26: Logistic Regression

Lisa Yan and Jerry Cain
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Quick slide reference

Background

1. Weighted sum

If $\boldsymbol{X} = (X_1, X_2, \ldots, X_m)$:

$$Z = \theta_1 X_1 + \theta_2 X_2 + \cdots + \theta_m X_m$$

$$= \sum_{j=1}^{m} \theta_j X_j$$ weighted sum

$$= \theta^T \boldsymbol{X}$$ dot product

$$[\theta_1 \quad \theta_2 \quad \quad \theta_m] \begin{bmatrix} X_1 \\ \\ X_m \end{bmatrix}$$

1. Weighted sum

Dot product/ weighted sum $\theta^T \boldsymbol{X} = \sum_{j=1}^{m} \theta_j X_j$

Recall the linear regression model, where $\boldsymbol{X} = (X_1, X_2, \dots, X_m)$ and $Y \in \mathbb{R}$:

$$\hat{Y} = g(\boldsymbol{X}) = \theta_0 + \sum_{j=1}^{m} \theta_j X_j$$

How would you rewrite this expression as a single dot product?

1. Weighted sum

Dot product/ weighted sum $\theta^T \boldsymbol{X} = \sum_{j=1}^{m} \theta_j X_j$

Recall the linear regression model, where $\boldsymbol{X} = (X_1, X_2, \dots, X_m)$ and $Y \in \mathbb{R}$:

$$g(\boldsymbol{X}) = \theta_0 + \sum_{j=1}^{m} \theta_j X_j$$

How would you rewrite this expression as a single dot product?

$$g(\boldsymbol{X}) = \theta_0 X_0 + \theta_1 X_1 + \theta_2 X_2 + \cdots + \theta_m X_m$$

Define $X_0 = 1$

$$= \theta^T \boldsymbol{X}$$

New $\boldsymbol{X} = (1, X_1, X_2, \dots, X_m)$, $\theta = (\theta_0, \theta_1, \dots, \theta_m)$

Prepending $X_0 = 1$ to each feature vector $\boldsymbol{X}$ makes matrix operators more accessible.

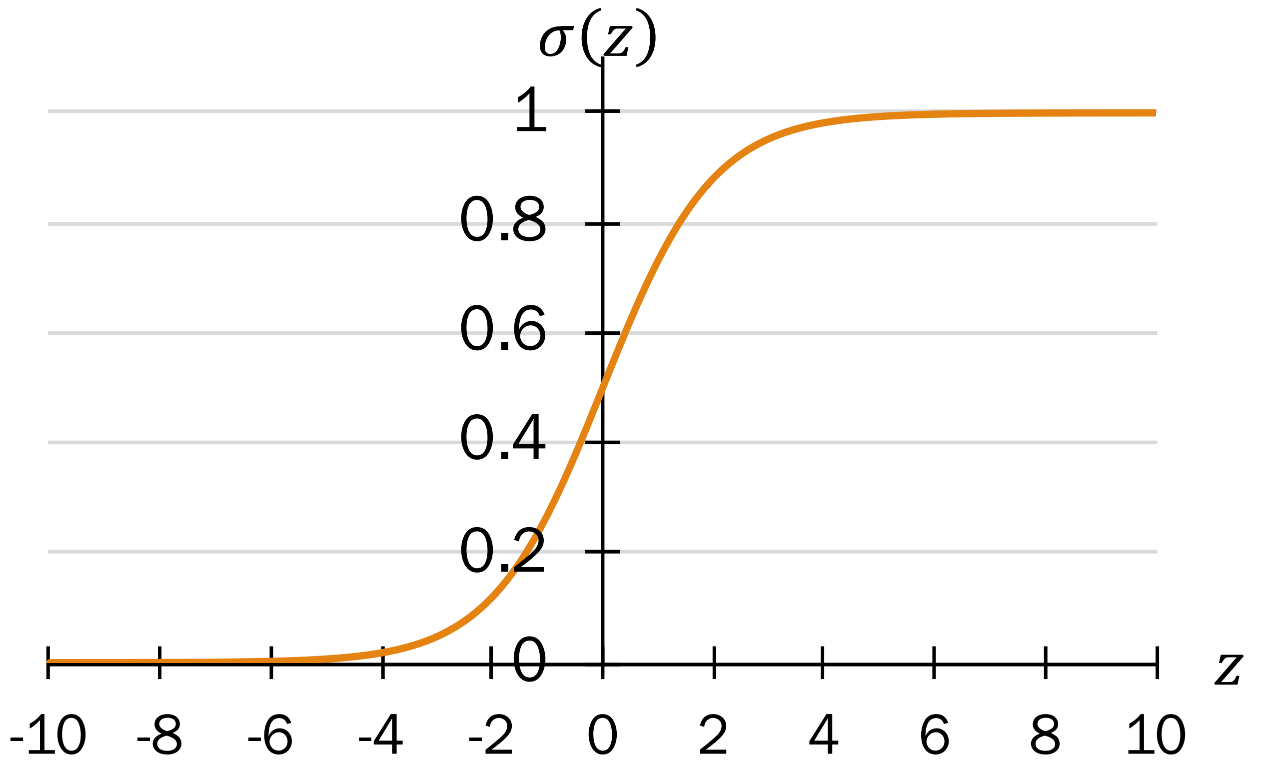
2. Sigmoid function $\sigma(z)$

- The sigmoid function:

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

- Sigmoid squashes z to a number between 0 and 1.

- Recall definition of probability: A number between 0 and 1



$\sigma(z)$ can represent a probability.

3. Conditional likelihood function

Review

Training data (n datapoints):

- $\left(\boldsymbol{x}^{(i)}, y^{(i)}\right)$ drawn i.i.d. from a distribution $f\left(\boldsymbol{X} = \boldsymbol{x}^{(i)}, Y = y^{(i)} | \theta\right) = f\left(\boldsymbol{x}^{(i)}, y^{(i)} | \theta\right)$

$$\theta_{MLE} = \arg\max_{\theta} \prod_{i=1}^{n} f\left(y^{(i)} | \boldsymbol{x}^{(i)}, \theta\right)$$

conditional likelihood of training data

$$= \arg\max_{\theta} \sum_{i=1}^{n} \log f\left(y^{(i)} | \boldsymbol{x}^{(i)}, \theta\right)$$

log conditional likelihood

$$= \arg\max_{\theta} LL(\theta)$$

- MLE in this lecture is estimator that maximizes conditional likelihood
- Confusingly, log conditional likelihood is also written as $LL(\theta)$

Logistic Regression

Prediction models so far

Linear Regression (Regression)

X ➡ $\boxed{\theta_0 + \sum_{j=1}^{m} \theta_j X_j}$ ➡ $\hat{Y}$

$\hat{Y} = \theta_0 + \sum_{j=1}^{m} \theta_j X_j$

✅ $\boldsymbol{X}$ can be dependent

🤷‍♀️ Regression model ($\hat{Y} \in \mathbb{R}$, not discrete)

Naïve Bayes (Classification)

$\boldsymbol{X}$, Y ➡ $\boxed{\hat{P}(\boldsymbol{X}|Y)\hat{P}(Y)}$ ➡ $\hat{P}(\boldsymbol{X}, Y)$

$$\hat{Y} = \arg\max_{y=\{0,1\}} \boxed{P(Y \mid \boldsymbol{X})}$$
$$= \arg\max_{y=\{0,1\}} P(\boldsymbol{X}|Y)P(Y)$$

✅ Tractable with NB assumption, but...

⚠️ Realistically, X_j features not necessarily conditionally independent

🤷‍♀️ Actually models $P(\boldsymbol{X}, Y)$, not $P(Y|\boldsymbol{X})$?

Introducing Logistic Regression!

Linear Regression ideas

Classification models

+ compute power

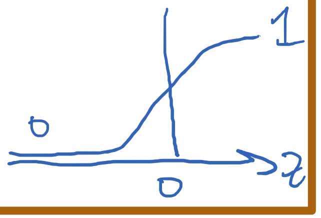
Logistic Regression

$z \in \mathbb{R}$

$\boldsymbol{X} \rightarrow \boxed{\theta_0 + \sum_{j=1}^{m} \theta_j X_j} \xrightarrow{z}$

sigmoid function

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



$\rightarrow P(Y = 1|\boldsymbol{X})$

Logistic Regression Model:

$$P(Y = 1|\boldsymbol{X} = \boldsymbol{x}) = \sigma\left(\theta_0 + \sum_{j=1}^{m} \theta_j x_j\right)$$

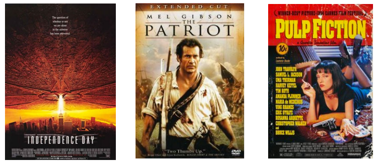
Predict $\hat{Y}$ as the most likely Y given our observation $\boldsymbol{X} = \boldsymbol{x}$:

$$\hat{Y} = \underset{y=\{0,1\}}{\arg\max}\, P(Y \mid \boldsymbol{X})$$

- Since $Y \in \{0,1\}$, $\quad P(Y = 0|\boldsymbol{X} = \boldsymbol{x}) = 1 - \sigma\left(\theta_0 + \sum_{j=1}^{m} \theta_j x_j\right)$
- Sigmoid function also known as “logit” function

Logistic Regression

$\boldsymbol{x} = [0,1,1]$



$\boldsymbol{X}$

input features

θ parameter

0.81

$P(Y = 1|\boldsymbol{X} = \boldsymbol{x})$

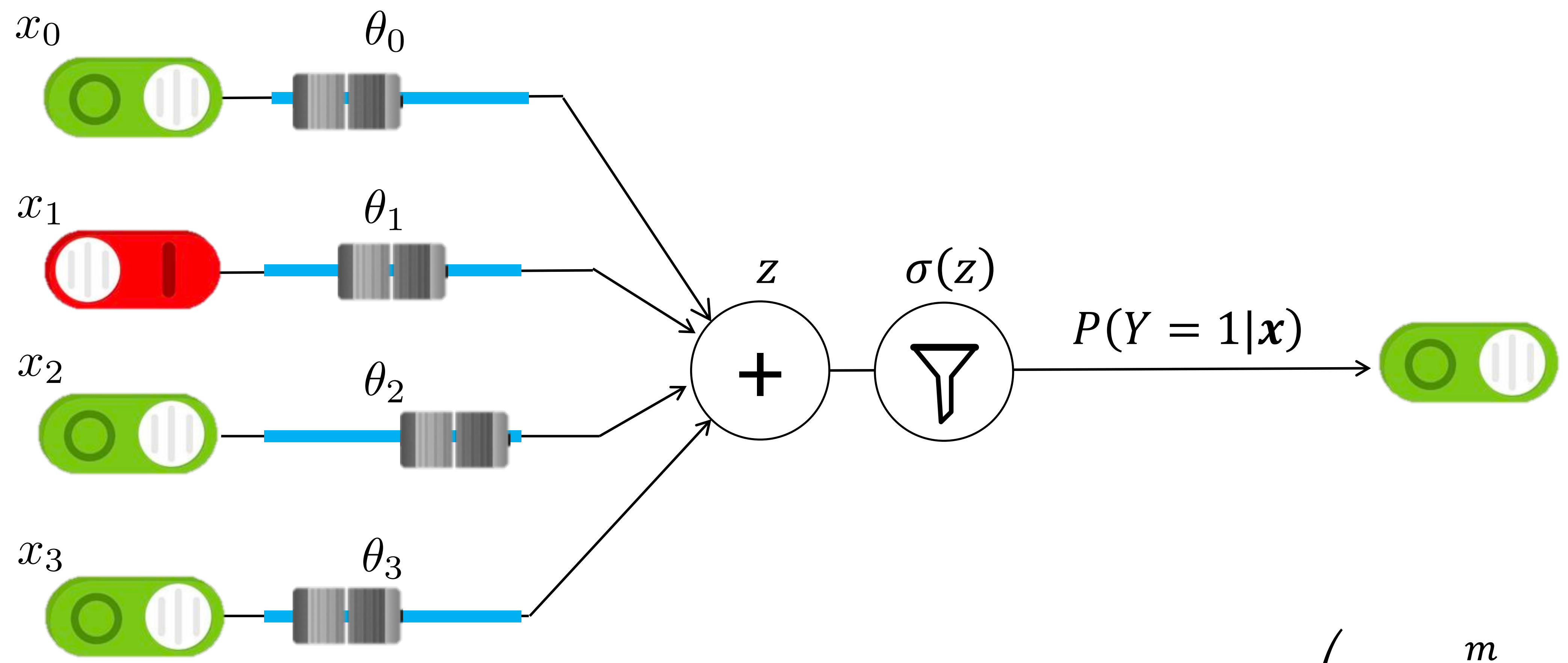
conditional likelihood

$$P(Y = 1|\boldsymbol{X} = x) = \sigma\left(\theta_0 + \sum_{j=1}^{m} \theta_j x_j\right)$$

