Logistic Regression

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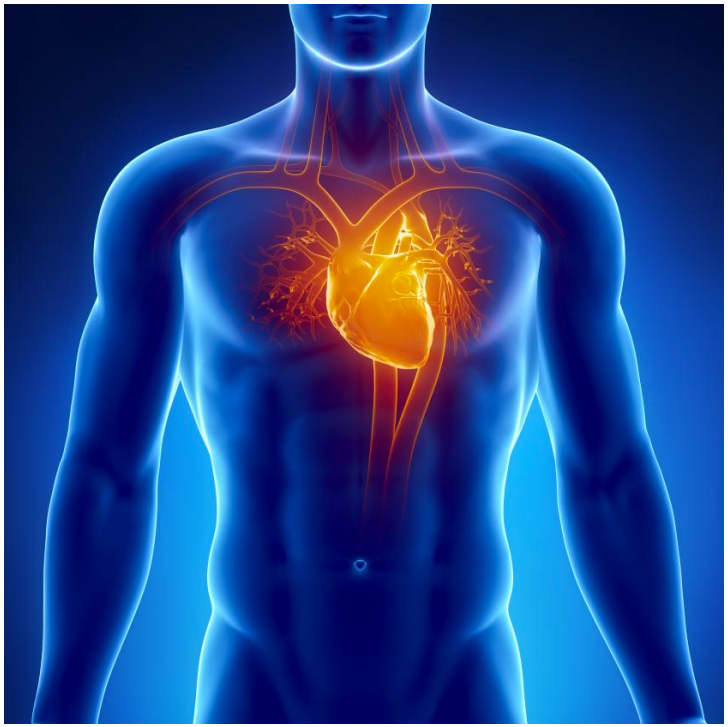
CS109, Stanford University

Review

Classification

Classification Task

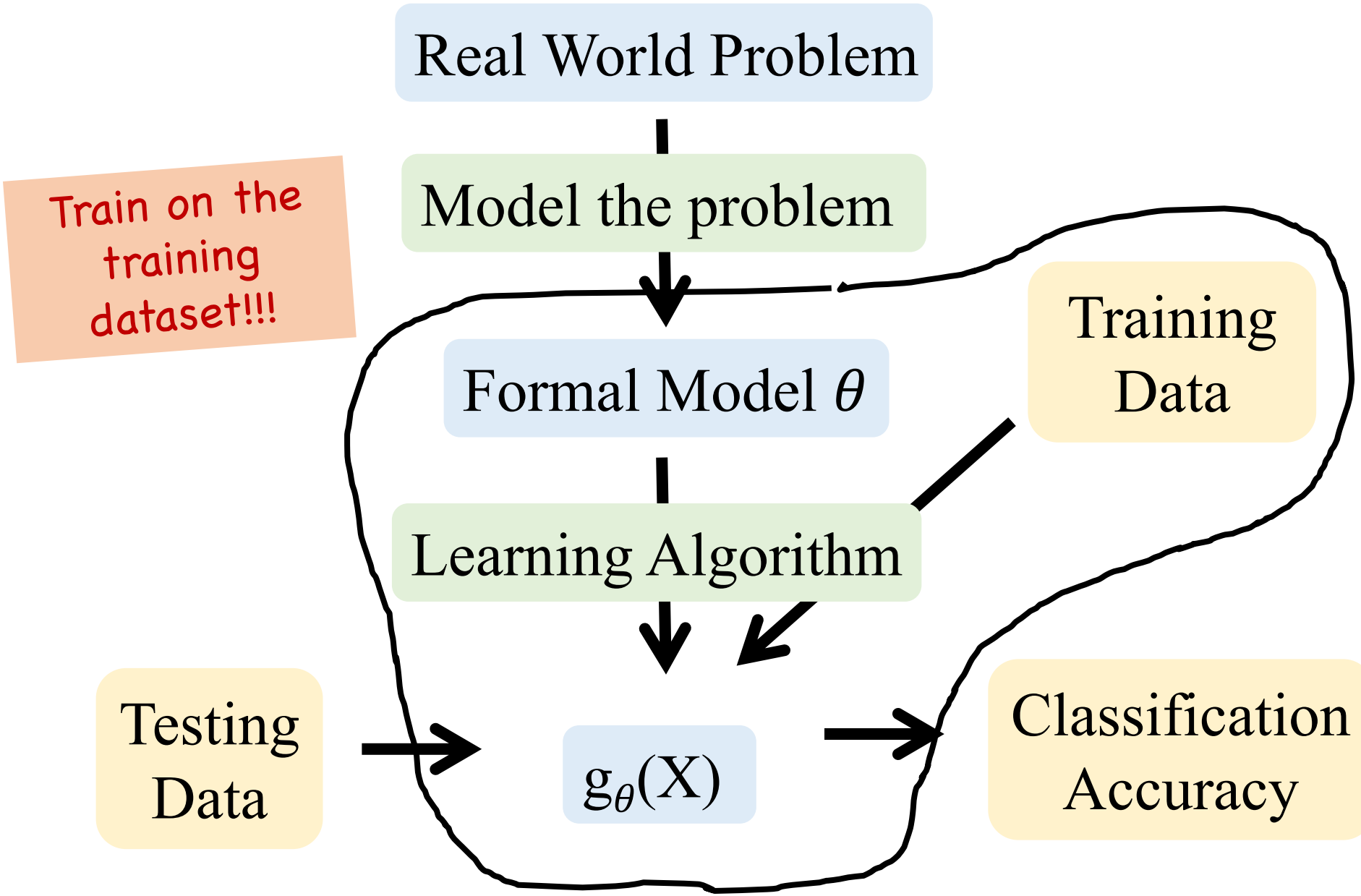
Heart



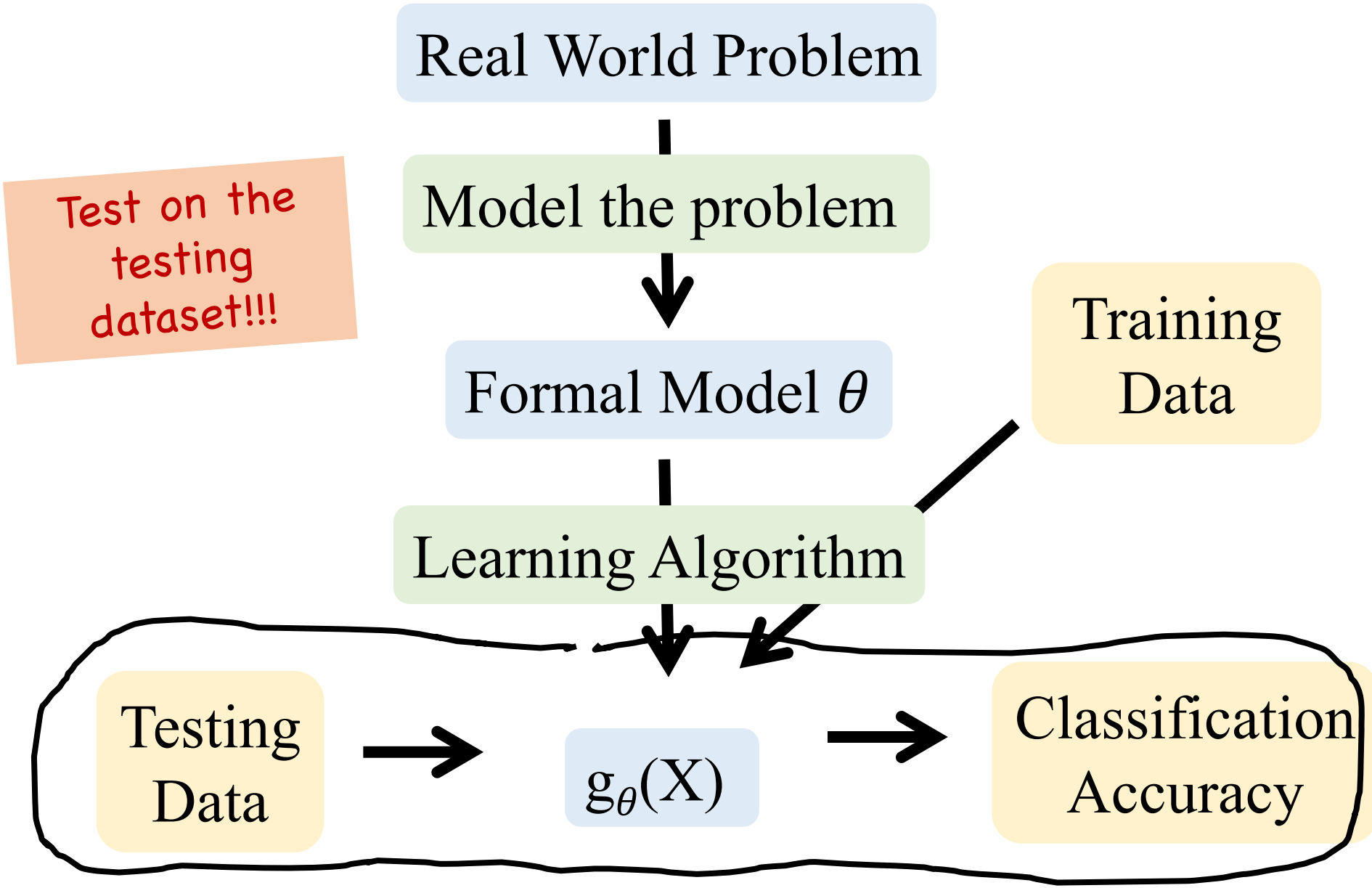
Ancestry

Netflix

Training


Real World Problem
Model the problem
Train on the training dataset!!!
Formal Model θ
Training Data
Learning Algorithm
Testing Data
$g_\theta(X)$
Classification Accuracy

