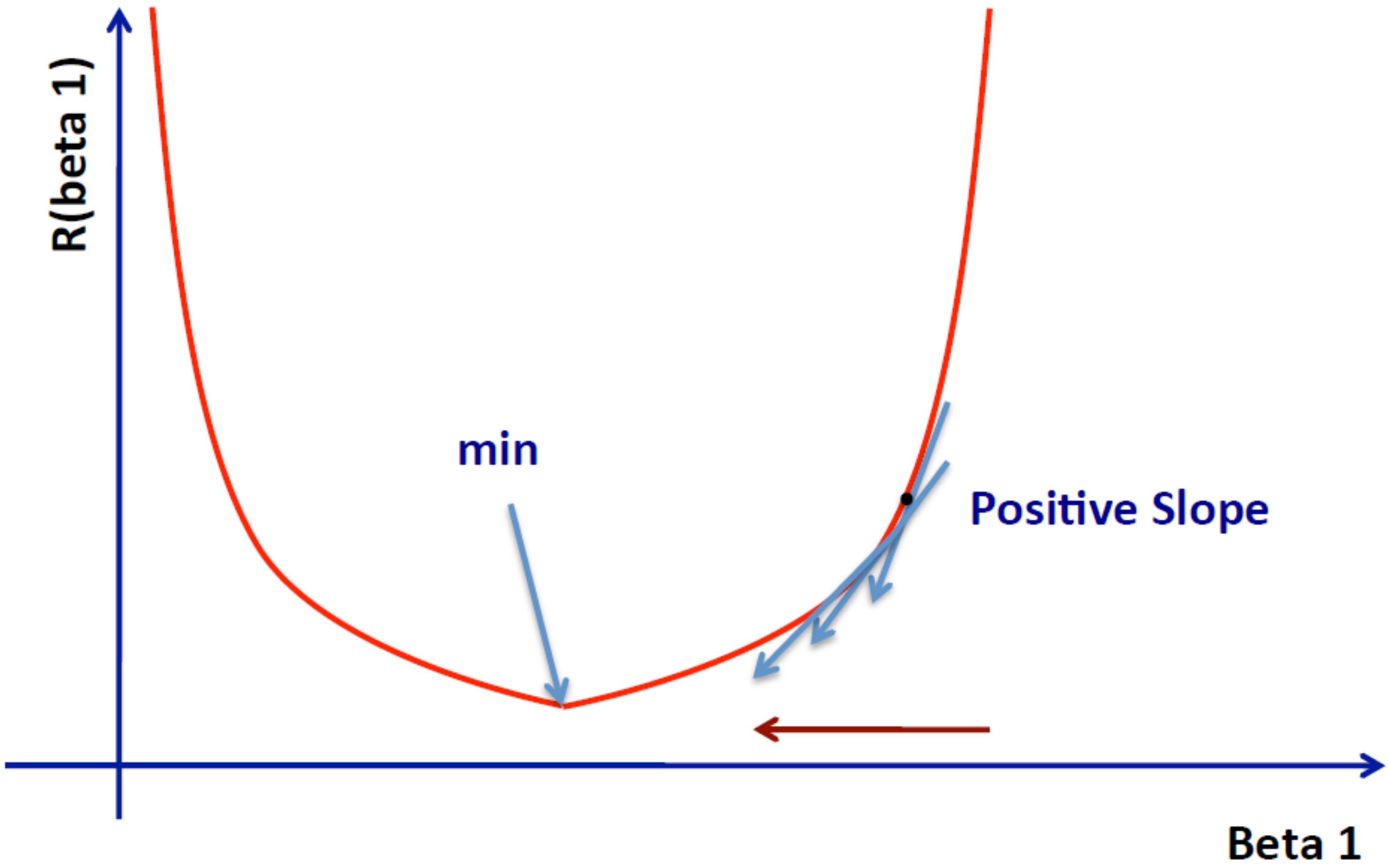
$$X^T(y - X\beta) = 0$$

$$X^T y = X^T X \beta$$

The unique solution is: $\boxed{\beta = (X^T X)^{-1} X^T y}$

Gradient descent

$(X^T X)^{-1} X^T y = \beta$



Gradient descent

Gradient Descent is an optimization method.