Logistic Regression cartoon

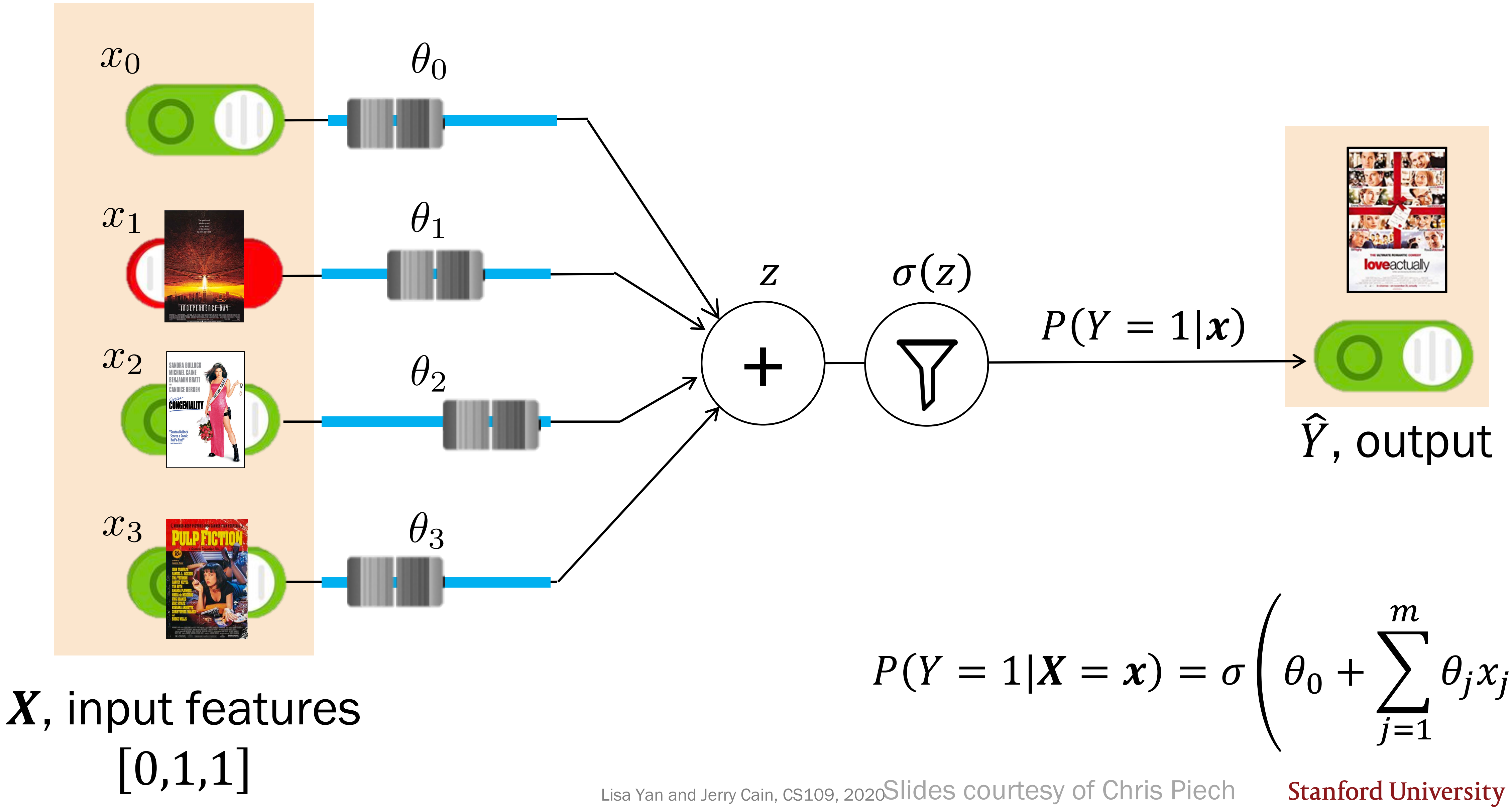
θ parameter

Logistic Regression cartoon



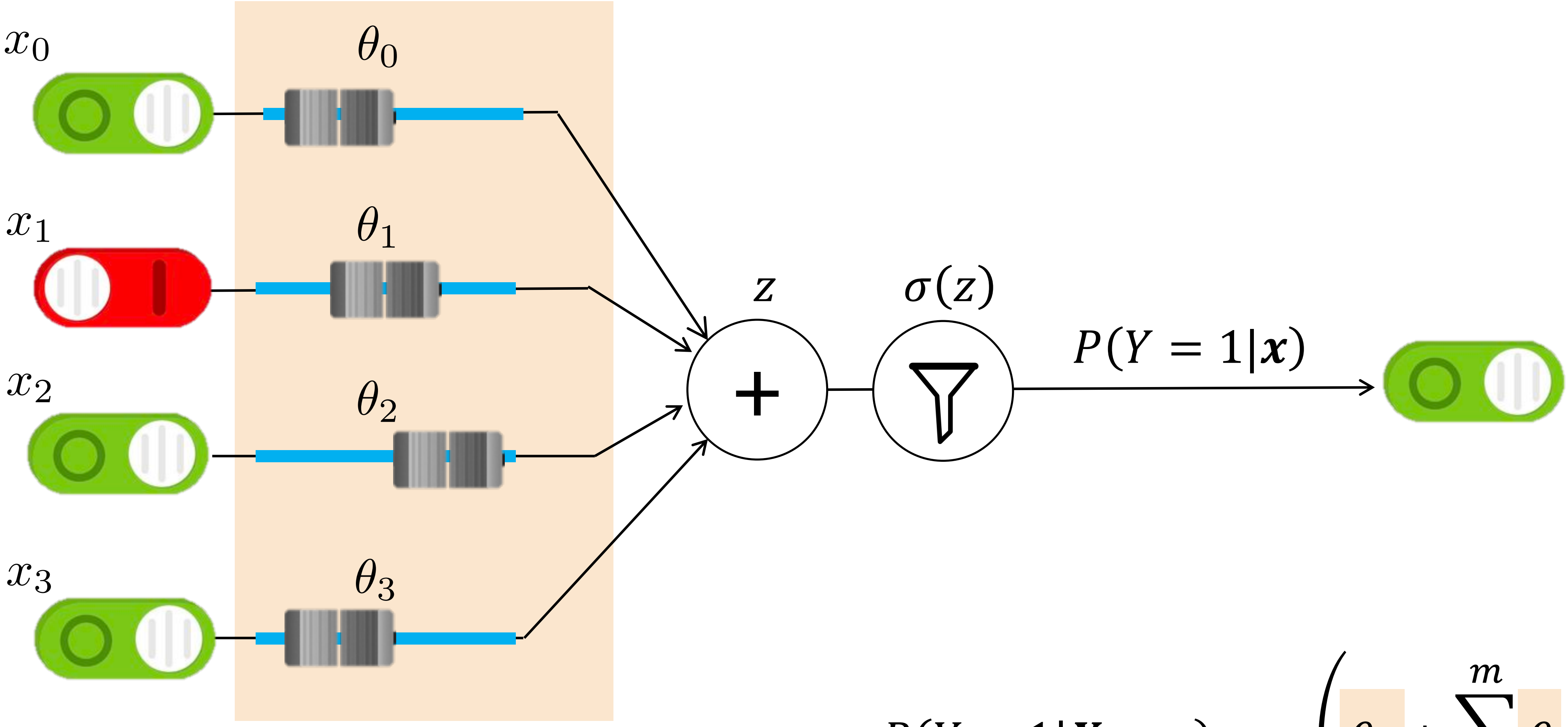
$$P(Y = 1|\boldsymbol{X} = \boldsymbol{x}) = \sigma\left(\theta_0 + \sum_{j=1}^{m} \theta_j x_j\right)$$

Logistic Regression cartoon



$$P(Y = 1|\boldsymbol{X} = \boldsymbol{x}) = \sigma\left(\theta_0 + \sum_{j=1}^{m} \theta_j x_j\right)$$

Components of Logistic Regression

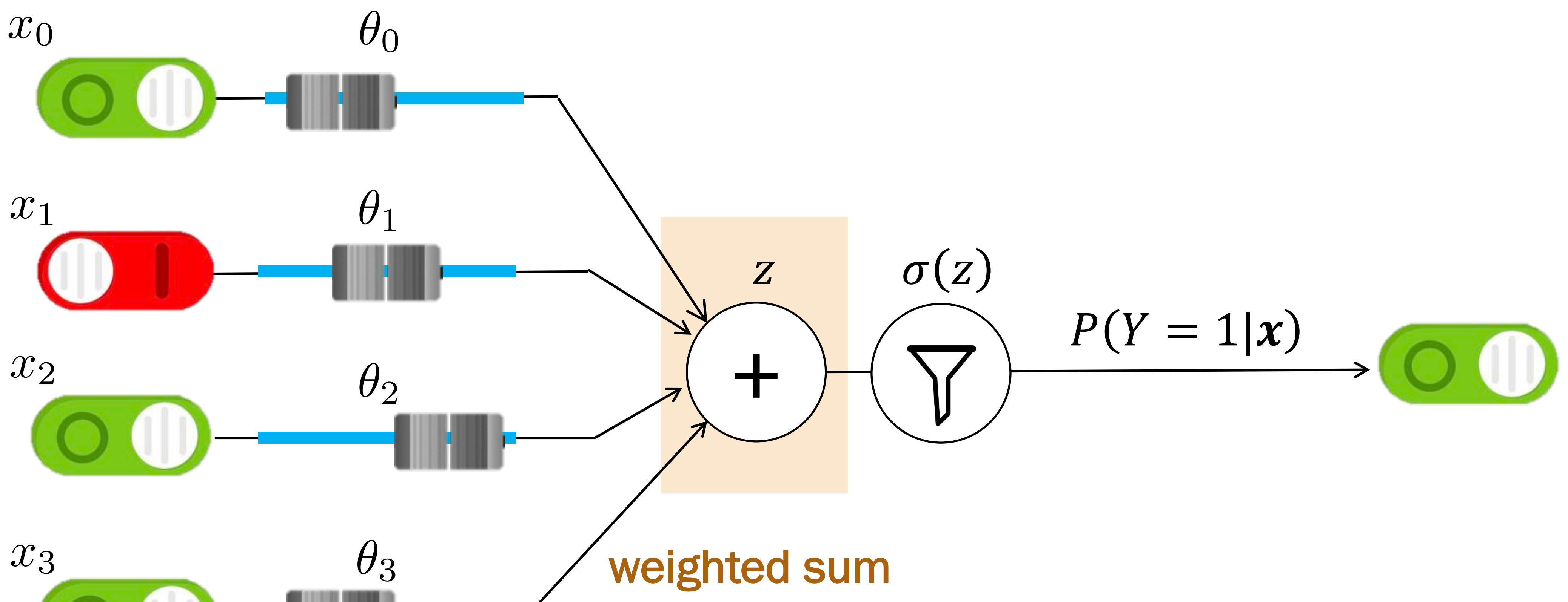


θ **weights**

(aka parameters)