Testing


Real World Problem
Model the problem
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Test on the testing dataset!!!
Testing Data
$g_\theta(X)$
Classification Accuracy

Training Data

Assume IID data:

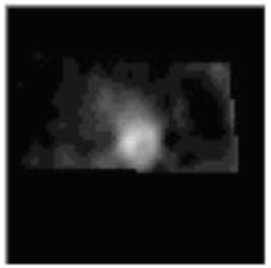
n training datapoints

$$(\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), \ldots (\mathbf{x}^{(n)}, y^{(n)})$$

$$m = |\mathbf{x}^{(i)}|$$

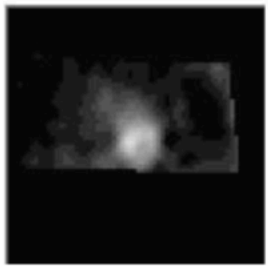
Each datapoint has m features and a single output

Healthy Heart Classifier

	ROI 1	ROI 2	...	ROI m	Output
					
Heart 1	0	1		1	0
Heart 2	1	1		1	0
			⋮		⋮
Heart n	0	0		0	1

$g_\theta(X)$

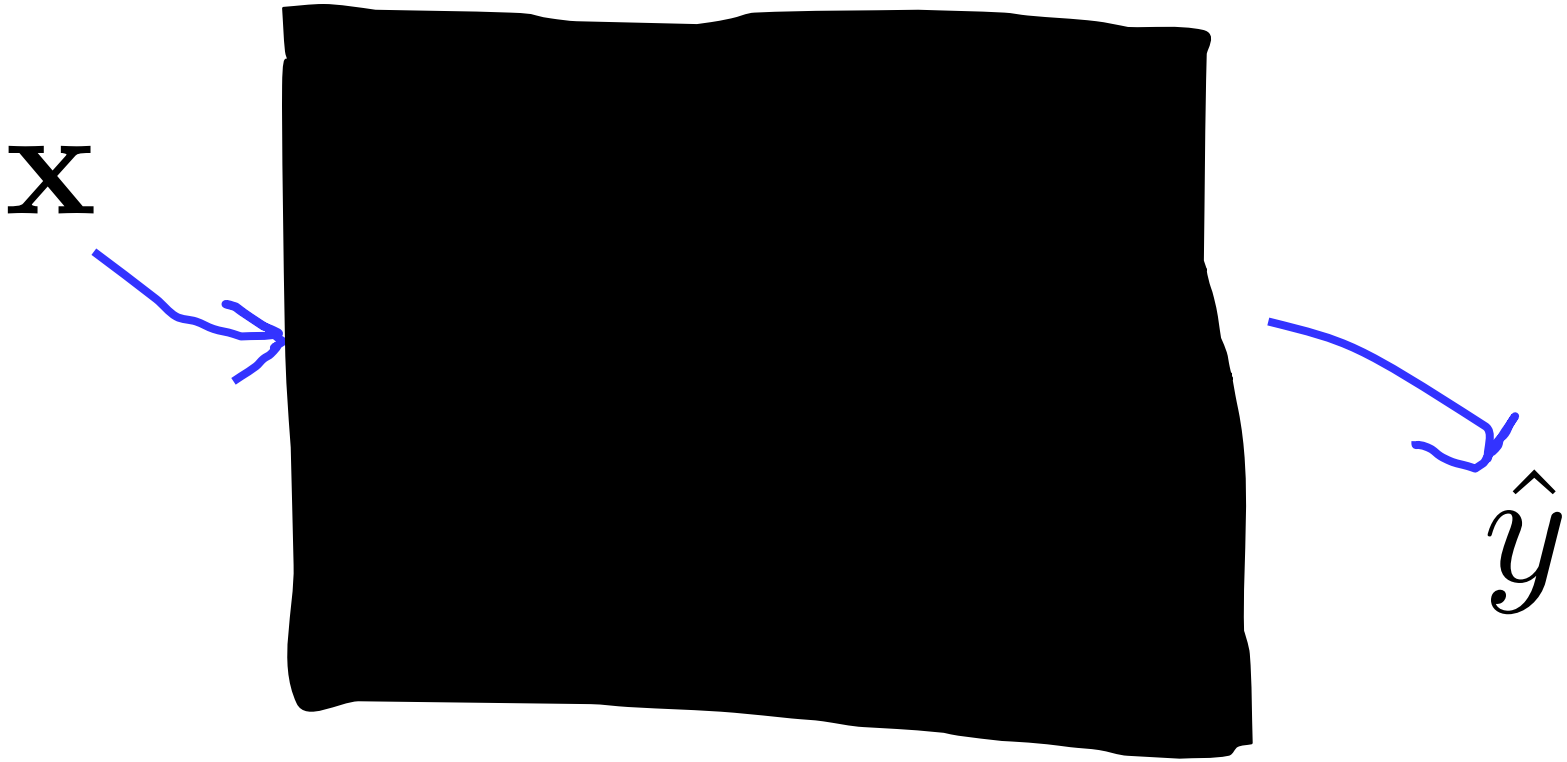
Healthy Heart Classifier

	ROI 1	ROI 2	ROI m	Output
			… 	
New Heart	1	0	1	1

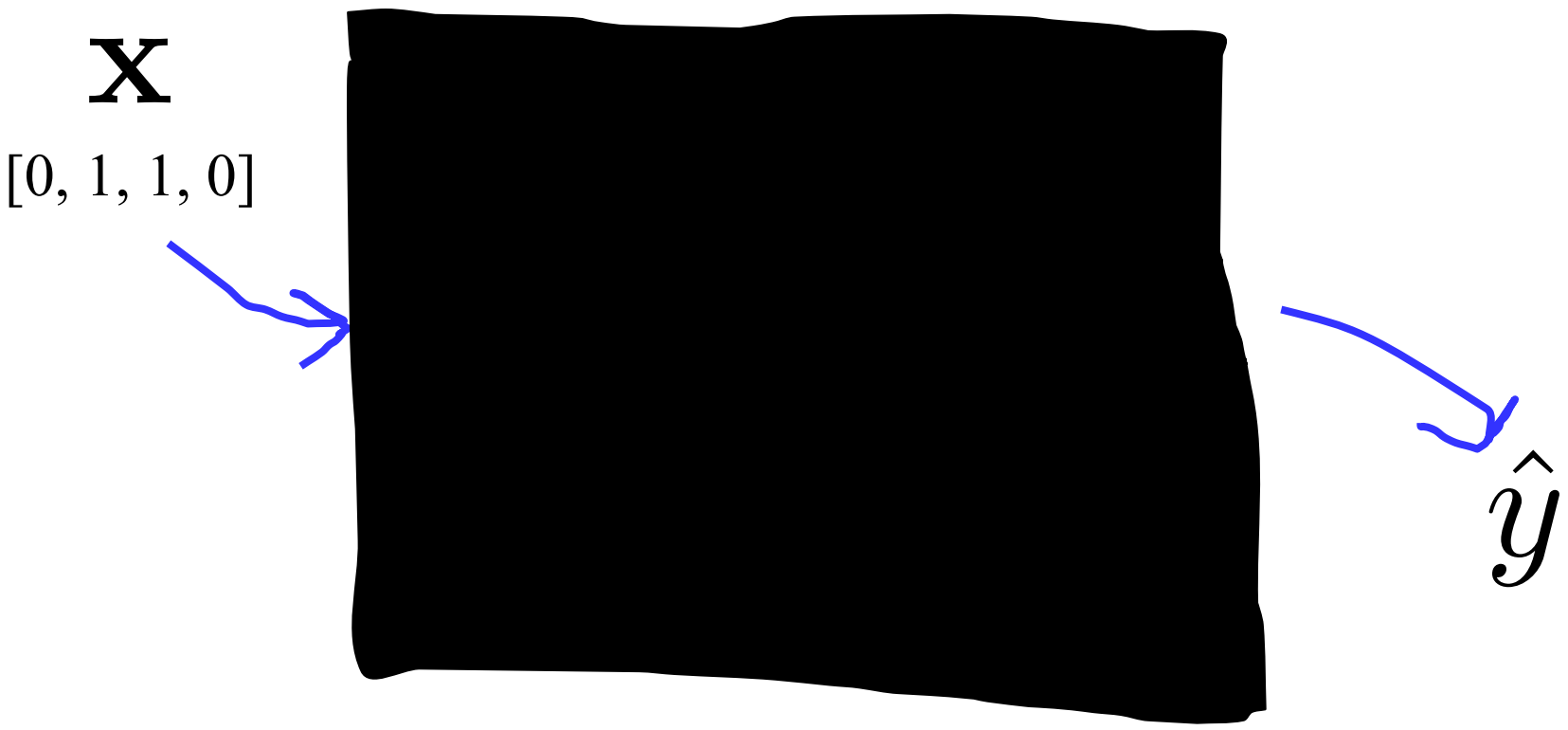
$$g_\theta(X)$$

Naïve Bayes Classification

$\mathbf{g}_\theta(\mathbf{x})$?