Repeat until convergence:

Update **simultaneously** all β_j for (j = 0 and j = 1)

$$\beta_0 := \beta_0 - \alpha \frac{\partial}{\partial \beta_0} R(\beta_0, \beta_1)$$

$$\beta_1 := \beta_1 - \alpha \frac{\partial}{\partial \beta_1} R(\beta_0, \beta_1)$$

α is a learning rate.

Gradient descent

In the linear case:

$$\frac{\partial R}{\partial \beta_0} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_i) \times (-1)$$

$$\frac{\partial R}{\partial \beta_1} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_i) \times (-x_i)$$

Repeat until convergence:

Update **simultaneously** all β_j for (j = 0 and j = 1)

$$\beta_0 := \beta_0 - \alpha\frac{1}{n}\sum_{i=1}^{n}(\beta_0 + \beta_1 x_i - y_i)$$

$$\beta_1 := \beta_1 - \alpha\frac{1}{n}\sum_{i=1}^{n}(\beta_0 + \beta_1 x_i - y_i)(x_i)$$

Pros and Cons

Analytical approach: Normal Equation

+ No need to specify a convergence rate or iterate.
- Works only if $X^T X$ is invertible
- Very slow if d is large $O(d^3)$ to compute $(X^T X)^{-1}$

Iterative approach: Gradient Descent

+ Effective and efficient even in high dimensions.
- Iterative (sometimes need many iterations to converge).
- Needs to choose the rate α.

Practical considerations

1. **Scaling**: Bring your features to a similar scale, e.g., $x_i := \frac{x_i - \mu_i}{stdev(x_i)}$

2. **Learning rate**: Don't use a rate that is too small or too large.
3. **R should decrease** after each iteration.
4. **Declare convergence** if it start decreasing by less ϵ
5. When $X^T X$ is not **invertible**?
   a) Too many features as compared to the number of examples (e.g., 50 examples and 500 features)
   b) Features linearly dependent: e.g., weight in pounds and in kilo.

Logistic Regression

Classification

Given: Training data: $(x_1, y_1), \dots, (x_n, y_n)$, $x_i \in \mathbb{R}^d$ and y_i is discrete (categorical/qualitative), $y_i \in Y$.

Example $Y = \{-1, +1\}$, $Y = \{0, 1\}$

Task: Learn a classification function, $f\colon \mathbb{R}^d \to Y$

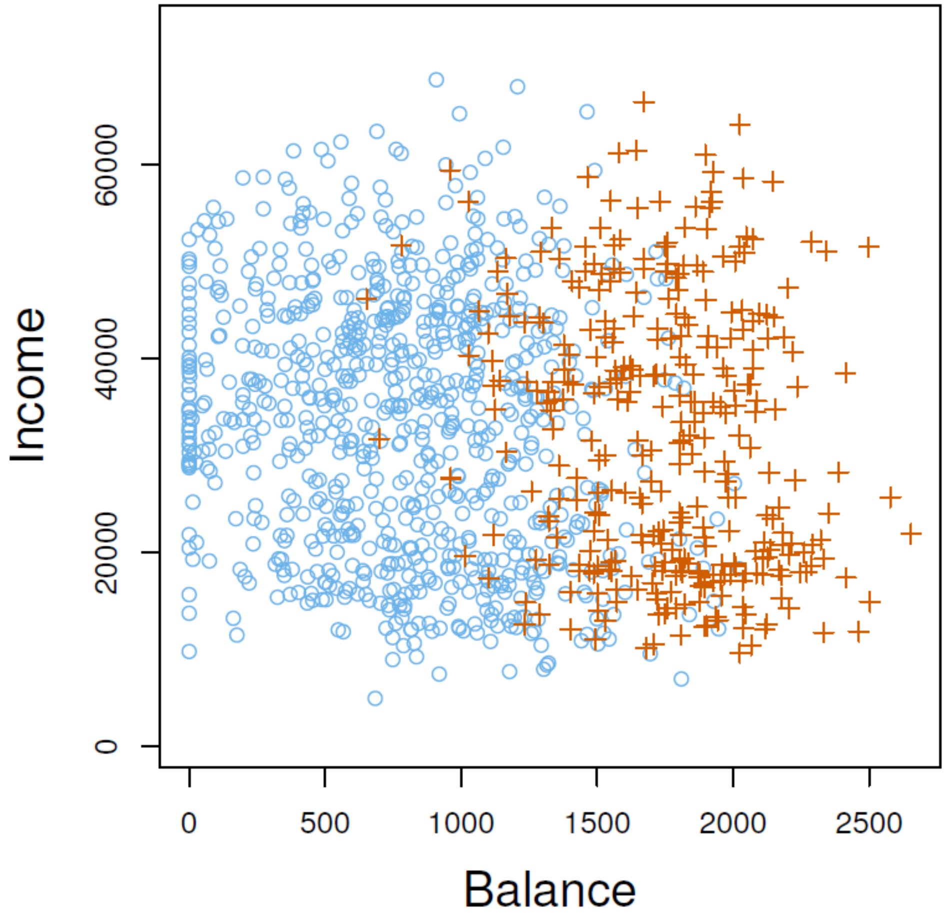
Linear Classification: A classification model is said to be linear if it is represented by a linear function f (linear hyperplane)