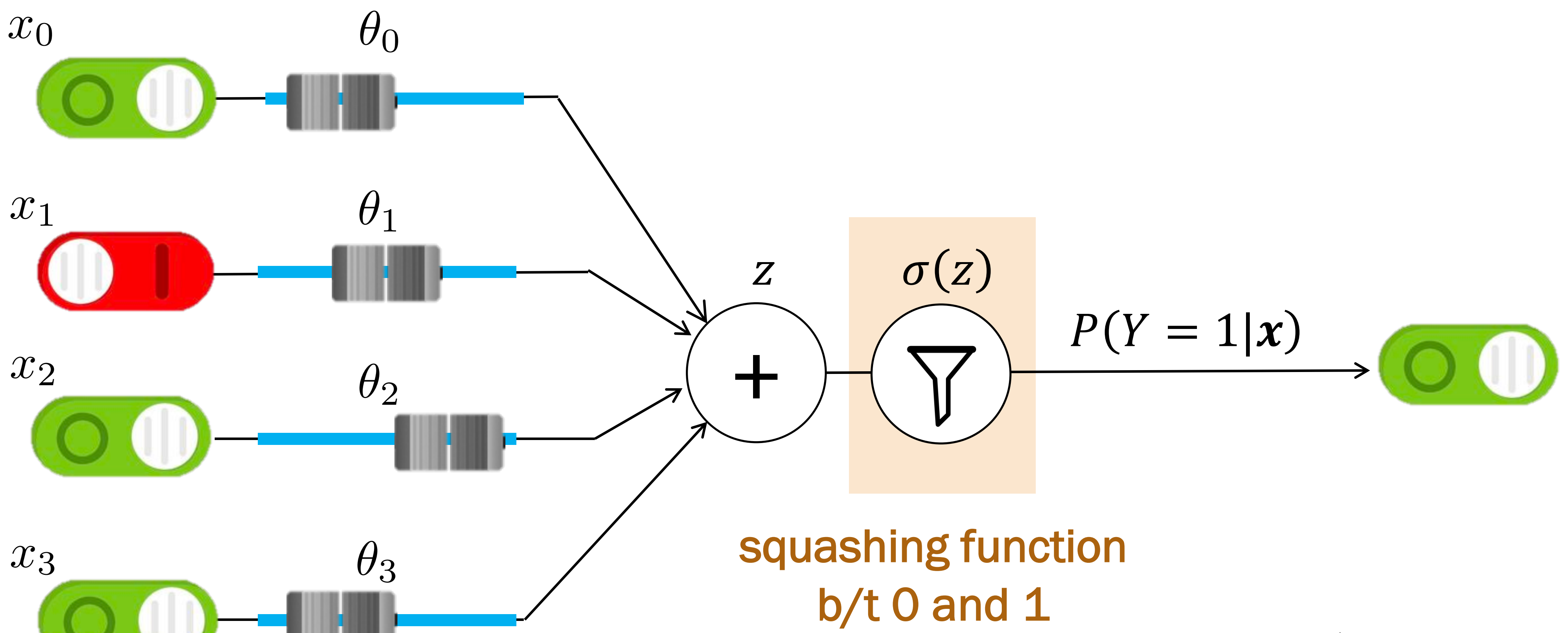
$$P(Y = 1|\boldsymbol{X} = \boldsymbol{x}) = \sigma\left(\theta_0 + \sum_{j=1}^{m} \theta_j x_j\right)$$

Components of Logistic Regression



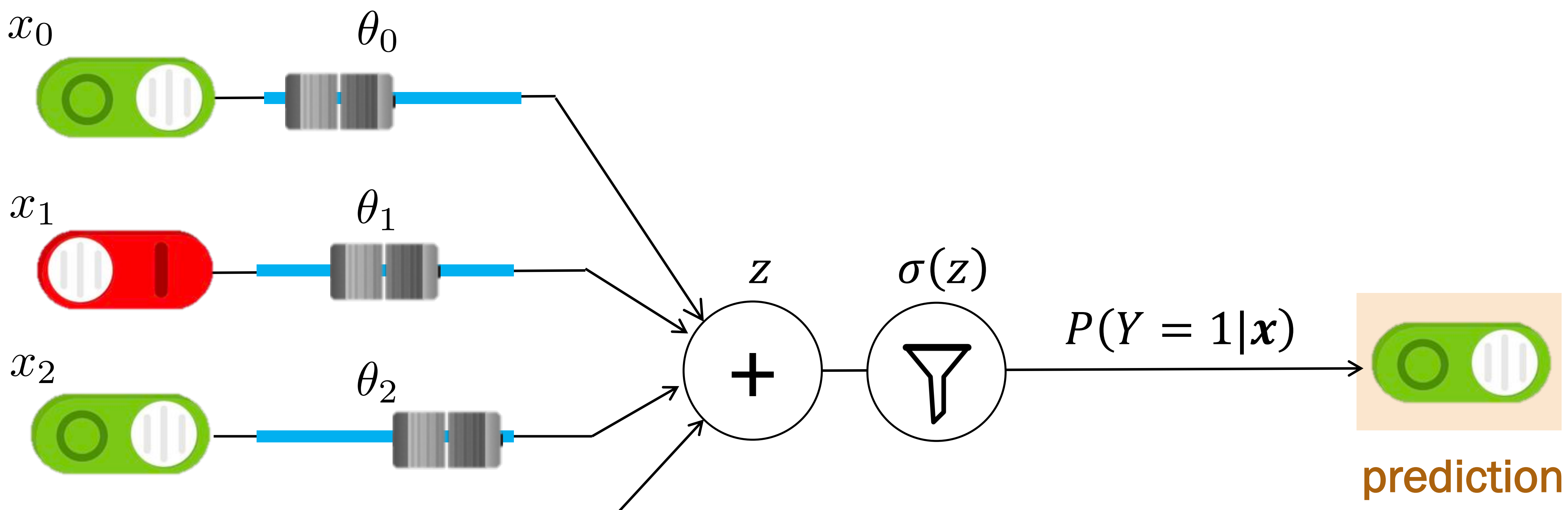
$$P(Y = 1|\boldsymbol{X} = \boldsymbol{x}) = \sigma\left(\theta_0 + \sum_{j=1}^{m} \theta_j x_j\right)$$

Components of Logistic Regression



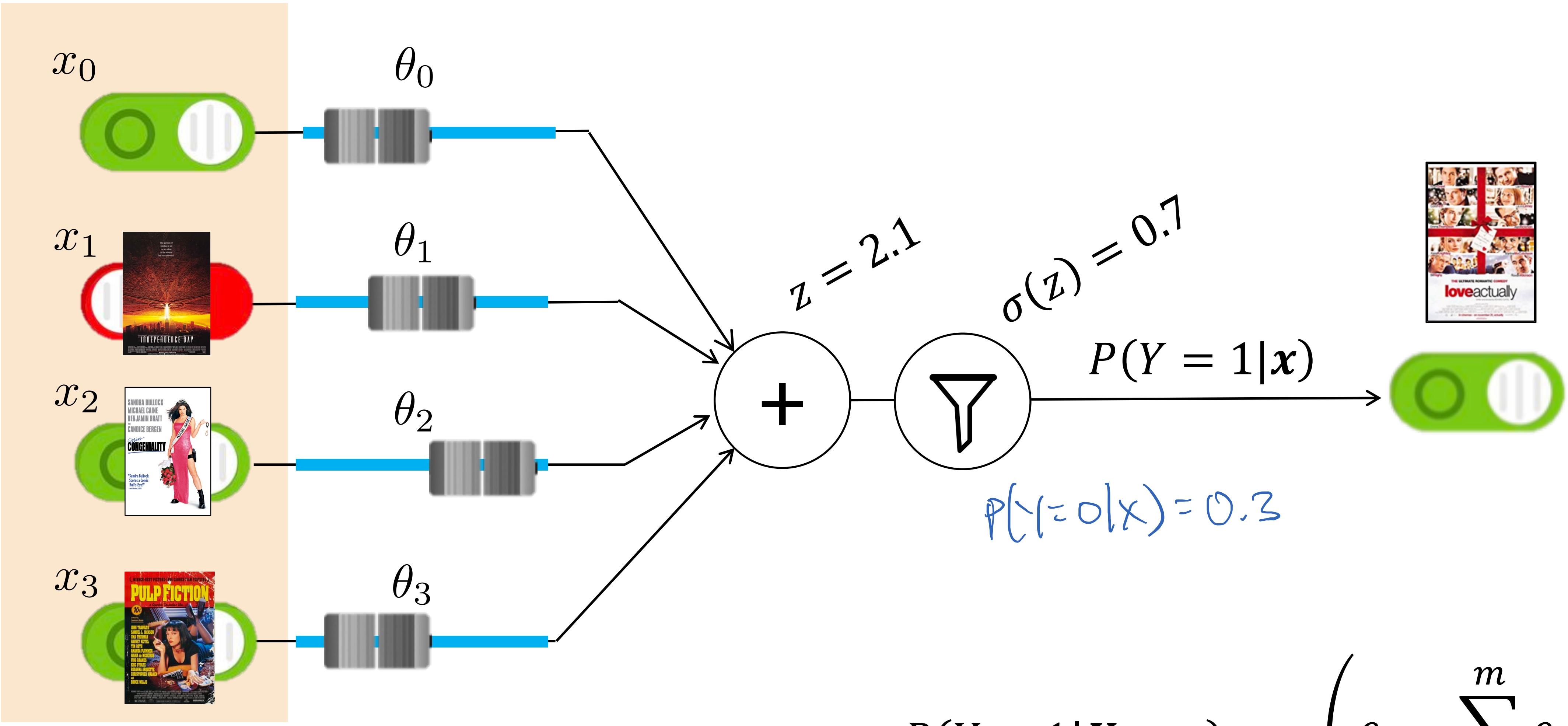
$$P(Y = 1|\boldsymbol{X} = \boldsymbol{x}) = \sigma\left(\theta_0 + \sum_{j=1}^{m} \theta_j x_j\right)$$

Components of Logistic Regression



$$P(Y = 1|\boldsymbol{X} = \boldsymbol{x}) = \sigma\left(\theta_0 + \sum_{j=1}^{m} \theta_j x_j\right)$$

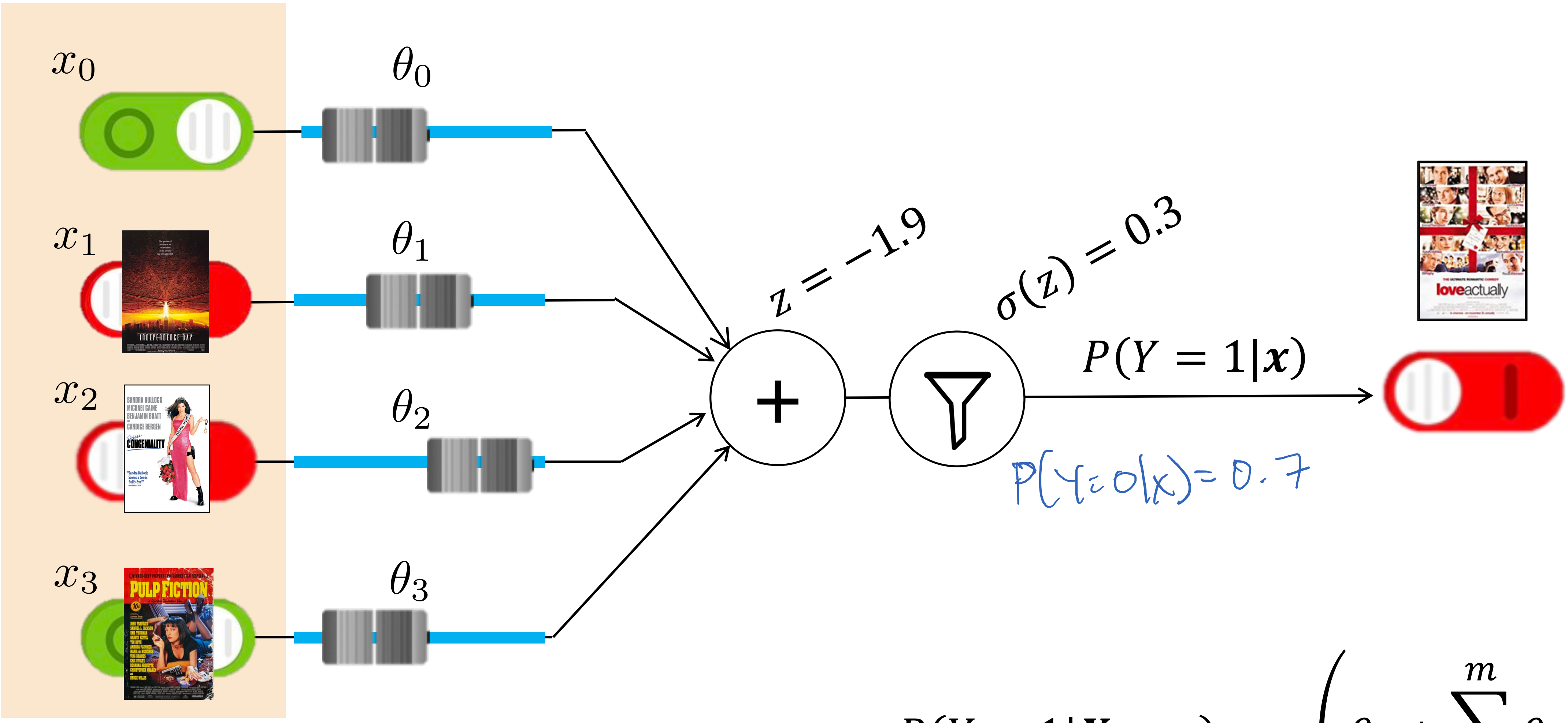
Different predictions for different inputs