$g_\theta(\mathbf{x})$?



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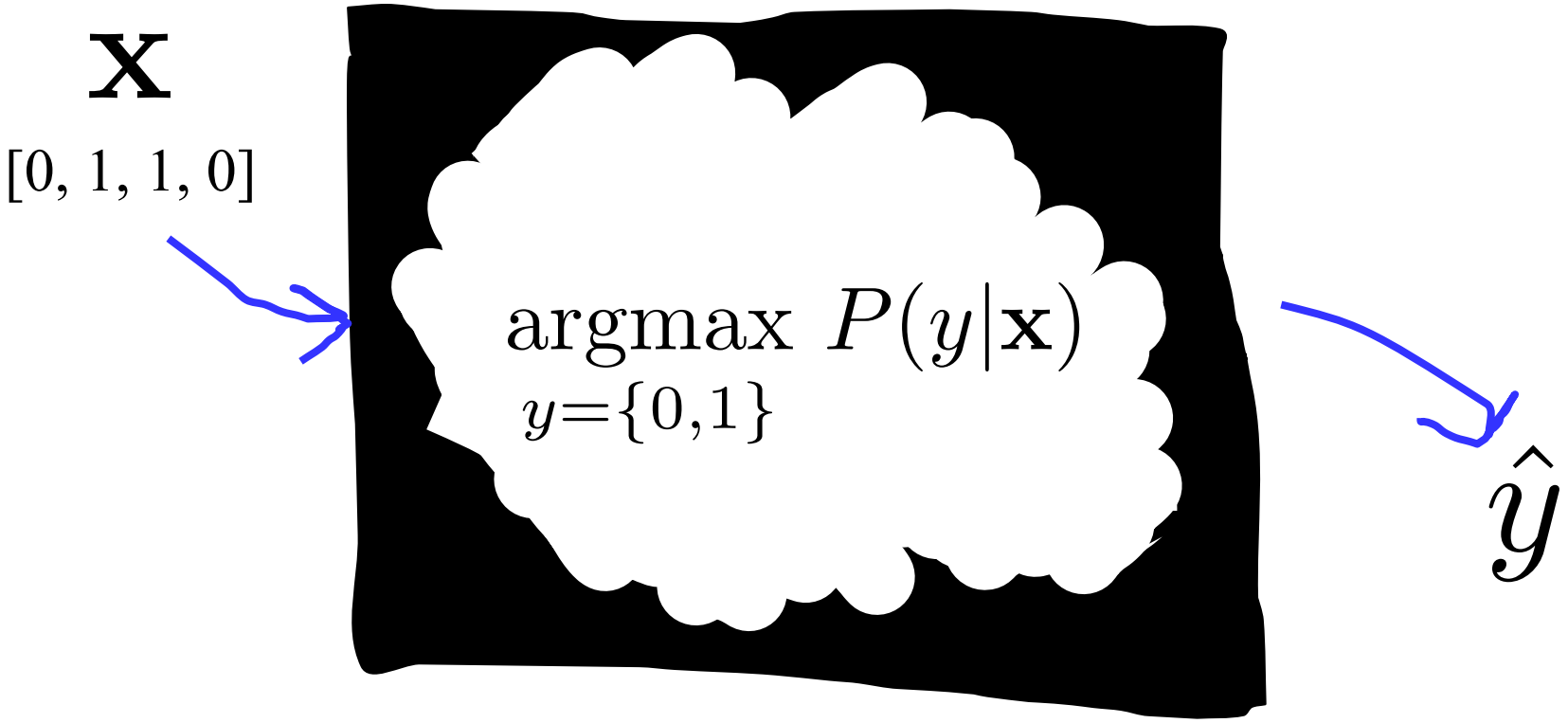

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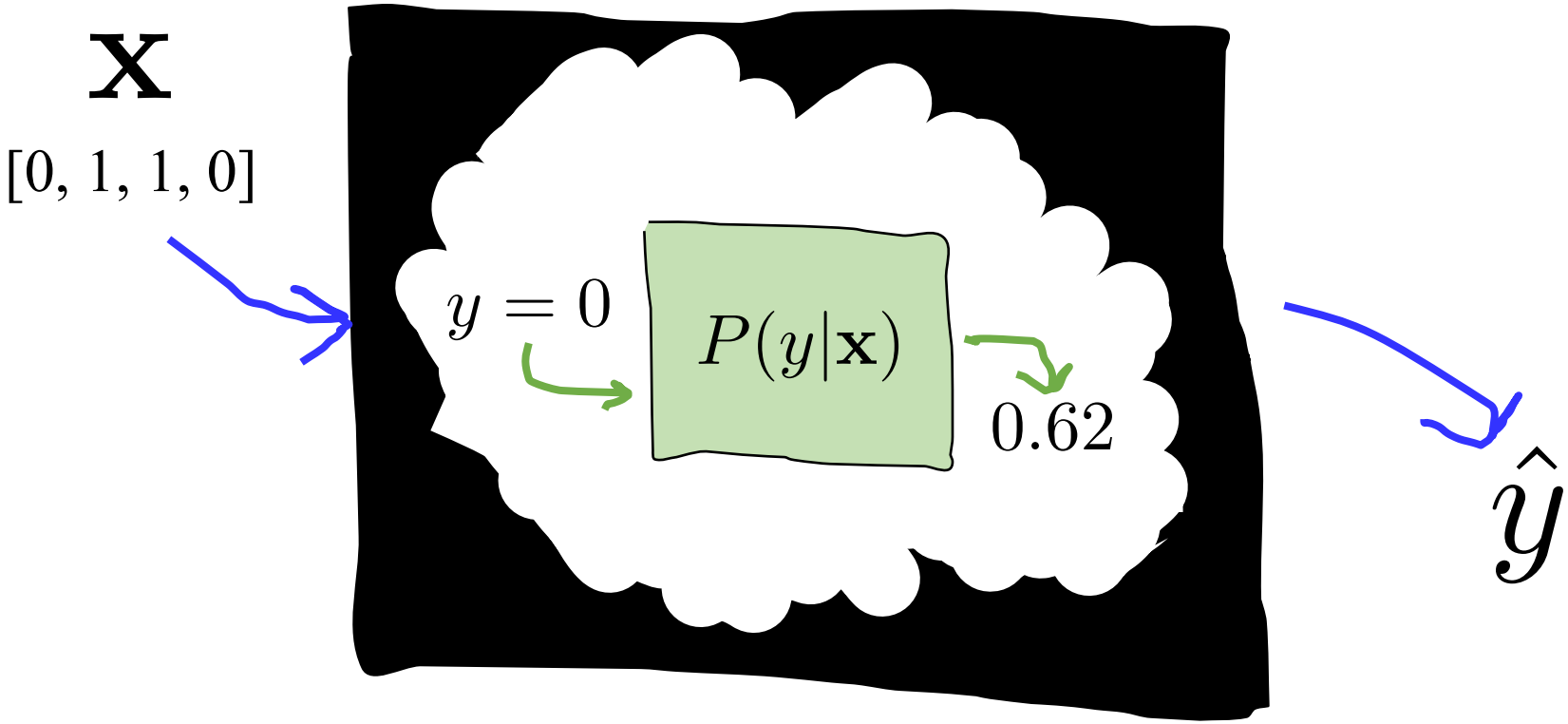