Classification: examples

1. Email Spam/Ham → Which email is junk?
2. Tumor benign/malignant → Which patient has cancer?
3. Credit default/not default → Which customers will default on their credit card debt?

Balance	Income	Default
300	$20,000.00	no
2000	$60,000.00	no
5000	$45,000.00	yes
.	.	.
.	.	.
.	.	.

Classification: examples



Classification

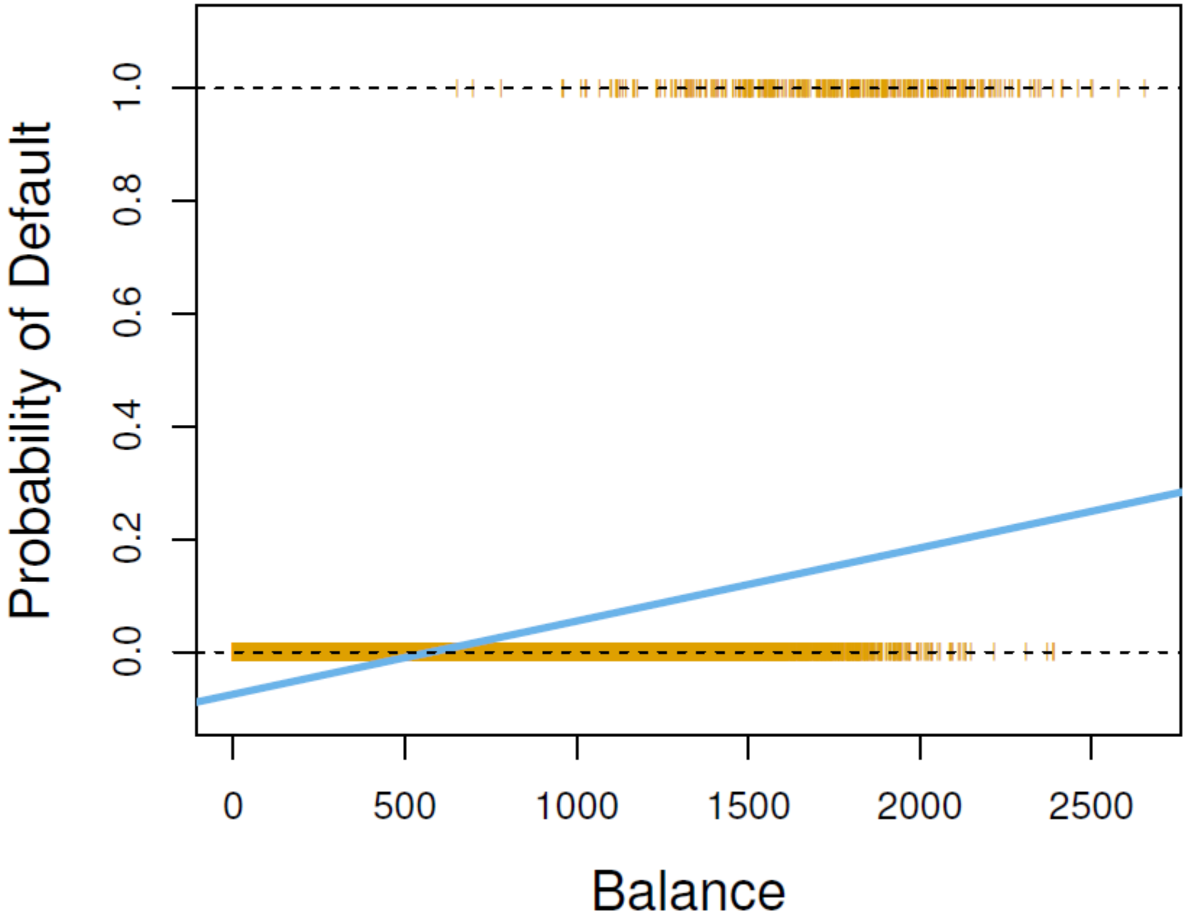
- We can't predict Credit Card Default with any certainty. Suppose we want to predict how likely is a customer to default. That is output a probability between 0 and 1 that a customer will default.
- It makes sense and would be suitable and practical.
- In this case, the output is real (regression) but is bounded (classification).