X, input features
[0,1,1]

$$P(Y = 1|\boldsymbol{X} = \boldsymbol{x}) = \sigma\left(\theta_0 + \sum_{j=1}^{m} \theta_j x_j\right)$$

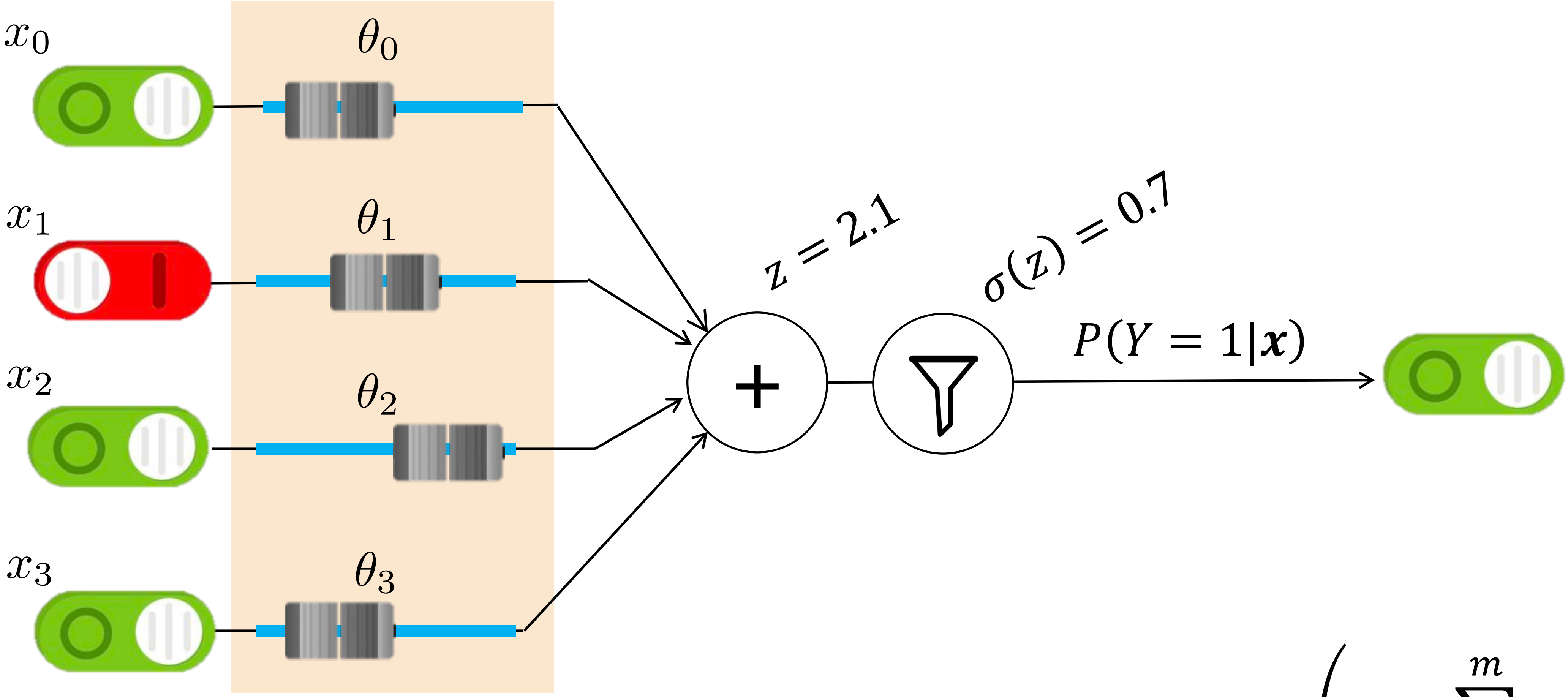
Different predictions for different inputs



$\boldsymbol{X}$, input features
[0,0,1]

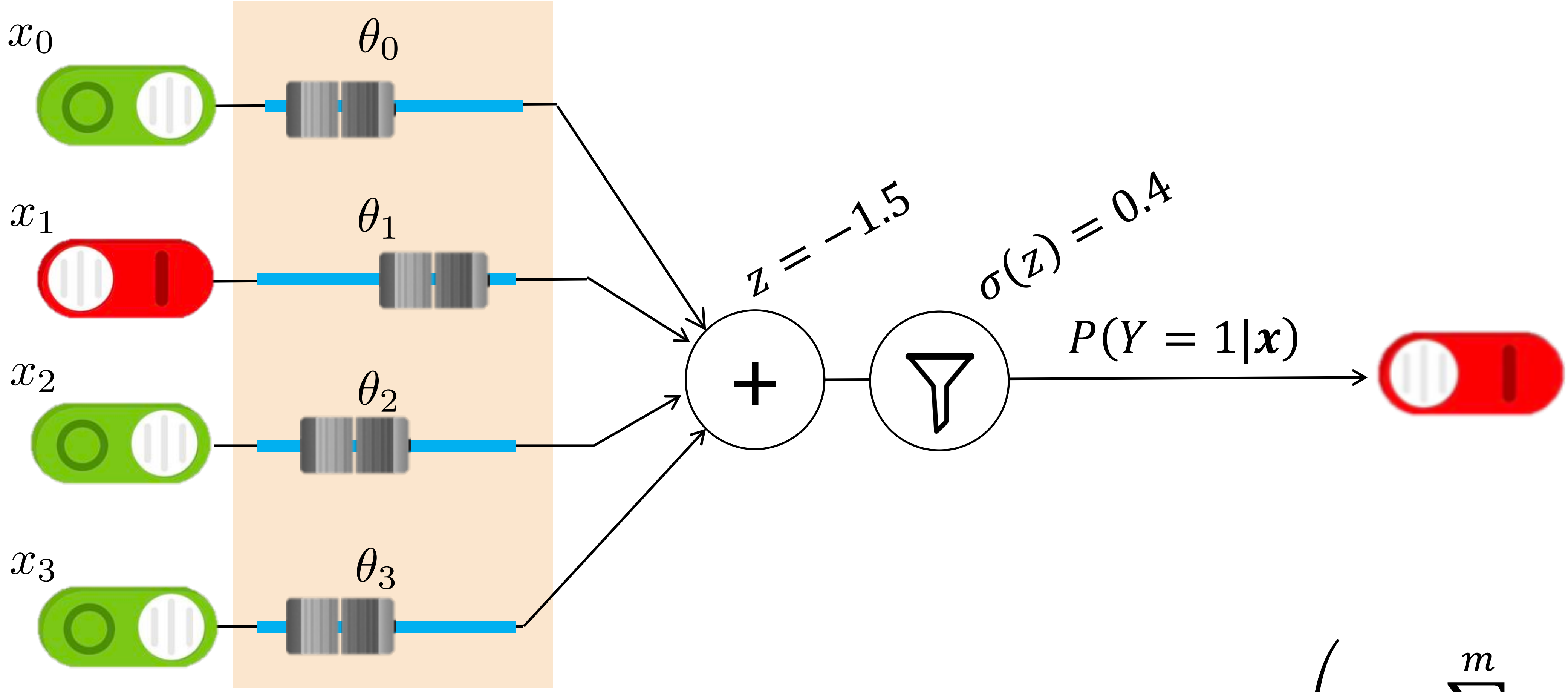
$$P(Y = 1|\boldsymbol{X} = \boldsymbol{x}) = \sigma\left(\theta_0 + \sum_{j=1}^{m} \theta_j x_j\right)$$

Parameters affect prediction



$$P(Y = 1|\boldsymbol{X} = \boldsymbol{x}) = \sigma\left(\theta_0 + \sum_{j=1}^{m} \theta_j x_j\right)$$

Parameters affect prediction



$$P(Y = 1|\boldsymbol{X} = \boldsymbol{x}) = \sigma\left(\theta_0 + \sum_{j=1}^{m} \theta_j x_j\right)$$

For simplicity

$$P(Y = 1|\boldsymbol{X} = \boldsymbol{x}) = \sigma\left(\theta_0 + \sum_{j=1}^{m} \theta_j x_j\right)$$

$$P(Y = 1|\boldsymbol{X} = \boldsymbol{x}) = \sigma\left(\sum_{j=0}^{m} \theta_j x_j\right) = \boxed{\sigma(\theta^T \boldsymbol{x})} \quad \text{where } x_0 = 1$$

$\theta = (\theta_0, \theta_1, \ldots, \theta_m)$

$X = (1, x_1, x_2, \ldots x_m)$

Logistic regression classifier

$$\hat{Y} = \arg\max_{y=\{0,1\}} P(Y|\boldsymbol{X})$$

$$P(Y = 1|\boldsymbol{X} = \boldsymbol{x}) = \sigma\left(\sum_{j=0}^{m} \theta_j x_j\right) = \sigma(\theta^T \boldsymbol{x})$$

Training

Estimate parameters from training data

$$\theta = (\theta_0, \theta_1, \theta_2, \dots, \theta_m)$$

Testing

Given an observation $\boldsymbol{X} = (X_1, X_2, \dots, X_m)$, predict

$$\hat{Y} = \arg\max_{y=\{0,1\}} P(Y|\boldsymbol{X})$$

Training: The big picture

Logistic regression classifier

$$\hat{Y} = \underset{y=\{0,1\}}{\arg\max}\, P(Y|\boldsymbol{X})$$

$$P(Y = 1|\boldsymbol{X} = \boldsymbol{x}) = \sigma\left(\sum_{j=0}^{m} \theta_j x_j\right) = \sigma(\theta^T \boldsymbol{x})$$

$(x^{(i)}, y^{(i)})$ $i = 1, \ldots, n$

Training

Estimate parameters from training data

$$\theta = (\theta_0, \theta_1, \theta_2, \ldots, \theta_m)$$

Choose θ that optimizes some objective:

1. Determine objective function
2. Find gradient with respect to θ
3. Solve analytically by setting to 0, or computationally with gradient ascent

We are modeling $P(Y|X)$ directly, so we maximize the **conditional likelihood** of training data.

Estimating θ

1. Determine objective function

$$\theta_{MLE} = \arg\max_{\theta} \prod_{i=1}^{n} f\left(y^{(i)} \mid \boldsymbol{x}^{(i)}, \theta\right)$$

2. Gradient w.r.t. θ_j, for $j = 0, 1, \ldots, m$

3. Solve
   - No analytical derivation of θ_{MLE}…
   - …but can still compute θ_{MLE} with gradient ascent!

```
initialize x
repeat many times:
  compute gradient
   x += η * gradient
```

1. Determine objective function

$$\theta_{MLE} = \boxed{\arg\max_{\theta} \prod_{i=1}^{n} f\left(y^{(i)} \mid \boldsymbol{x}^{(i)}, \theta\right)} = \boxed{\arg\max_{\theta} \; LL(\theta)}$$

$$P(Y = 1 | \boldsymbol{X} = \boldsymbol{x}) = \sigma\left(\sum_{j=0}^{m} \theta_j x_j\right) = \sigma(\theta^T \boldsymbol{x})$$

First: Interpret conditional likelihood with Logistic Regression

Second: Write a differentiable expression for log conditional likelihood

1. Determine objective function (interpret)

$$\theta_{MLE} = \arg\max_\theta \prod_{i=1}^{n} f\left(y^{(i)} \mid \boldsymbol{x}^{(i)}, \theta\right) = \arg\max_\theta \; LL(\theta)$$

$$P(Y = 1 | \boldsymbol{X} = \boldsymbol{x}) = \sigma\left(\textstyle\sum_{j=0}^{m} \theta_j x_j\right) = \sigma(\theta^T \boldsymbol{x})$$

Suppose you have $n = 2$ training datapoints: $\left(\boldsymbol{x}^{(1)}, \underset{y^{(1)}}{1}\right), \left(\boldsymbol{x}^{(2)}, \underset{y^{(2)}}{0}\right)$

Consider the following expressions for a given θ:

A. $\sigma\left(\theta^T \boldsymbol{x}^{(1)}\right) \sigma\left(\theta^T \boldsymbol{x}^{(2)}\right)$

B. $\left(1 - \sigma\left(\theta^T \boldsymbol{x}^{(1)}\right)\right) \sigma\left(\theta^T \boldsymbol{x}^{(2)}\right)$

C. $\sigma\left(\theta^T \boldsymbol{x}^{(1)}\right) \left(1 - \sigma\left(\theta^T \boldsymbol{x}^{(2)}\right)\right)$

D. $\left(1 - \sigma\left(\theta^T \boldsymbol{x}^{(1)}\right)\right) \left(1 - \sigma\left(\theta^T \boldsymbol{x}^{(2)}\right)\right)$

1. Interpret the above expressions as probabilities.
2. If we let $\theta = \theta_{MLE}$, which probability should be highest?