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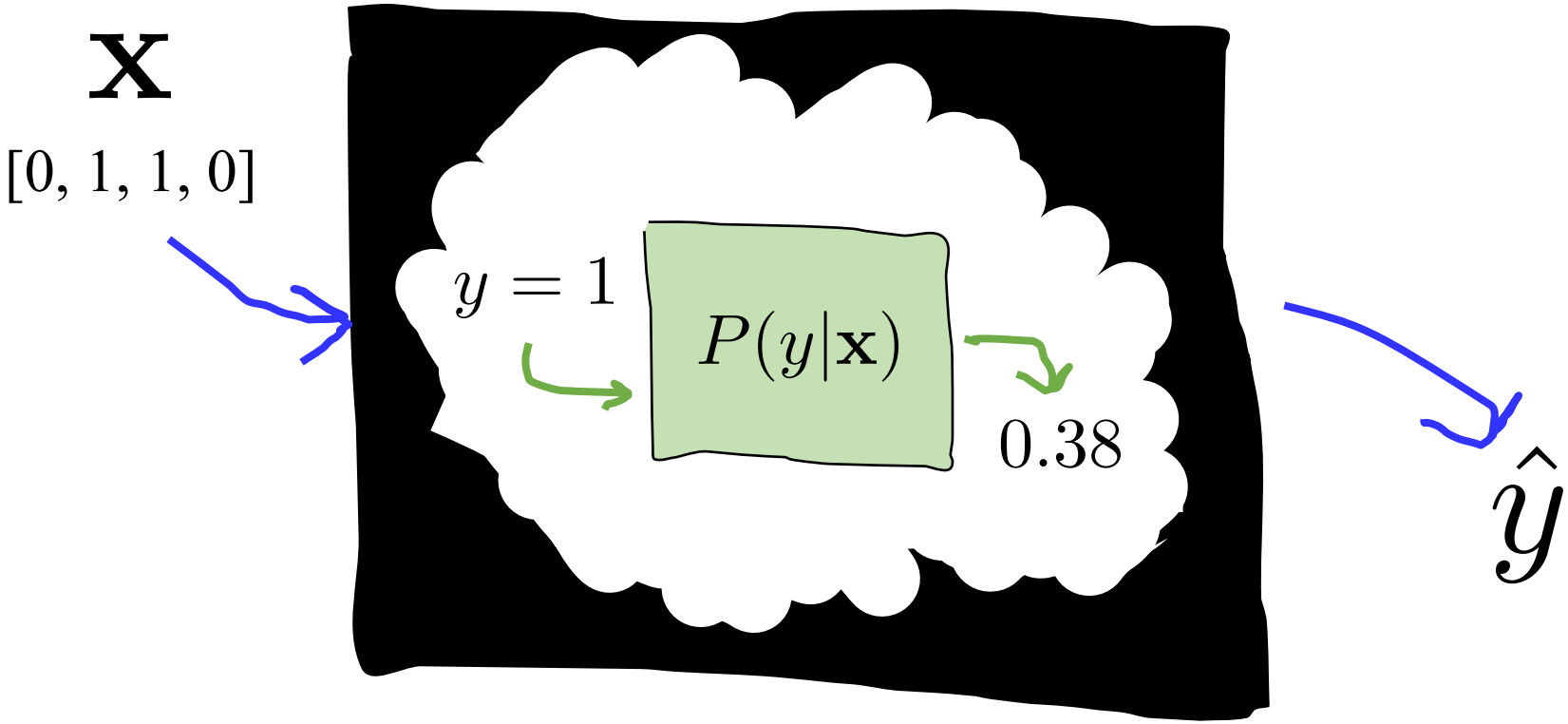

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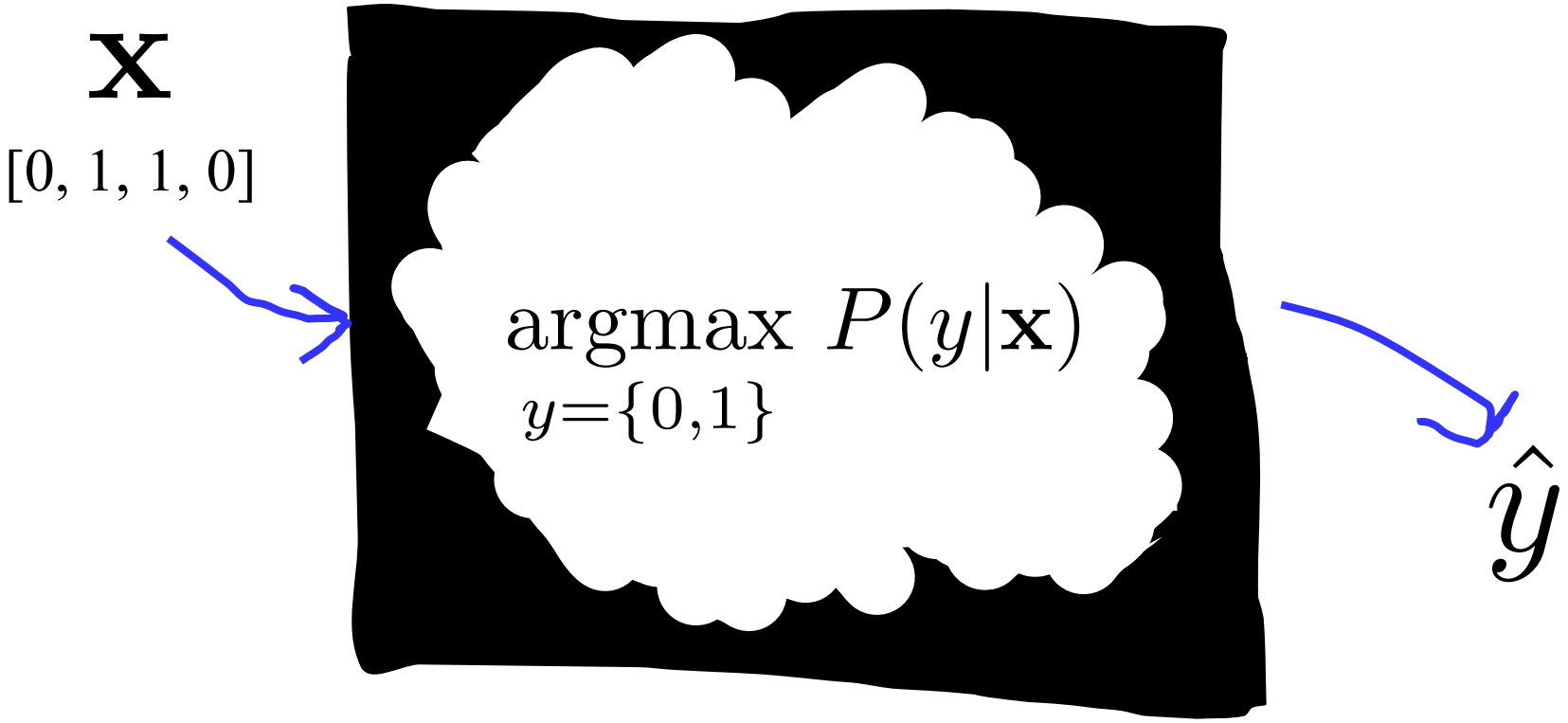

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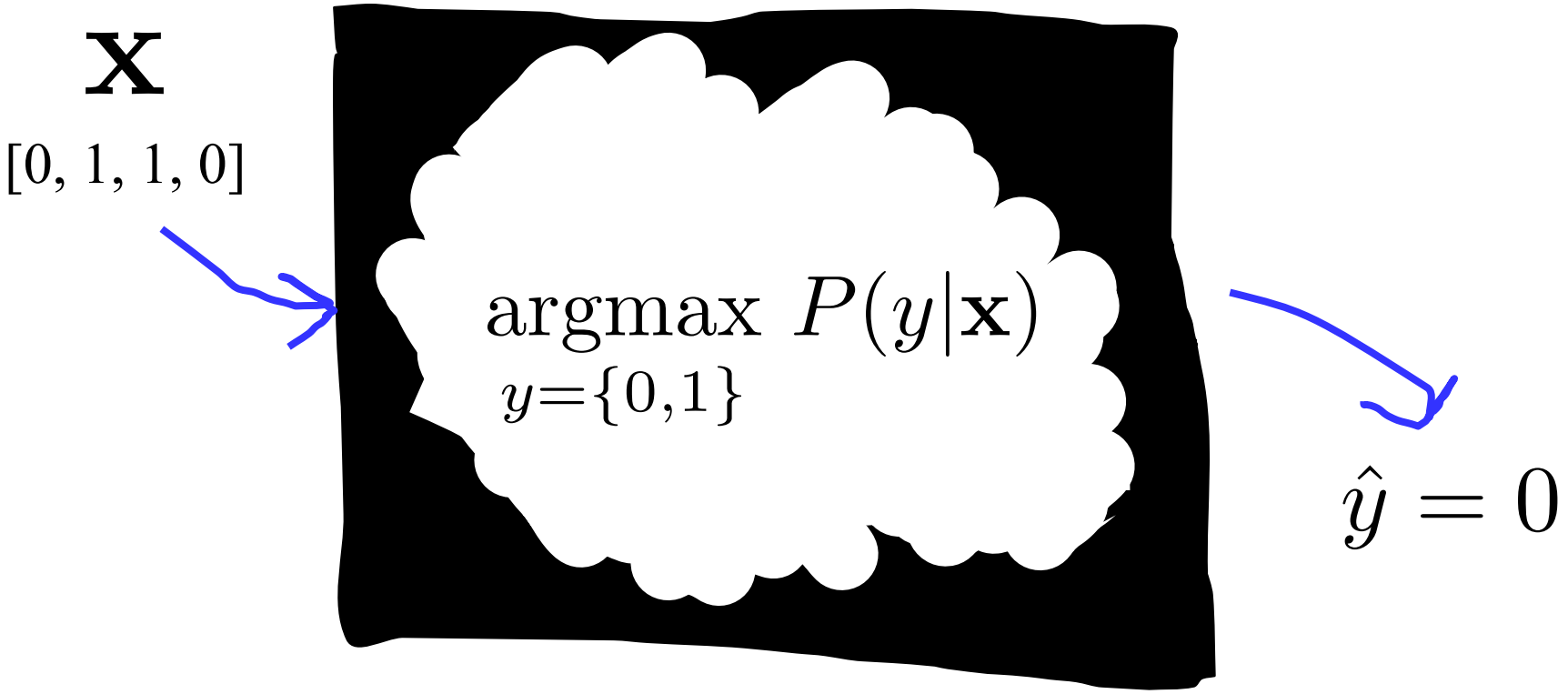

Simply chose the class label that is the most likely given the data. Make Naïve Bayes assumption

$$\hat{y} = \mathrm{g}(\mathbf{x})$$
$$= \underset{y=\{0,1\}}{\arg\max}\ P(Y = y|\mathbf{X} = \mathbf{x})$$

Naïve Bayes

Simply chose the class label that is the most likely given the data. Make Naïve Bayes assumption

$$
\begin{aligned}
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&= \arg\max_{y=\{0,1\}} \frac{P(Y = y) P(\mathbf{X} = \mathbf{x} | Y = y)}{P(\mathbf{X} = \mathbf{x})} \\
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&= \arg\max_{y=\{0,1\}} \log P(Y = y) + \sum_i \log P(X_i = x_i | Y = y)
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Woot, Bayes!