$$P(y|x) = P(\text{default} = \text{yes} \,|\text{balance})$$

Classification

- Can we use linear regression?
- Yes. However…
  - If we use linear regression, some of the predictions will be outside of [0, 1].
  - Model can be poor.

Classification: example



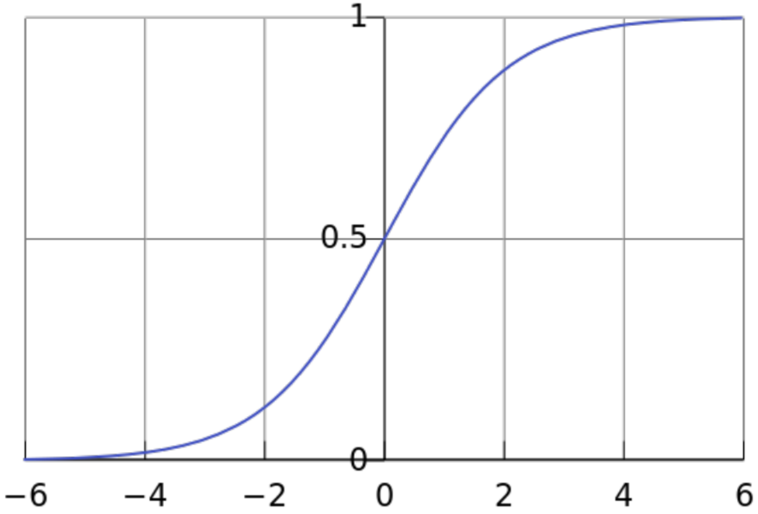
Classification

$$y = f(x) = \beta_0 + \beta_1 x$$

$$\text{Default} = \beta_0 + \beta_1 \times \text{Balance}$$

We want $0 \leq f(x) \leq 1$; $f(x) = P(y = 1|x)$

We use the sigmoid function: $$g(z) = \frac{e^z}{1+e^z} = \frac{1}{1+e^{-z}}$$



$g(z) \rightarrow 1$ when $z \rightarrow +\infty$

$g(z) \rightarrow 0$ when $z \rightarrow -\infty$

Logistic Regression

$$g(\beta_0 + \beta_1 x) = \frac{e^{(\beta_0 + \beta_1 x)}}{1 + e^{(\beta_0 + \beta_1 x)}}$$