1. Determine objective function (interpret)

$$\theta_{MLE} = \arg\max_{\theta} \prod_{i=1}^{n} f\left(y^{(i)} \mid \boldsymbol{x}^{(i)}, \theta\right) = \arg\max_{\theta} LL(\theta)$$

$$P(Y = 1 | \boldsymbol{X} = \boldsymbol{x}) = \sigma\left(\textstyle\sum_{j=0}^{m} \theta_j x_j\right) = \sigma(\theta^T \boldsymbol{x})$$

Suppose you have $n = 2$ training datapoints: $\left(\boldsymbol{x}^{(1)}, 1\right), \left(\boldsymbol{x}^{(2)}, 0\right)$

$1 = y^{(1)}$, $0 = y^{(2)}$

Consider the following expressions for a given θ:

$P(Y = y^{(1)} \mid X = x^{(1)})\, P(Y = y^{(2)} \mid X = x^{(2)})$

A. $\sigma\left(\theta^T \boldsymbol{x}^{(1)}\right) \sigma\left(\theta^T \boldsymbol{x}^{(2)}\right)$

$P(Y=1 \mid X = x^{(1)})\, P(Y=1 \mid X = x^{(2)})$

B. $\left(1 - \sigma\left(\theta^T \boldsymbol{x}^{(1)}\right)\right) \sigma\left(\theta^T \boldsymbol{x}^{(2)}\right)$

$P(Y=0 \mid X = x^{(1)})\, P(Y=1 \mid X = x^{(2)})$

C. $\sigma\left(\theta^T \boldsymbol{x}^{(1)}\right) \left(1 - \sigma\left(\theta^T \boldsymbol{x}^{(2)}\right)\right)$

$P(Y=1 \mid X = x^{(1)})\, P(Y=0 \mid X = x^{(2)})$

D. $\left(1 - \sigma\left(\theta^T \boldsymbol{x}^{(1)}\right)\right)\left(1 - \sigma\left(\theta^T \boldsymbol{x}^{(2)}\right)\right)$

$P(Y=0 \mid X = x^{(1)})\, P(Y=0 \mid X = x^{(2)})$

1. Interpret the above expressions as probabilities.
2. If we let $\theta = \theta_{MLE}$, which probability should be highest?

1. Determine objective function (write)

$$\theta_{MLE} = \arg\max_{\theta} \prod_{i=1}^{n} f\left(y^{(i)} \mid \boldsymbol{x}^{(i)}, \theta\right) = \arg\max_{\theta} \; LL(\theta)$$

$$P(Y = 1 | \boldsymbol{X} = \boldsymbol{x}) = \sigma\left(\textstyle\sum_{j=0}^{m} \theta_j x_j\right) = \sigma(\theta^T \boldsymbol{x})$$

1. What is a differentiable expression for $P(Y = y | \boldsymbol{X} = \boldsymbol{x})$?

$$P(Y = y | \boldsymbol{X} = \boldsymbol{x}) = \begin{cases} \sigma(\theta^T \boldsymbol{x}) & \text{if } y = 1 \\ 1 - \sigma(\theta^T \boldsymbol{x}) & \text{if } y = 0 \end{cases}$$

2. What is a differentiable expression for $LL(\theta)$, log conditional likelihood?

$$LL(\theta) = \log \prod_{i=1}^{n} f\left(y^{(i)} \mid \boldsymbol{x}^{(i)}, \theta\right)$$

1. Determine objective function (write)

$$\theta_{MLE} = \arg\max_{\theta} \prod_{i=1}^{n} f\left(y^{(i)} \mid \boldsymbol{x}^{(i)}, \theta\right) = \arg\max_{\theta} LL(\theta)$$

$$P(Y=1 \mid \boldsymbol{X}=\boldsymbol{x}) = \sigma\left(\sum_{j=0}^{m} \theta_j x_j\right) = \sigma(\theta^T \boldsymbol{x})$$

1. What is a differentiable expression for $P(Y=y \mid \boldsymbol{X}=\boldsymbol{x})$?

$$P(Y=y \mid \boldsymbol{X}=\boldsymbol{x}) = \begin{cases} \sigma(\theta^T \boldsymbol{x}) & \text{if } y=1 \\ 1-\sigma(\theta^T \boldsymbol{x}) & \text{if } y=0 \end{cases}$$

Recall Bernoulli MLE!

$B \sim Ber(p)$

$$P(B=b) = \begin{cases} p & b=1 \\ 1-p & b=0 \end{cases}$$

$$p^b (1-p)^{1-b}$$

$$\sigma(\theta^T x)^y \left(1-\sigma(\theta^T x)\right)^{1-y}$$

2. What is a differentiable expression for $LL(\theta)$, log conditional likelihood?

$$LL(\theta) = \log \prod_{i=1}^{n} f\left(y^{(i)} \mid \boldsymbol{x}^{(i)}, \theta\right)$$

$$\sum_{i=1}^{n} \log\left[\sigma(\theta^T x^{(i)})^{y^{(i)}} \left(1-\sigma(\theta^T x^{(i)})\right)^{1-y^{(i)}}\right] = \sum_{i=1}^{n} \log \sigma(\theta^T x^{(i)})^{y^{(i)}} + \log\left(1-\sigma(\theta^T x^{(i)})\right)^{1-y^{(i)}}$$

$$= \sum_{i=1}^{n} y^{(i)} \log\left(\sigma(\theta^T x^{(i)})\right) + (1-y^{(i)}) \log\left(1-\sigma(\theta^T x^{(i)})\right)$$

1. Determine objective function (write)

$$\theta_{MLE} = \arg\max_{\theta} \prod_{i=1}^{n} f\left(y^{(i)} | \boldsymbol{x}^{(i)}, \theta\right) = \arg\max_{\theta} LL(\theta)$$

$$P(Y = 1|\boldsymbol{X} = \boldsymbol{x}) = \sigma\left(\sum_{j=0}^{m} \theta_j x_j\right) = \sigma(\theta^T \boldsymbol{x})$$

1. What is a differentiable expression for $P(Y = y| \boldsymbol{X} = \boldsymbol{x})$?

$$P(Y = y|\boldsymbol{X} = \boldsymbol{x}) = \left(\sigma(\theta^T \boldsymbol{x})\right)^y \left(1 - \sigma(\theta^T \boldsymbol{x})\right)^{1-y}$$

2. What is a differentiable expression for $LL(\theta)$, log conditional likelihood?

$$LL(\theta) = \sum_{i=1}^{n} y^{(i)} \log \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right)\right)$$

2. Find gradient with respect to θ

Optimization problem:

$$\theta_{MLE} = \arg\max_{\theta} \prod_{i=1}^{n} f\left(y^{(i)} \mid \boldsymbol{x}^{(i)}, \theta\right) = \arg\max_{\theta} \; LL(\theta)$$

$$LL(\theta) = \sum_{i=1}^{n} y^{(i)} \log \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right)\right)$$

Gradient w.r.t. θ_j, for $j = 0, 1, \ldots, m$:

$$\theta = (\theta_0, \theta_1, \theta_2, \ldots, \theta_m)$$

$$\theta^T x^{(i)} = \sum_{j=0}^{m} \theta_j x_j^{(i)}$$

$$\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=1}^{n} \left[y^{(i)} - \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right)\right] x_j^{(i)}$$

(derived later)

How do we interpret the gradient contribution of the i-th training datapoint?

2. Find gradient with respect to θ

Optimization problem:

$$\theta_{MLE} = \arg\max_{\theta} \prod_{i=1}^{n} f\left(y^{(i)} \mid \boldsymbol{x}^{(i)}, \theta\right) = \arg\max_{\theta} \; LL(\theta)$$

$$LL(\theta) = \sum_{i=1}^{n} y^{(i)} \log \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right)\right)$$

Gradient w.r.t. θ_j, for $j = 0, 1, \ldots, m$:

$$\theta^T x^{(i)} = \sum_{j=0}^{m} \theta_j x_j^{(i)}$$

$$\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=1}^{n} \left[y^{(i)} - \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right)\right] x_j^{(i)}$$

(derived later)

scale by j-th feature

2. Find gradient with respect to θ

Optimization problem:

$$\theta_{MLE} = \arg\max_{\theta} \prod_{i=1}^{n} f\left(y^{(i)} \mid \boldsymbol{x}^{(i)}, \theta\right) = \arg\max_{\theta} \; LL(\theta)$$

$$LL(\theta) = \sum_{i=1}^{n} y^{(i)} \log \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right)\right)$$

Gradient w.r.t. θ_j, for $j = 0, 1, \ldots, m$:

$$\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=1}^{n} \left[\underbrace{y^{(i)}}_{\text{1 or 0}} - \underbrace{\sigma\left(\theta^T \boldsymbol{x}^{(i)}\right)}_{P\left(Y = 1 \mid \boldsymbol{X} = \boldsymbol{x}^{(i)}\right)}\right] x_j^{(i)}$$

(derived later)

2. Find gradient with respect to θ

Optimization problem:

$$\theta_{MLE} = \arg\max_{\theta} \prod_{i=1}^{n} f\left(y^{(i)} \mid \boldsymbol{x}^{(i)}, \theta\right) = \arg\max_{\theta} \; LL(\theta)$$

$$LL(\theta) = \sum_{i=1}^{n} y^{(i)} \log \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right)\right)$$

Gradient w.r.t. θ_j, for $j = 0, 1, \ldots, m$:

$$\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=1}^{n} \underbrace{\left[y^{(i)} - \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right)\right]} x_j^{(i)}$$

(derived later)

Suppose $y^{(i)} = 1$ (the true class label for i-th datapoint):

- If $\sigma\left(\theta^T \boldsymbol{x}^{(i)}\right) \geq 0.5$, correct
- If $\sigma\left(\theta^T \boldsymbol{x}^{(i)}\right) < 0.5$, incorrect → change θ_j more

3. Solve

1. Optimization problem:

$$\theta_{MLE} = \arg\max_{\theta} \prod_{i=1}^{n} f\left(y^{(i)} \mid \boldsymbol{x}^{(i)}, \theta\right) = \arg\max_{\theta} LL(\theta)$$

$$LL(\theta) = \sum_{i=1}^{n} y^{(i)} \log \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right)\right)$$

2. Gradient w.r.t. θ_j, for $j = 0, 1, \ldots, m$:

$$\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=1}^{n} \left[y^{(i)} - \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right)\right] x_j^{(i)}$$

3. Solve

Stay tuned!