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$$= \arg\max_{y=\{0,1\}} \frac{P(Y = y)P(\mathbf{X} = \mathbf{x}|Y = y)}{P(\mathbf{X} = \mathbf{x})}$$

argmax is unaffected by P(X)

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

$$= \arg\max_{y=\{0,1\}} P(Y = y)\prod_i P(X_i = x_i|Y = y)$$

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Naïve Bayes Assumption

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\end{aligned}
$$

Argmax of log

Computing Probabilities from Data

- Various probabilities you will need to compute for Naive Bayesian Classifier (using MLE here):

$$\hat{p}(X_i = 1|Y = 0) = \frac{(\#\text{ training examples where } X_i = 1 \text{ and } Y = 0)}{(\#\text{ training examples where } Y = 0)}$$

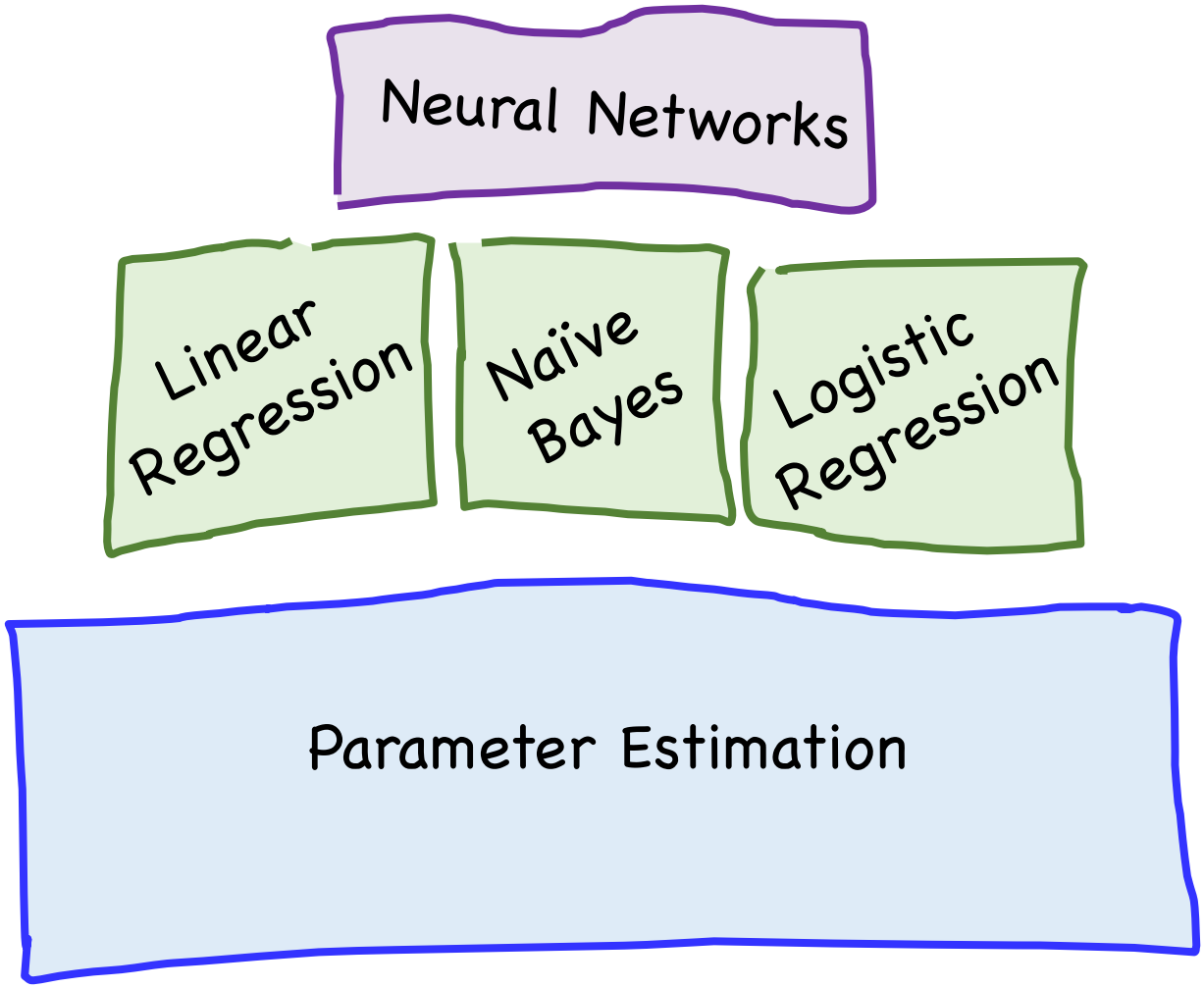
$$\hat{p}(Y = 1) = \frac{(\#\text{ training examples where } Y = 1)}{(\#\text{ training examples})}$$

Training Naïve Bayes, is estimating parameters for a multinomial.

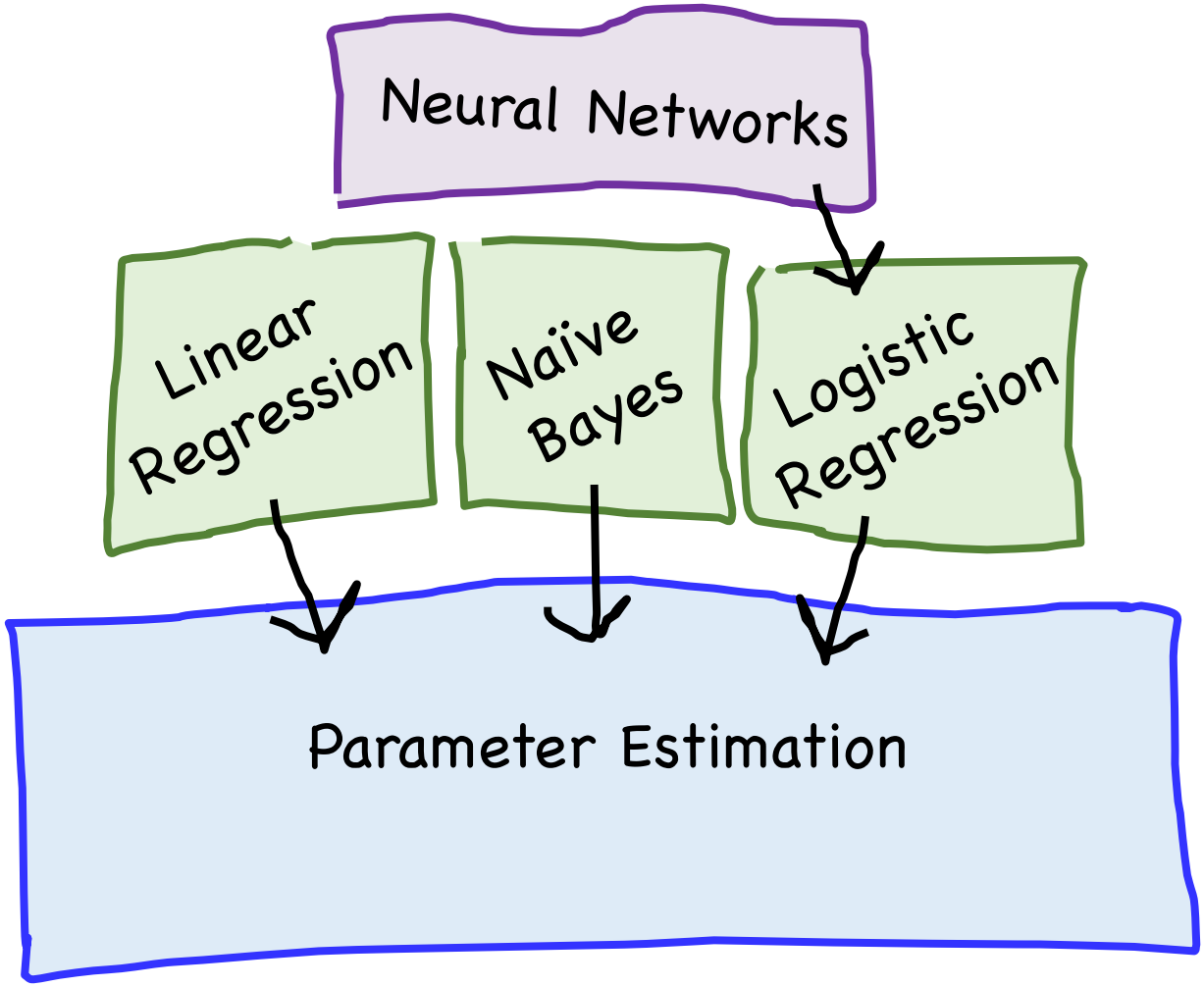
Thus training is just counting (sometimes with laplace smoothing).