$$\boxed{\text{New } f(x) = g(\beta_0 + \beta_1 x)}$$

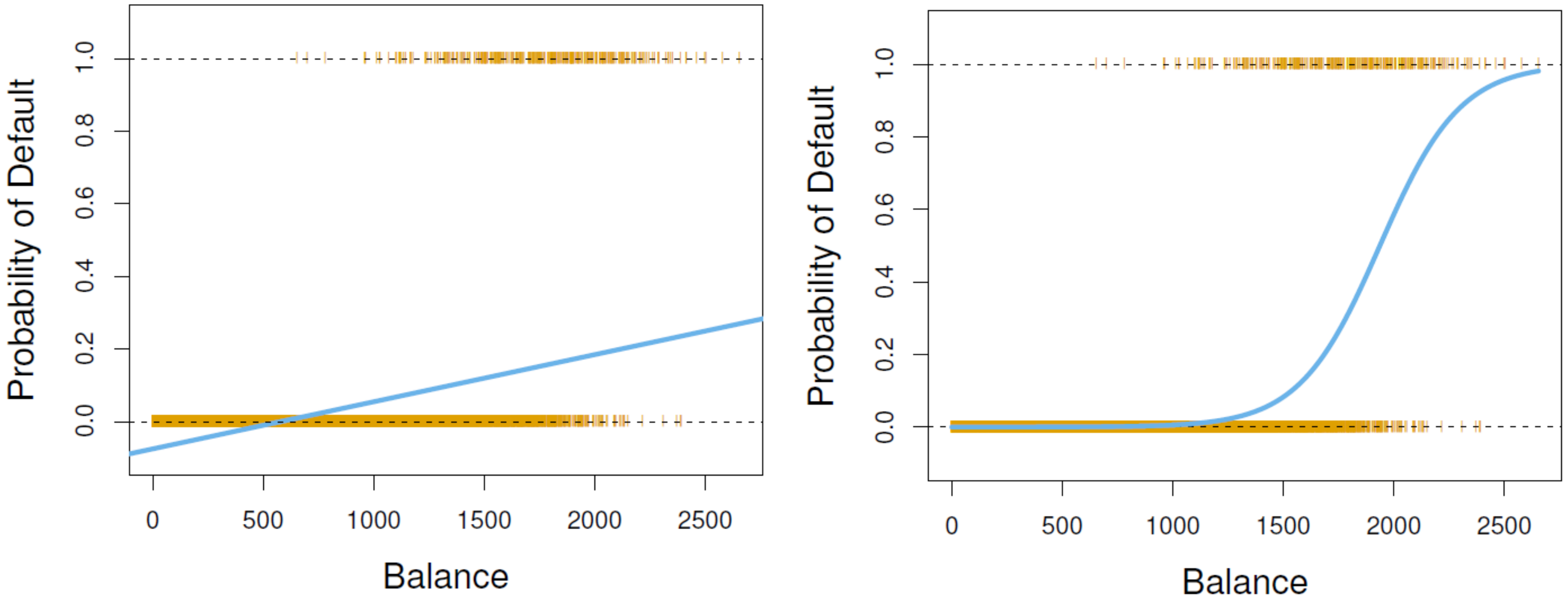
In general:

$$f(x) = g\left(\sum_{j=1}^{d} \beta_j x_j\right)$$

In other words, cast the output to bring the linear function quantity between 0 and 1.

Note: One can use other S-shaped functions.

Logistic Regression



Logistic regression is not a regression method but a classification method!

Logistic Regression

How to make a prediction?

- Suppose β_0 = -10.65 and β_1 = 0.0055. What is the probability of default for a customer with $1,000 balance?

$$P(default = yes|balance = 1000) = \frac{1}{1 + e^{10.65 - 0.0055 * 1000}}$$

$$P(default = yes|balance = 1000) = 0.00576$$

- To predict the class:

$$\text{If} g(z) \geq 0.5 \text{ predict } y = 1 \quad (z \geq 0)$$

$$\text{If} g(z) < 0.5 \text{ predict } y = 0 \quad (z < 0)$$

Logistic Regression

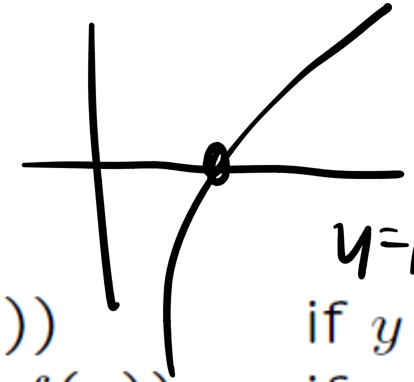
How to find the β 's?