(live)
26: Logistic Regression

Lisa Yan and Jerry Cain

November 11, 2020

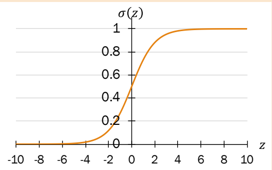
Logistic Regression Model

$$\hat{Y} = \underset{y=\{0,1\}}{\arg\max}\, P(Y|\boldsymbol{X})$$

$$P(Y = 1|\boldsymbol{X} = \boldsymbol{x}) = \sigma\left(\textstyle\sum_{j=0}^{m} \theta_j x_j\right) = \sigma(\theta^T \boldsymbol{x})$$

where $x_0 = 1$

$\boldsymbol{X}$ → $\theta_0 + \sum_{j=1}^{m} \theta_j X_j$ → **sigmoid function** $\sigma(z) = \frac{1}{1+e^{-z}}$ → $P(Y = 1|\boldsymbol{X})$



$\mathbb{R}$

Introducing notation $\hat{y}$

$$\hat{Y} = \arg\max_{y=\{0,1\}} P(Y|\boldsymbol{X})$$

$$P(Y = 1|\boldsymbol{X} = \boldsymbol{x}) = \sigma\left(\sum_{j=0}^{m} \theta_j x_j\right) = \sigma(\theta^T \boldsymbol{x})$$

$\hat{Y}$ is prediction of Y. $\hat{Y} \in \{0,1\}$

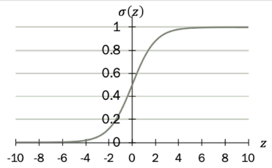
where $x_0 = 1$

$\boldsymbol{X}$

$$\theta_0 + \sum_{j=1}^{m} \theta_j X_j$$

sigmoid function

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



$$P(Y = 1|\boldsymbol{X}) = \hat{y}$$

$$\hat{y} = P(Y = 1|\boldsymbol{X} = \boldsymbol{x}) = \sigma(\theta^T \boldsymbol{x})$$

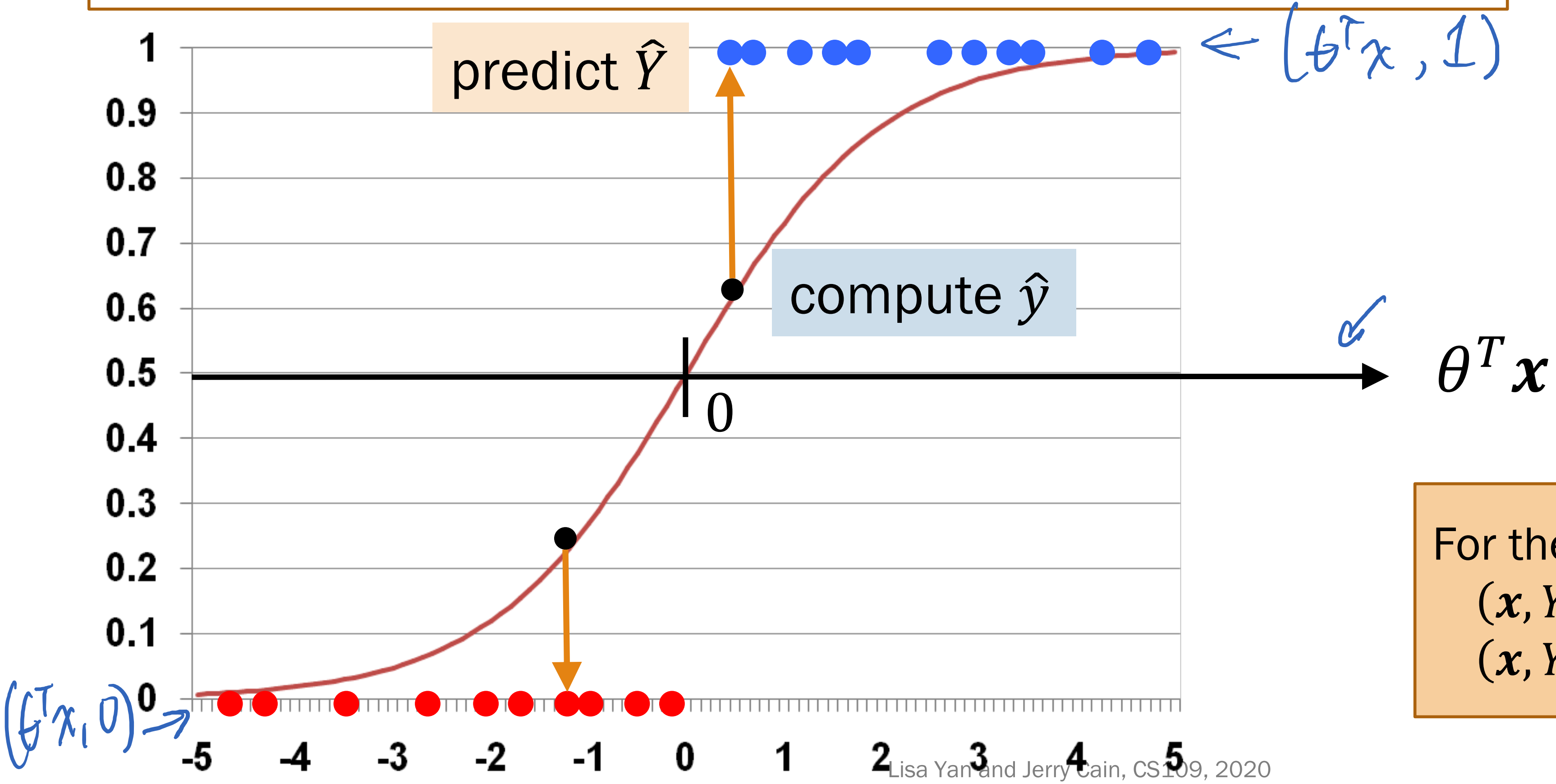
$$P(Y = y|\boldsymbol{X} = \boldsymbol{x}) = \begin{cases} \hat{y} & \text{if } y = 1 \\ 1 - \hat{y} & \text{if } y = 0 \end{cases}$$

Small $\hat{y}$ is conditional probability of $Y = 1$ given $\boldsymbol{X} = \boldsymbol{x}$. $\hat{y} \in [0,1]$

Another view of Logistic Regression

$$\hat{Y} = \arg\max_{y=\{0,1\}} P(Y|\boldsymbol{X})$$

$$\hat{y} = P(Y = 1|\boldsymbol{X} = \boldsymbol{x}) = \sigma\left(\sum_{j=0}^{m} \theta_j x_j\right) = \sigma(\theta^T \boldsymbol{x})$$



For the "correct" parameters θ:
$(\boldsymbol{x}, Y = 1)$ should have $\theta^T \boldsymbol{x} > 0$
$(\boldsymbol{x}, Y = 0)$ should have $\theta^T \boldsymbol{x} \leq 0$

Today's goals: Logistic Regresison

✅ At a high level
- Understand the model
- Training: Use gradient ascent

Details
- Gradient ascent pseudocode
- Testing

For the problem set

Philosophy
- Logistic Regression vs Naïve Bayes
- Linearly separable functions

Derivation of gradient (Calculus)

Machine learning insights

Training: The details

Training: Learning parameters

$(x^{(i)}, y^{(i)})$

$i=1,\dots,n$

Review

Training

Learn parameters $\theta = (\theta_0, \theta_1, \dots, \theta_m)$

that maximize log conditional likelihood of training data

Some reminders:

- Log conditional likelihood:

$$LL(\theta) = \sum_{i=1}^{n} y^{(i)} \log \overbrace{\sigma\left(\theta^T \boldsymbol{x}^{(i)}\right)}^{\hat{y}} + \left(1 - y^{(i)}\right) \log \overbrace{\left(1 - \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right)\right)}^{1-\hat{y}}$$

- Gradient with respect to θ:

$$\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=1}^{n} \left[y^{(i)} - \overbrace{\sigma\left(\theta^T \boldsymbol{x}^{(i)}\right)}^{\hat{y}}\right] x_j^{(i)} \quad \text{for } j = 0, 1, \dots, m$$

(derived at end of lecture)

- No analytical solution; optimize with gradient ascent

Training: Gradient ascent step

$$\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=1}^{n} \left[y^{(i)} - \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right) \right] x_j^{(i)} \qquad \text{for } j = 0, 1, \ldots, m$$

```
repeat many times:

    for all thetas:
```

$j = 0, 1, \ldots, m$

$$\theta_j^{\text{new}} = \theta_j^{\text{old}} + \eta \cdot \frac{\partial LL(\theta^{\text{old}})}{\partial \theta_j^{\text{old}}}$$

$$= \theta_j^{\text{old}} + \eta \cdot \underbrace{\sum_{i=1}^{n} \left[y^{(i)} - \sigma\left({\theta^{\text{old}}}^T \boldsymbol{x}^{(i)}\right) \right] x_j^{(i)}}_{\text{gradient w.r.t. } \theta_j}$$

learning rate

What does this look like in code?

Think

Slide 50 has code to think over by yourself.

Post any clarifications here or in chat!

https://us.edstem.org/courses/2678/discussion/171556

Think by yourself: 2 min

(by yourself)

Training: Gradient Ascent

Gradient Ascent Step

for $j = 0, 1, \dots, m$:

$$\theta_j^{\text{new}} = \theta_j^{\text{old}} + \eta \cdot \sum_{i=1}^{n} \left[y^{(i)} - \sigma\left(\theta^{\text{old}^T} \boldsymbol{x}^{(i)} \right) \right] x_j^{(i)}$$

```
initialize θ_j = 0 for 0 ≤ j ≤ m
repeat many times:
    gradient[j] = 0 for 0 ≤ j ≤ m
    // TODO: your code here
    // compute all gradient[j]'s
    // based on n training examples

    θ_j += η  * gradient[j] for all 0 ≤ j ≤ m
```

(by yourself)

Training: Gradient Ascent

inner loop

Gradient Ascent Step

for $j = 0, 1, \dots, m$:

$$\theta_j^{\text{new}} = \theta_j^{\text{old}} + \eta \cdot \underbrace{\sum_{i=1}^{n} \underbrace{\left[y^{(i)} - \sigma\left(\theta^{\text{old}^T} \boldsymbol{x}^{(i)}\right)\right] x_j^{(i)}}_{\text{compute}}}_{\text{outer loop}}$$

compute

outer loop

```
initialize θ_j = 0 for 0 ≤ j ≤ m
repeat many times:
    gradient[j] = 0 for 0 ≤ j ≤ m
    for each training example (x,y):
        for each 0 ≤ j ≤ m:
            // update gradient[j] for
            // current (x,y) example
    θ_j += η  * gradient[j] for all 0 ≤ j ≤ m
```

Training: Gradient Ascent

inner loop

Gradient Ascent Step

$$\text{for } j = 0, 1, \ldots, m:$$
$$\theta_j^{\text{new}} = \theta_j^{\text{old}} + \eta \cdot \sum_{i=1}^{n} \underbrace{\left[y^{(i)} - \sigma\left({\theta^{\text{old}}}^T \boldsymbol{x}^{(i)} \right) \right] x_j^{(i)}}_{\text{compute}}$$

outer loop

compute

```
initialize θ_j = 0 for 0 ≤ j ≤ m
repeat many times:
    gradient[j] = 0 for 0 ≤ j ≤ m
    for each training example (x,y):
        for each 0 ≤ j ≤ m:
            gradient[j] +=  [y − 1/(1 + e^(−θ^T x))] x_j
    θ_j += η * gradient[j] for all 0 ≤ j ≤ m
```

$\left[y - \frac{1}{1 + e^{-\theta^T \boldsymbol{x}}} \right] x_j$

$\hat{y} = \sigma(\theta^T x)$

Some important details…

Training: Gradient Ascent

Gradient Ascent Step $\theta_j^{\text{new}} = \theta_j^{\text{old}} + \eta \cdot \sum_{i=1}^{n} \left[y^{(i)} - \underbrace{\sigma\left({\theta^{\text{old}}}^T \boldsymbol{x}^{(i)} \right)}_{\hat{y}} \right] x_j^{(i)}$

```
initialize θ_j = 0 for 0 ≤ j ≤ m
repeat many times:
    gradient[j] = 0 for 0 ≤ j ≤ m
    for each training example (x,y):
        for each 0 ≤ j ≤ m:
            gradient[j] += [y − 1/(1 + e^(−θ^T x))] x_j
    θ_j += η * gradient[j] for all 0 ≤ j ≤ m
```

$\sigma(\theta^T x) = \hat{y}$

- Finish computing gradient with θ^{old} prior to any θ update

Training: Gradient Ascent

Gradient Ascent Step $\theta_j^{\text{new}} = \theta_j^{\text{old}} + \eta \cdot \sum_{i=1}^{n} \left[y^{(i)} - \sigma\left(\theta^{\text{old}^T} \boldsymbol{x}^{(i)} \right) \right] x_j^{(i)}$

```
initialize θ_j = 0 for 0 ≤ j ≤ m
repeat many times:
    gradient[j] = 0 for 0 ≤ j ≤ m
    for each training example (x,y):
        for each 0 ≤ j ≤ m:
            gradient[j] += [y − 1/(1 + e^(−θ^T x))] x_j
    θ_j += η * gradient[j] for all 0 ≤ j ≤ m
```

$$\text{gradient[j]} \mathrel{+}= \left[y - \frac{1}{1 + e^{-\theta^T \boldsymbol{x}}} \right] x_j$$

$$\theta_j \mathrel{+}= \boxed{\eta} * \text{gradient[j] for all } 0 \le j \le m$$

α 1×10^{-6}

- Finish computing gradient with θ^{old} prior to any θ update
- Learning rate η is a constant you set before training