End Review

Our Path


Neural Networks
Linear Regression
Naïve Bayes
Logistic Regression
Parameter Estimation

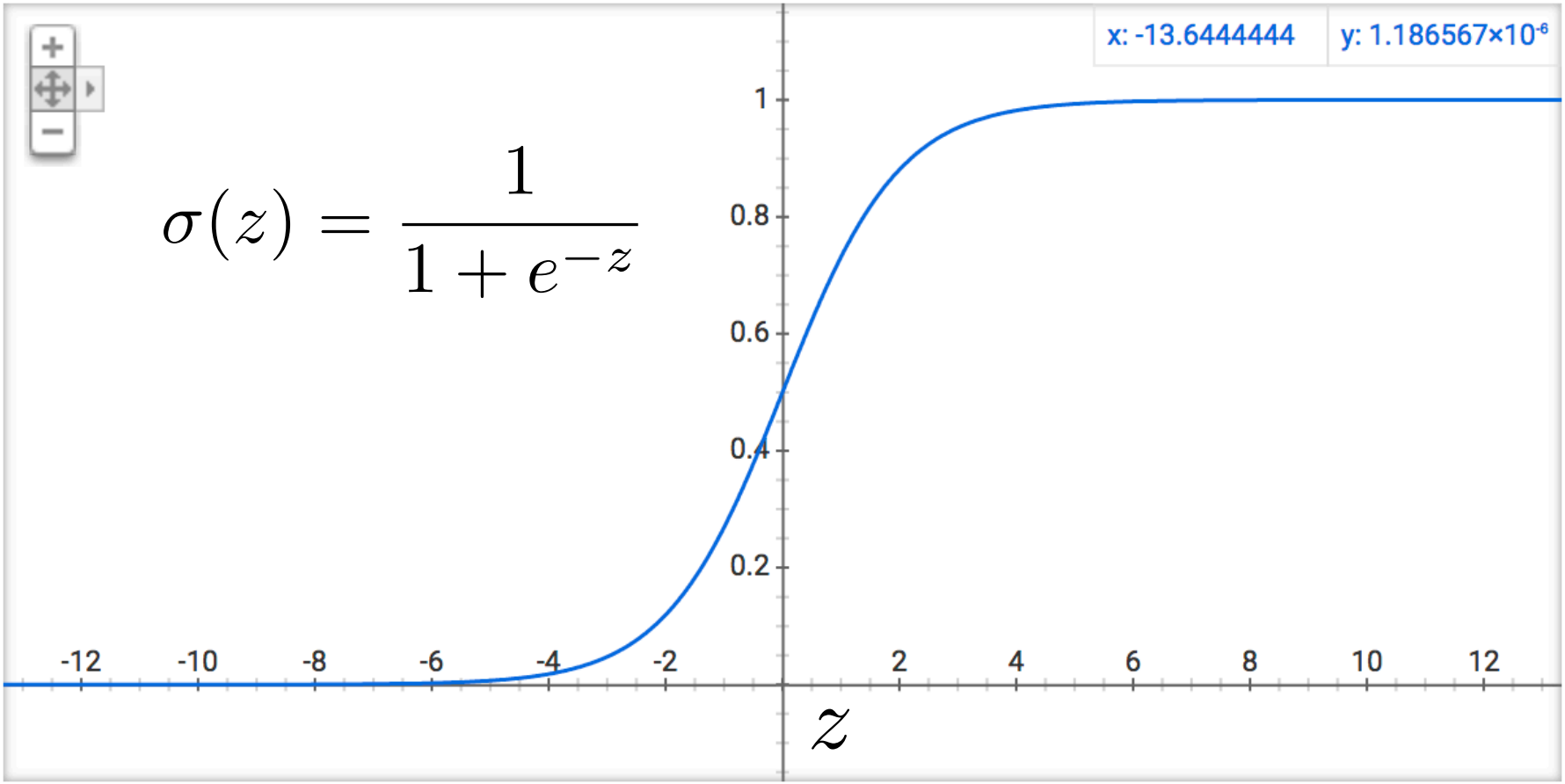
Knowledge Dependency



Logistic Regression

Chapter 0: Background

Background: Sigmoid Function



The sigmoid function squashes z to be a number between 0 and 1

Background: Key Notation

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

Sigmoid function

$$\theta^T \mathbf{x} = \sum_{i=1}^{n} \theta_i x_i$$

$$= \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n$$

Weighted sum
(aka dot product)

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

Sigmoid function of
weighted sum

Background: Chain Rule

It's called chain rule

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

Chapter 1: Big Picture

From Naïve Bayes to Logistic Regression

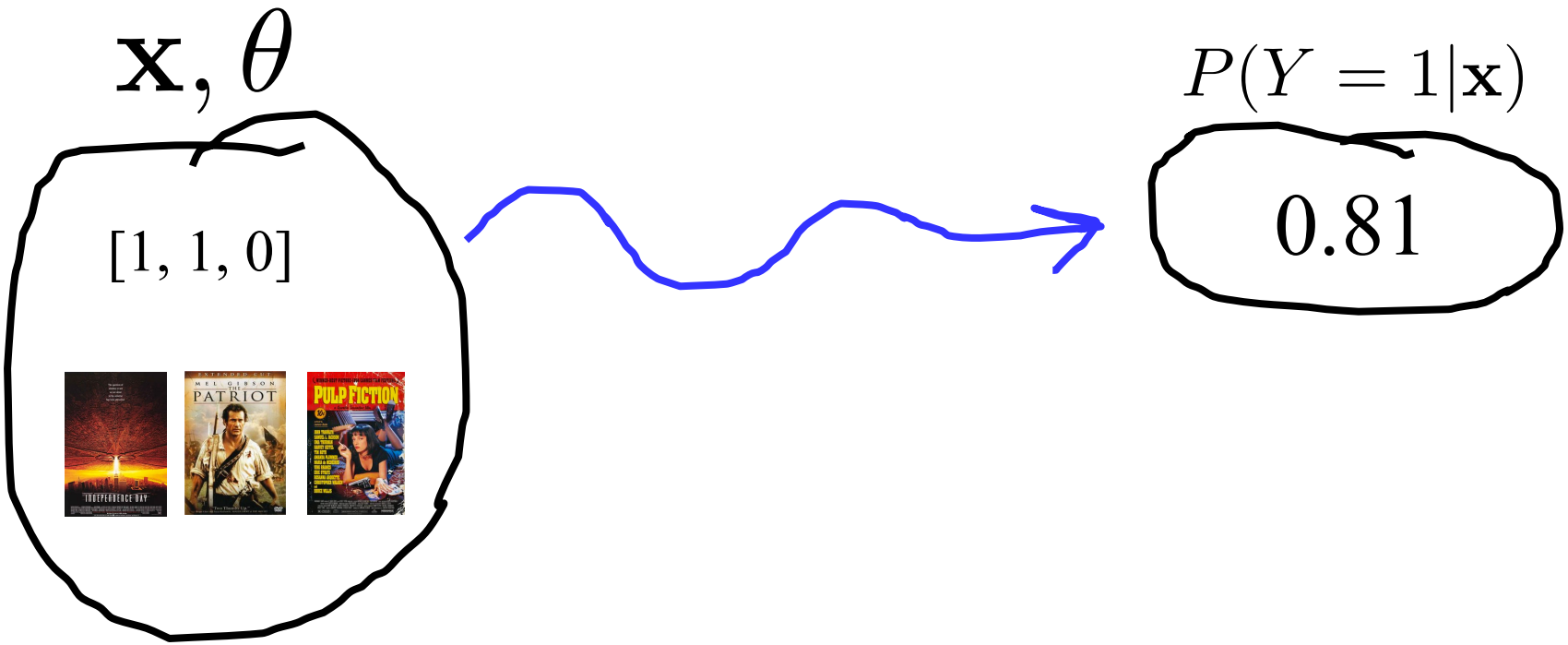
- In classification we care about P(Y | **X**)

- Recall the Naive Bayes Classifier
  - Predict P(Y | **X**)
  - Use assumption that $P(\boldsymbol{X} \mid Y) = P(X_1, X_2, \ldots X_m \mid Y) = \prod_{i=1}^{m} P(X_i \mid Y)$
  - That is a pretty big assumption…