$$R(\beta) = \frac{1}{m}\sum_{i=1}^{m}\frac{1}{2}(f(x) - y)^2$$

$$Loss = \frac{1}{2}(f(x) - y)^2$$

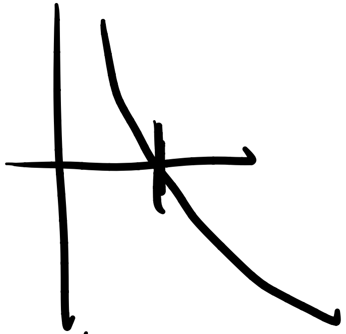
- Remember, $f(x)$ is now the logistic function so the $(f(x) - y)^2$ is not the quadratic function we had when f was linear.
- Cost/risk is a complicated non-linear function!
- Many local optima, hence Gradient Descent will not find the global optimum!
- We need a different function that is convex.

Logistic Regression

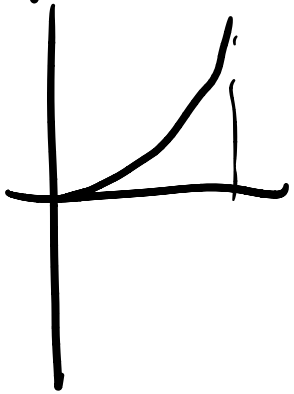


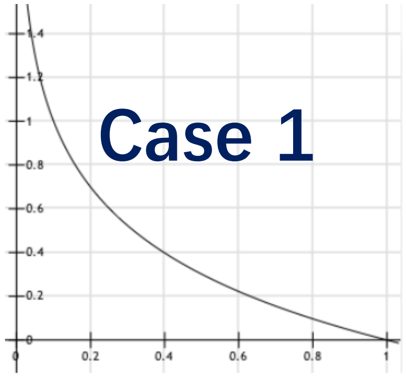
$y=1$ ↗ cost ↓

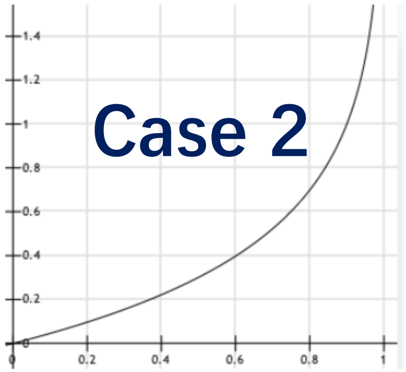
New Convex function: $$Cost(f(x),y) = \begin{cases} -log(f(x)) & \text{if } y=1 \\ -log(1-f(x)) & \text{if } y=0 \end{cases}$$



1. If $y = 1$ if the prediction $f(x) = 1$ then cost $= 0$
2. If $y = 1$ if the prediction $f(x) = 0$ then cost $\rightarrow \infty$
3. If $y = 0$ if the prediction $f(x) = 0$ then cost $\rightarrow 0$
4. If $y = 0$ if the prediction $f(x) = 1$ then cost $= \infty$







Logistic Regression 逻辑回归

Nice convex functions! 凸函数

Let's combine them in a compact function (because $y = 0$ or $y = 1$!):

$$Loss(f(x), y) = -y log f(x) - (1-y) log(1 - f(x))$$

$$R(\beta) = -\frac{1}{m}[\sum_{i=1}^{m} y log f(x) + (1-y) log(1 - f(x))]$$

/β

Gradient Descent

Repeat {

Simultaneously update for all β's

$$\beta_j := \beta_j - \alpha \frac{\partial}{\partial \beta_j} R(\beta)$$

}

After some calculus:

Repeat {

Simultaneously update for all β's

$$\beta_j := \beta_j - \alpha \sum_{i=1}^{m} (f(x) - y) x_j$$

}

Note: Same as linear regression BUT with the new function *f*.

To be continued