Training: Gradient Ascent

Gradient Ascent Step $\theta_j^{\text{new}} = \theta_j^{\text{old}} + \eta \cdot \sum_{i=1}^{n} \left[y^{(i)} - \sigma\left({\theta^{\text{old}}}^T \boldsymbol{x}^{(i)} \right) \right] x_j^{(i)}$

```
initialize θ_j = 0 for 0 ≤ j ≤ m
repeat many times:
    gradient[j] = 0 for 0 ≤ j ≤ m
    for each training example (x,y):
        for each 0 ≤ j ≤ m:
            gradient[j] += [y − 1/(1 + e^(−θ^T x))] x_j
    θ_j += η * gradient[j] for all 0 ≤ j ≤ m
```

$$\text{gradient[j]} \mathrel{+}= \left[y - \frac{1}{1+e^{-\theta^T \boldsymbol{x}}} \right] \boxed{x_j}$$

- Finish computing gradient with θ^{old} prior to any θ update
- Learning rate η is a constant you set before training
- x_j is j-th feature of input $\boldsymbol{x} = (x_1, \ldots, x_m)$

Training: Gradient Ascent

Gradient Ascent Step $\theta_j^{\text{new}} = \theta_j^{\text{old}} + \eta \cdot \sum_{i=1}^{n} \left[y^{(i)} - \sigma\left(\theta^{\text{old}^T} \boldsymbol{x}^{(i)} \right) \right] x_j^{(i)}$

$(x_1, x_2, \ldots, x_m) \rightarrow (1, x_1, x_2, \ldots, x_m)$ $\theta^T x = \theta_0 + \sum_{j=1}^{m} \theta_j x_j$

insert $x_0 = 1$ into all traing data x

```
initialize θj = 0 for 0 ≤ j ≤ m
repeat many times:
    gradient[j] = 0 for 0 ≤ j ≤ m
    for each training example (x,y):
        for each 0 ≤ j ≤ m:
            gradient[j] +=  [y − 1/(1 + e^(−θ^T x))] xj
    θj += η * gradient[j] for all 0 ≤ j ≤ m
```

$$\text{gradient[j]} \mathrel{+}= \left[y - \frac{1}{1 + \boxed{e^{-\theta^T \boldsymbol{x}}}} \right] x_j$$

- Finish computing gradient with θ^{old} prior to any θ update
- Learning rate η is a constant you set before training
- x_j is j-th feature of input $\boldsymbol{x} = (x_1, \ldots, x_m)$
- Insert $x_0 = 1$ before training

Training: Gradient Ascent

Gradient Ascent Step $\theta_j^{\text{new}} = \theta_j^{\text{old}} + \eta \cdot \sum_{i=1}^{n} \left[y^{(i)} - \sigma\left({\theta^{\text{old}}}^T \boldsymbol{x}^{(i)} \right) \right] x_j^{(i)}$

$(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \dots \rightarrow (x^{(n)}, y^{(n)})$

initialize θ_j = 0 for 0 ≤ j ≤ m
repeat many times:

    gradient[j] = 0 for 0 ≤ j ≤ m

    for each training example $(\boldsymbol{x}, y)$:

        for each 0 ≤ j ≤ m:

            gradient[j] += $\left[y - \overbrace{\frac{1}{1 + e^{-\theta^T \boldsymbol{x}}}}^{\hat{y}} \right] x_j$

    θ_j += η * gradient[j] for all 0 ≤ j ≤ m

- Finish computing gradient with θ^{old} prior to any θ update
- Learning rate η is a constant you set before training
- x_j is j-th feature of input $\boldsymbol{x} = (x_1, \dots, x_m)$
- Insert $x_0 = 1$ before training

Testing

Testing: Classification with Logistic Regression

Training

Learn parameters $\theta = (\theta_0, \theta_1, \dots, \theta_m)$

via gradient ascent:

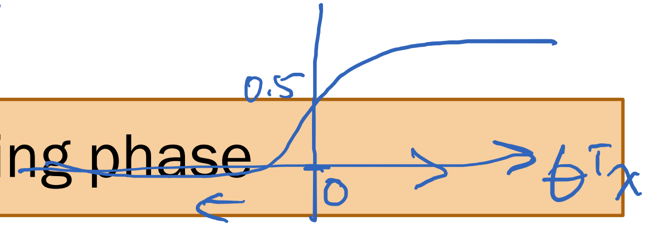
$$\theta_j^{\text{new}} = \theta_j^{\text{old}} + \eta \cdot \sum_{i=1}^{n} \left[y^{(i)} - \sigma\left(\theta^{\text{old}^T} \boldsymbol{x}^{(i)} \right) \right] x_j^{(i)}$$

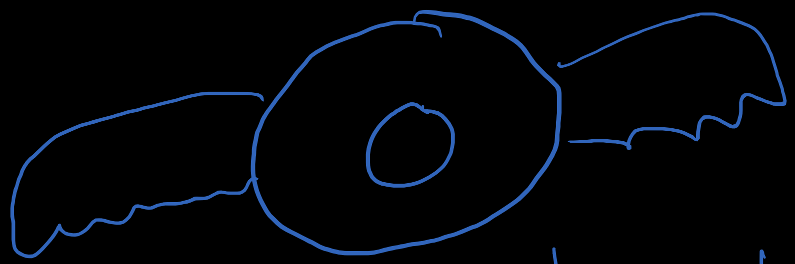
Testing

- Compute $\hat{y} = P(Y = 1 | \boldsymbol{X} = \boldsymbol{x}) = \sigma(\theta^T \boldsymbol{x}) = \dfrac{1}{1 + e^{-\theta^T \boldsymbol{x}}}$
- Classify instance as: 1 if $P(Y=1|X=x) > P(Y=0|X=x)$

$$\hat{Y} = \begin{cases} 1 & \hat{y} > 0.5, \text{ equivalently } \theta^T \boldsymbol{x} > 0 \\ 0 & \text{otherwise} \end{cases}$$

⚠ Parameters θ_j are **not** updated during testing phase





plane bagel

schmear
schmear
campaign

Interlude for jokes/announcements

https://www.bagelbakerygainesville.com/top-8-bagel-jokes-of-all-time/

Announcements

Quiz #3

Time frame: Wednesday 11/18 2:00pm – Friday 11/20 12:59pm PT
Covers: Up to and including logistic regression
Info and practice: Quizzes page

Next week: Last section

Review session for Quiz #3

Probability Reference (Overleaf)

Updated to include all of Quiz 3-relevant material (sampling defs, MLE/MAP, classifiers)

Interesting probability news

The Time Everyone "Corrected" the World's Smartest Woman

https://priceonomics.com/the-time-everyone-corrected-the-worlds-smartest/

Today's goals: Logistic Regression

✅ At a high level
- Understand the model
- Training: Use gradient ascent

Details
✅
- Gradient ascent pseudocode
- Testing

For the problem set

Philosophy
- Logistic Regression vs Naïve Bayes
- Linearly separable functions

Derivation of gradient (Calculus)

Machine learning insights

Philosophy

Think

Slide 64 asks you to think over by yourself.

Post any clarifications here or in chat!

https://us.edstem.org/courses/2678/discussion/171556

Think by yourself: 2 min

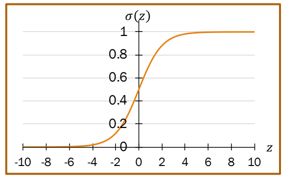
(by yourself)

Naïve Bayes vs Logistic Regression

$\boldsymbol{X}$, Y → $\hat{P}(\boldsymbol{X}|Y)\hat{P}(Y)$ (parameters θ) → $\hat{P}(\boldsymbol{X}, Y)$

$$\hat{Y} = \underset{y=\{0,1\}}{\arg\max}\, P(Y \mid \boldsymbol{X}) = \underset{y=\{0,1\}}{\arg\max}\, P(\boldsymbol{X}|Y)P(Y)$$

$\boldsymbol{X}$ → $\theta^T \boldsymbol{x}$ →



→ $P(Y = 1|\boldsymbol{X})$

$$\hat{Y} = \underset{y=\{0,1\}}{\arg\max}\, P(Y|\boldsymbol{X})$$

Compare/contrast:

1. What **distributions** are we modeling?
2. After learning our parameters, could we randomly **generate** a new datapoint $(\boldsymbol{x}, y)$?
3. Could we model a **continuous** X_j feature (e.g., X_j~Normal, or X_j~Unknown)?
4. Could we model a non-binary **discrete** X_j (e.g., $X_j \in \{1,2,\ldots,6\}$)?

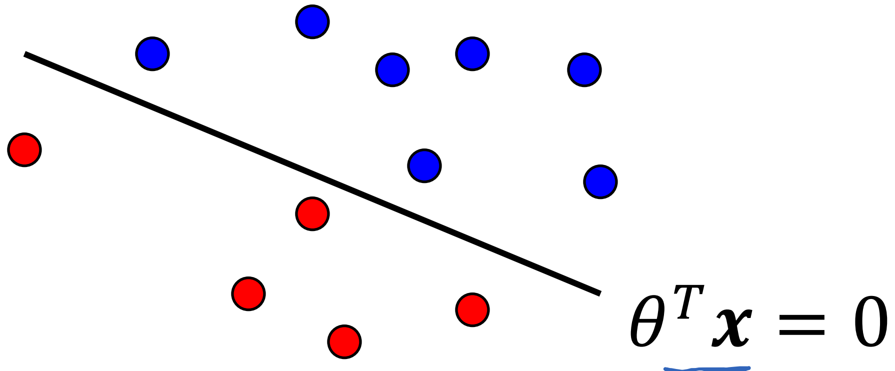
(by yourself)

Tradeoffs: Naïve Bayes vs Logistic Regression

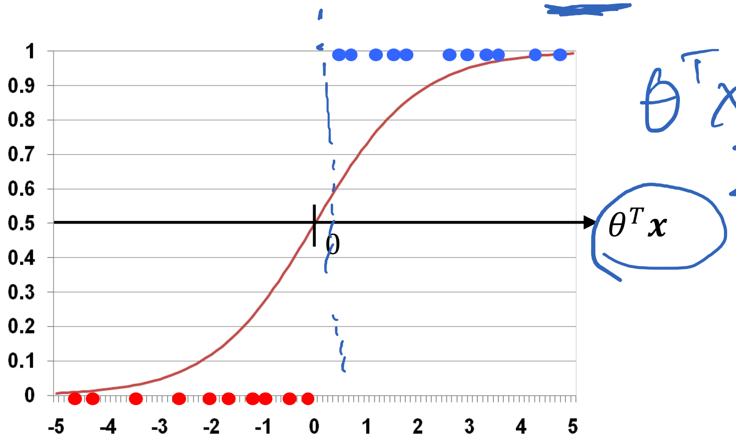
Tradeoffs:	Naïve Bayes	Logistic Regression
1. Modeling goal	$P(\boldsymbol{X}, Y)$	$P(Y \mid \boldsymbol{X})$
2. Generative or discriminative?	**Generative**: could use joint distribution to generate new points (⚠️ but you might not need this extra effort)	**Discriminative**: just tries to discriminate $y = 0$ vs $y = 1$ (❌ cannot generate new points b/c no $P(\boldsymbol{X}, Y)$)
3. Continuous input features $0 - 100$	$X \sim N(\mu, \sigma^2)$ ⚠️ Needs parametric form (e.g., Gaussian) or discretized buckets (for multinomial features)	$\underline{\theta^T x}$ ✅ Yes, easily
$\{$apple, banana, orange$\}$ 4. Discrete input features	✅ Yes, multi-value discrete data = multinomial $P(X_i \mid Y)$	⚠️ Multi-valued discrete data hard (e.g., if $X_i \in \{A, B, C\}$, not necessarily good to encode as $\{1, 2, 3\}$

Linearly separable data

Logistic Regression is trying to fit a <u>line</u> that separates data instances where $y = 1$ from those where $y = 0$:



- We call such data (or functions generating the data) **<u>linearly separable</u>.**