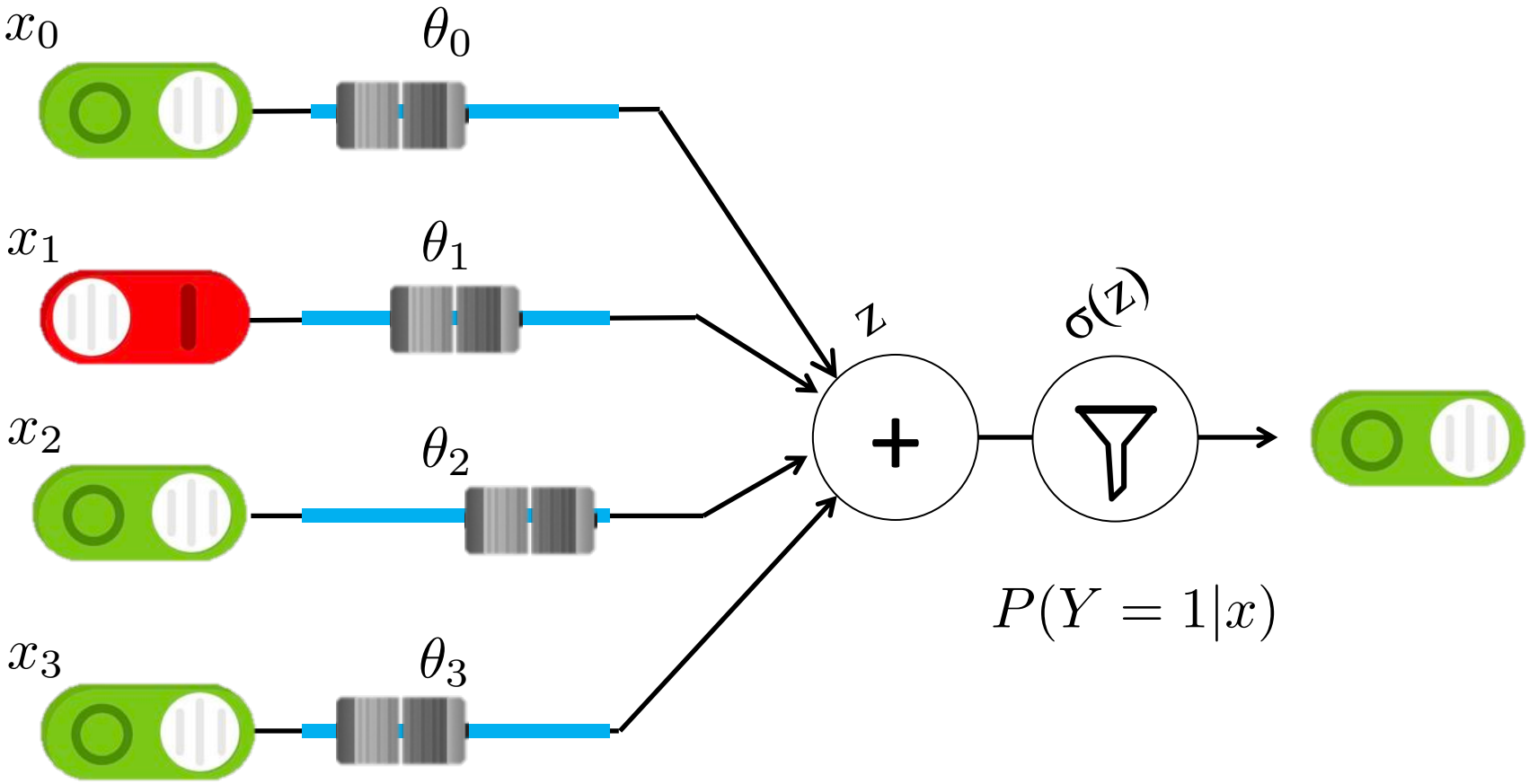
- Could we model P(Y | **X**) directly?
  - Welcome our friend: logistic regression!

Logistic Regression Assumption

- Could we model P(Y | **X**) directly?
  - Welcome our friend: logistic regression!