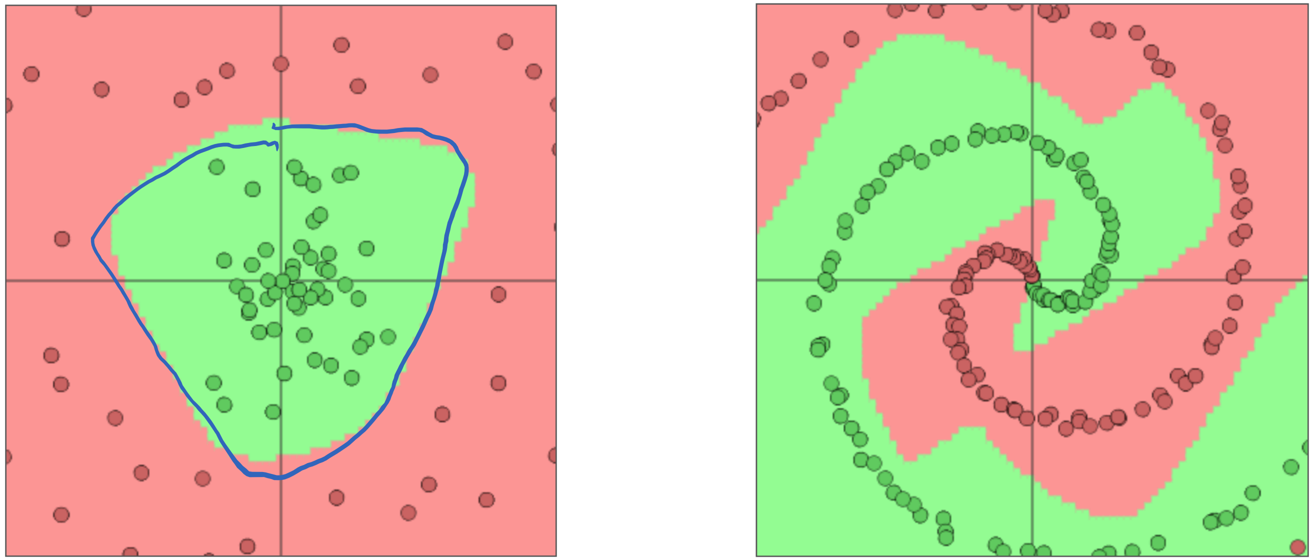


$\theta^T x = \sum_{j=0}^{m} \theta_j x_j$

- Naïve Bayes is linear too, because there is <u>one parameter for each feature</u> (and no parameters that involve multiple features).

$$\hat{P}(\boldsymbol{X}|Y) = \prod_{j=1}^{m} \hat{P}(X_j|Y)$$

Data is often not linearly separable



- Not possible to draw a line that successfully separates all the $y = 1$ points (green) from the $y = 0$ points (red)
- Despite this fact, Logistic Regression and Naive Bayes still often work well in practice

Gradient Derivation

Background: Calculus

Calculus refresher #1:
Derivative(sum) = sum(derivative)

$$\frac{\partial}{\partial x}\sum_{i=1}^{n} f_i(x) = \sum_{i=1}^{n} \frac{\partial f_i(x)}{\partial x}$$

Calculus refresher #2:
Chain rule 🌟 🌟 🌟

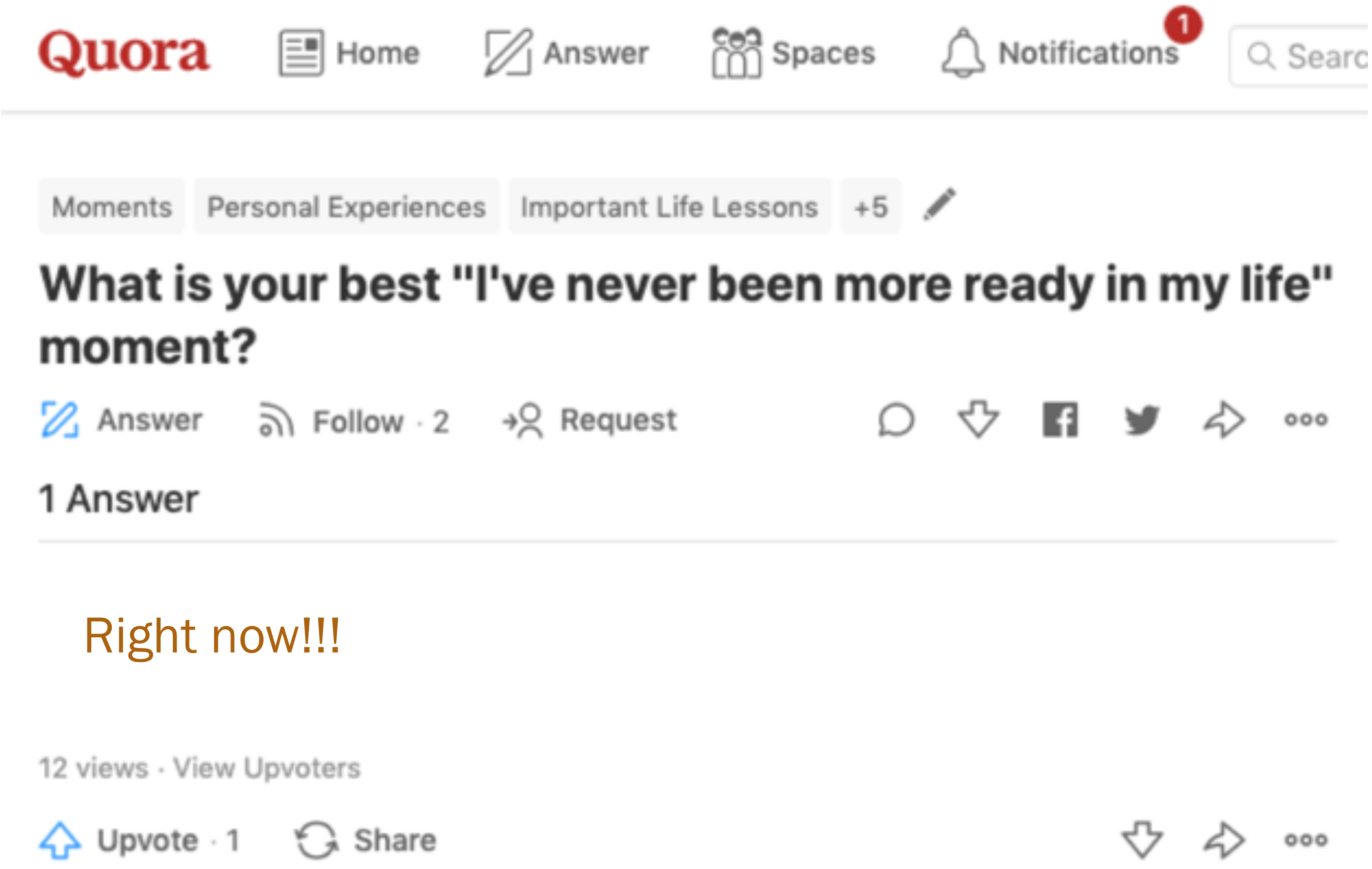
$$\frac{\partial f(x)}{\partial x} = \frac{\partial f(z)}{\partial z}\frac{\partial z}{\partial x}$$

Calculus Chain Rule

$$f(x) = f\big(z(x)\big)$$

aka decomposition of composed functions

Are you ready?



Our goal

Find: $\dfrac{\partial LL(\theta)}{\partial \theta_j}$ where

$$LL(\theta) = \sum_{i=1}^{n} y^{(i)} \log \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right)\right)$$

log conditional likelihood

Think

Slide 72 has code to think over by yourself.

Post any clarifications here or in chat!

https://us.edstem.org/courses/2678/discussion/171556

Think by yourself: 2 min

🤔 (by yourself)

Aside: Sigmoid has a beautiful derivative

Sigmoid function:

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

Derivative:

$$\frac{d}{dz}\sigma(z) = \sigma(z)[1 - \sigma(z)]$$

What is $\frac{\partial}{\partial \theta_j} \sigma(\theta^T \boldsymbol{x})$?

A. $\sigma(x_j)[1 - \sigma(x_j)]x_j$
B. $\sigma(\theta^T \boldsymbol{x})[1 - \sigma(\theta^T \boldsymbol{x})]\boldsymbol{x}$
C. $\sigma(\theta^T \boldsymbol{x})[1 - \sigma(\theta^T \boldsymbol{x})]x_j$
D. $\sigma(\theta^T \boldsymbol{x})x_j[1 - \sigma(\theta^T \boldsymbol{x})x_j]$
E. None/other

🤔 (by yourself)

Aside: Sigmoid has a beautiful derivative

Sigmoid function:

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

Derivative:

$$\frac{d}{dz}\sigma(z) = \sigma(z)[1-\sigma(z)]$$

What is $\frac{\partial}{\partial \theta_j}\sigma(\theta^T \boldsymbol{x})$?

A. $\sigma(x_j)[1-\sigma(x_j)]x_j$

B. $\sigma(\theta^T \boldsymbol{x})[1-\sigma(\theta^T \boldsymbol{x})]\boldsymbol{x}$

C. $\sigma(\theta^T \boldsymbol{x})[1-\sigma(\theta^T \boldsymbol{x})]x_j$

D. $\sigma(\theta^T \boldsymbol{x})x_j[1-\sigma(\theta^T \boldsymbol{x})x_j]$

E. None/other

Let $z = \theta^T \boldsymbol{x} = \sum_{k=0}^{m} \theta_k x_k$.

$$\frac{\partial}{\partial \theta_j}\sigma(\theta^T \boldsymbol{x}) = \frac{\partial}{\partial z}\sigma(z) \cdot \frac{\partial z}{\partial \theta_j}$$ (Chain Rule)

$$= \sigma(\theta^T \boldsymbol{x})[1-\sigma(\theta^T \boldsymbol{x})]x_j$$

Our goal: Re-introducing notation $\hat{y}$

Find: $\dfrac{\partial LL(\theta)}{\partial \theta_j}$ where

$$LL(\theta) = \sum_{i=1}^{n} y^{(i)} \log \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right)\right)$$

log conditional likelihood

$$\boxed{LL(\theta) = \sum_{i=1}^{n} y^{(i)} \log \hat{y}^{(i)} + \left(1 - y^{(i)}\right) \log\left(1 - \hat{y}^{(i)}\right)}$$

Let $\hat{y}^{(i)} = \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right)$

Compute gradient of log conditional likelihood

$$\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=1}^{n} \frac{\partial}{\partial \theta_j}\left[y^{(i)} \log\left(\hat{y}^{(i)}\right) + \left(1 - y^{(i)}\right)\log\left(1 - \hat{y}^{(i)}\right)\right]$$

Let $\hat{y}^{(i)} = \sigma\left(\theta^T \boldsymbol{x}^{(\boldsymbol{i})}\right)$

$$= \sum_{i=1}^{n} \frac{\partial}{\partial \hat{y}^{(i)}}\left[y^{(i)} \log\left(\hat{y}^{(i)}\right) + \left(1 - y^{(i)}\right)\log\left(1 - \hat{y}^{(i)}\right)\right] \cdot \frac{\partial \hat{y}^{(i)}}{\partial \theta_j}$$

(Chain Rule)

$$= \sum_{i=1}^{n} \left[y^{(i)} \frac{1}{\hat{y}^{(i)}} - \left(1 - y^{(i)}\right)\frac{1}{1 - \hat{y}^{(i)}}\right] \cdot \hat{y}^{(i)}\left(1 - \hat{y}^{(i)}\right) x_j^{(i)}$$

(calculus)

$$= \sum_{i=1}^{n} \left[y^{(i)} - \hat{y}^{(i)}\right] x_j^{(i)} \qquad = \sum_{i=1}^{n} \left[y^{(i)} - \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right)\right] x_j^{(i)}$$

(simplify)

Compute gradient of log conditional likelihood

$$\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=1}^{n} \frac{\partial}{\partial \theta_j}\left[y^{(i)} \log\left(\hat{y}^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - \hat{y}^{(i)}\right)\right]$$

Let $\hat{y}^{(i)} = \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right)$

$$= \sum_{i=1}^{n} \frac{\partial}{\partial \hat{y}^{(i)}}\left[y^{(i)} \log\left(\hat{y}^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - \hat{y}^{(i)}\right)\right] \cdot \frac{\partial \hat{y}^{(i)}}{\partial \theta_j}$$

(Chain Rule)

$$= \sum_{i=1}^{n} \left[y^{(i)} \frac{1}{\hat{y}^{(i)}} - \left(1 - y^{(i)}\right) \frac{1}{1 - \hat{y}^{(i)}}\right] \cdot \hat{y}^{(i)}\left(1 - \hat{y}^{(i)}\right) x_j^{(i)}$$

(calculus)

$$= \sum_{i=1}^{n} \left[y^{(i)} - \hat{y}^{(i)}\right] x_j^{(i)} \qquad = \sum_{i=1}^{n} \left[y^{(i)} - \sigma\left(\theta^T \boldsymbol{x}^{(i)}\right)\right] x_j^{(i)}$$

(simplify)