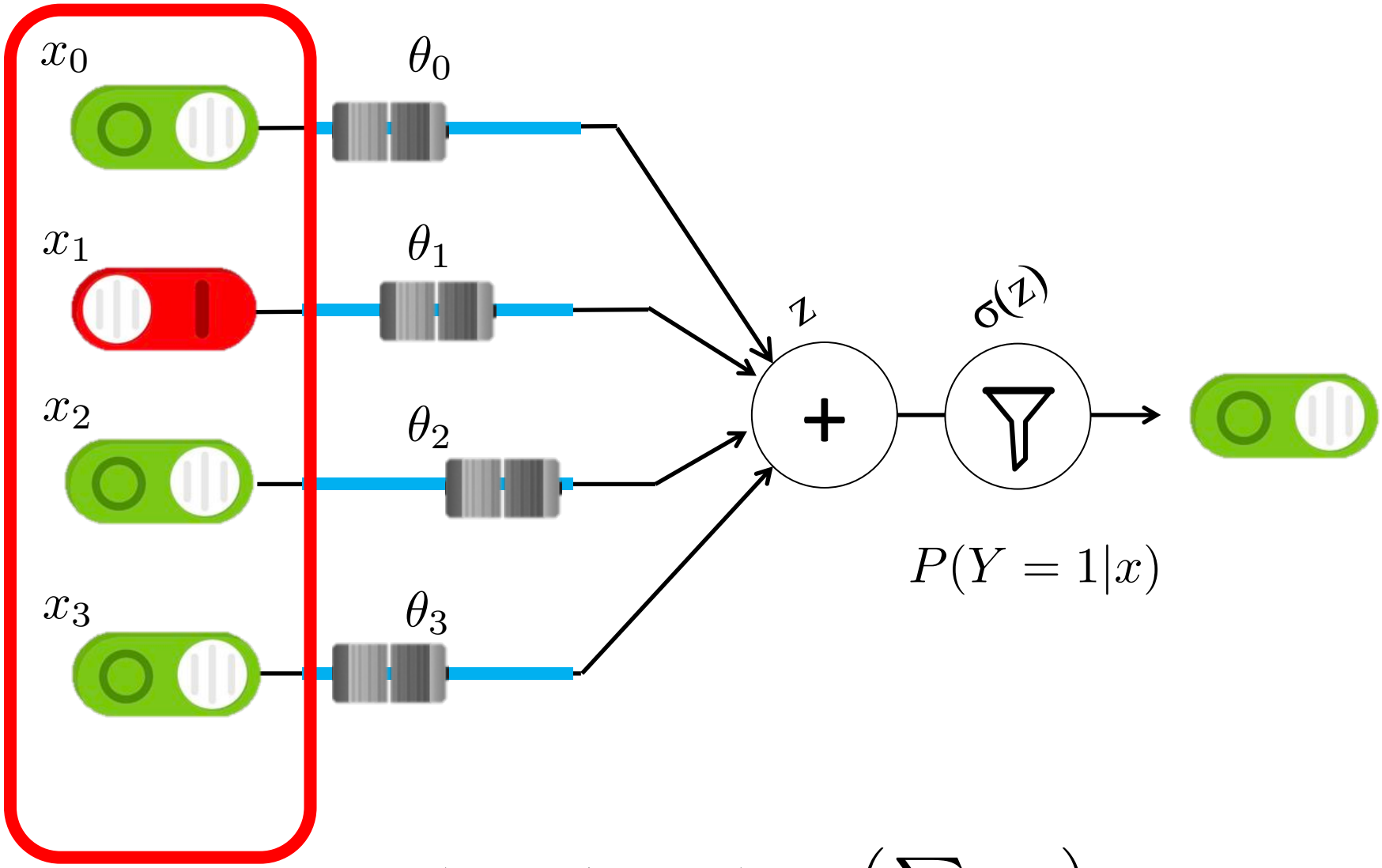


Logistic Regression Cartoon



$$P(Y = 1|\mathbf{X} = \mathbf{x}) = \sigma\left(\sum_i \theta_i x_i\right)$$

Inputs $x = [0, 1, 1]$



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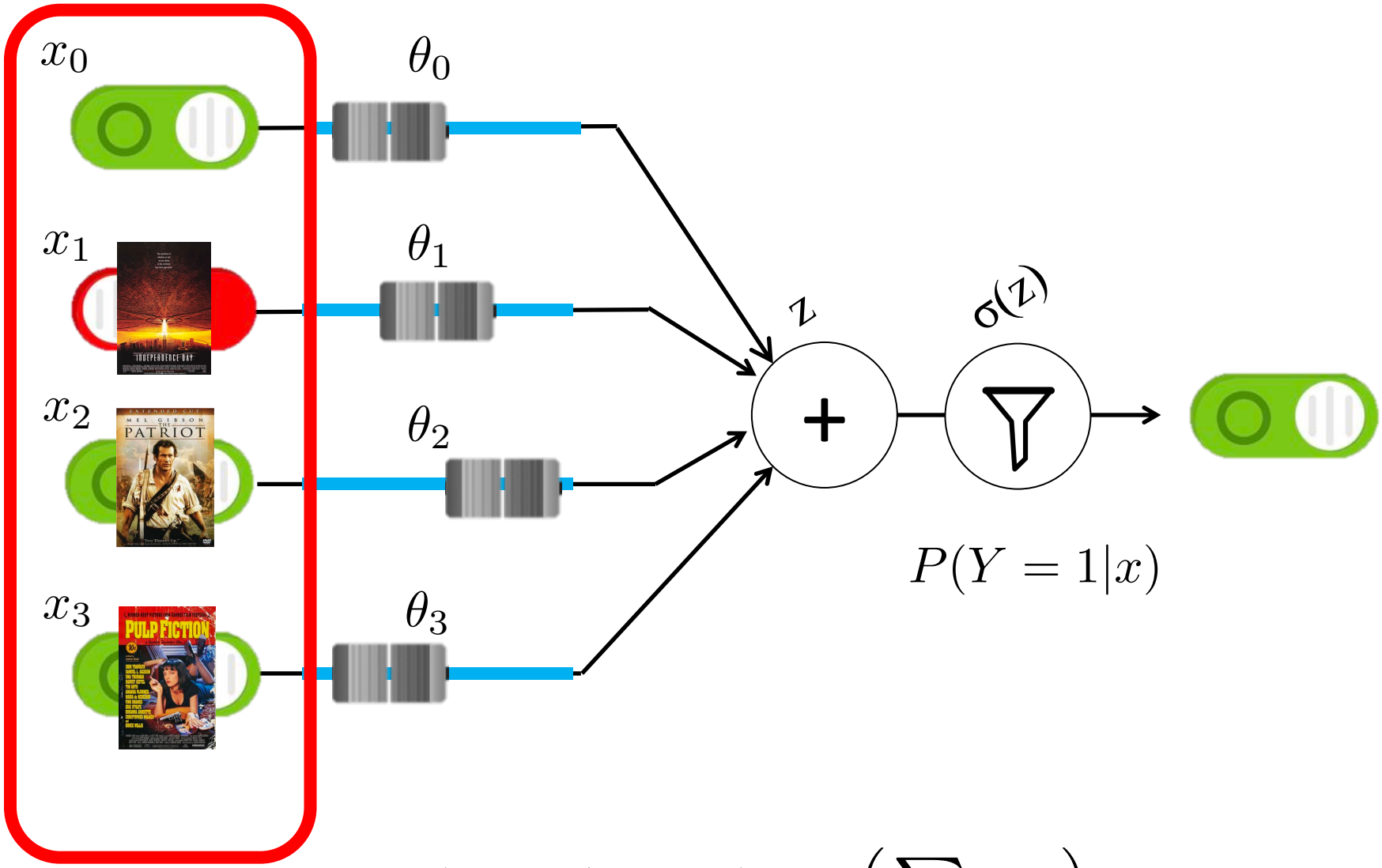
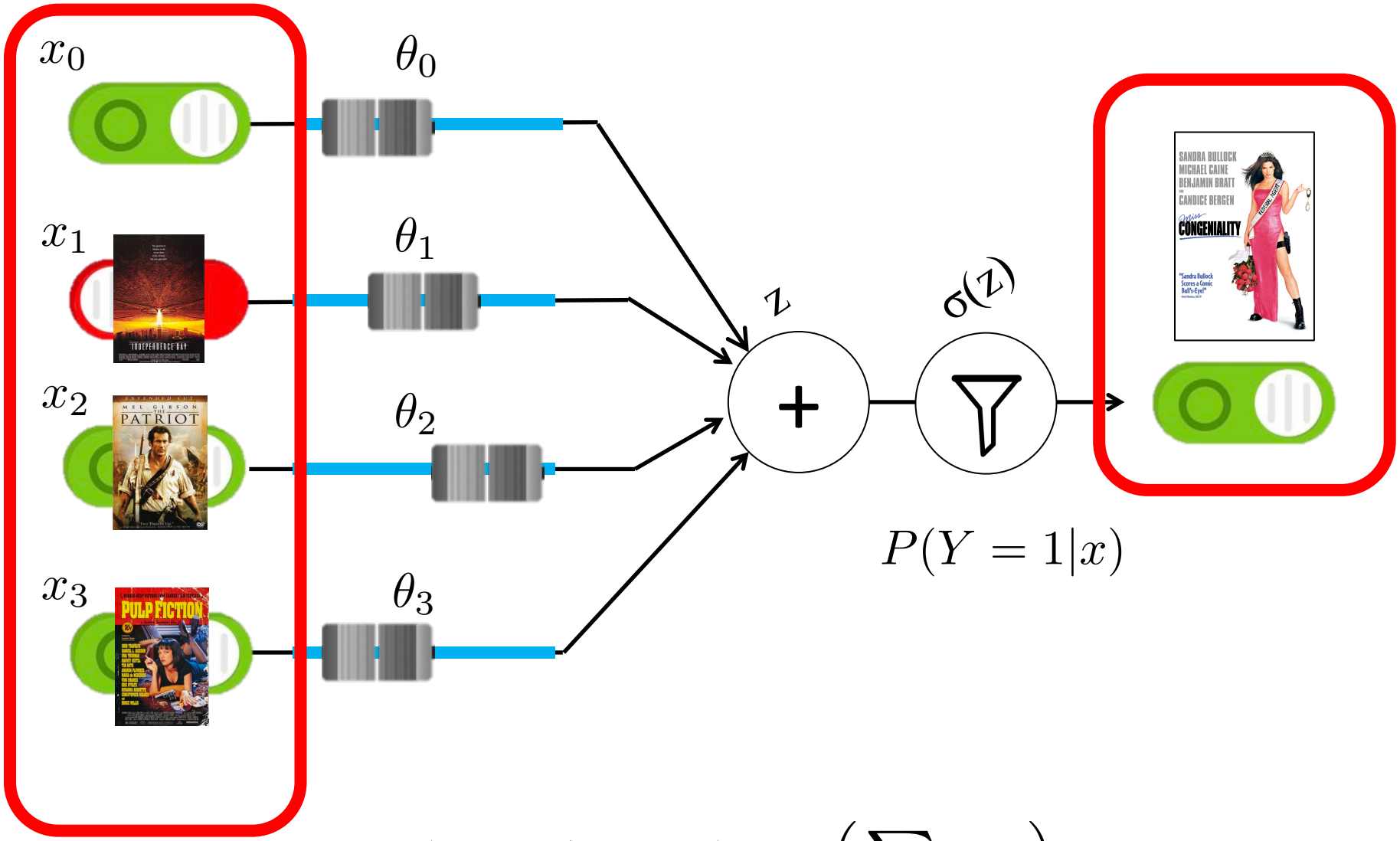


$$P(Y = 1|\mathbf{X} = \mathbf{x}) = \sigma\left(\sum_i \theta_i x_i\right)$$

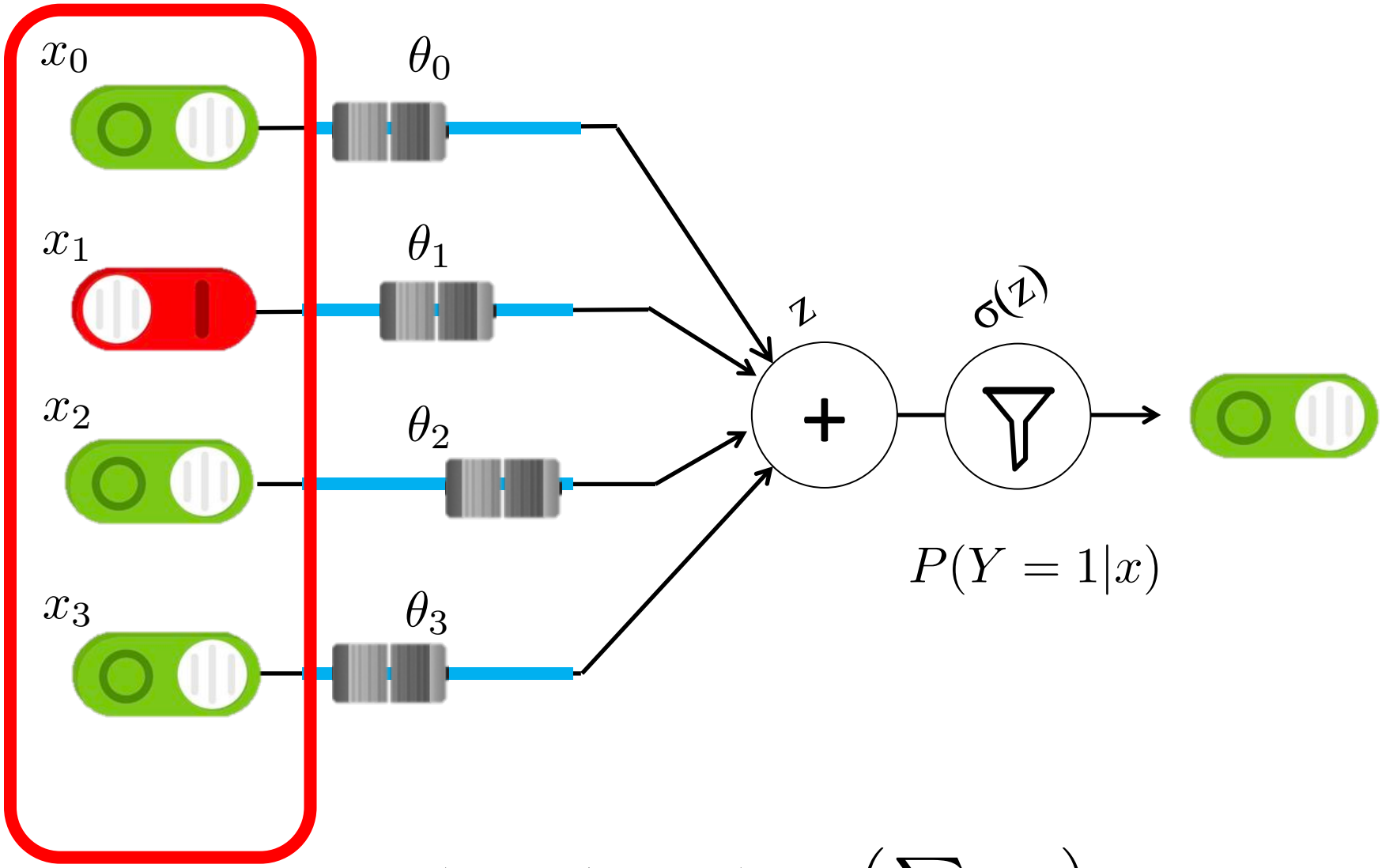
Inputs + Output



$$P(Y = 1|x)$$

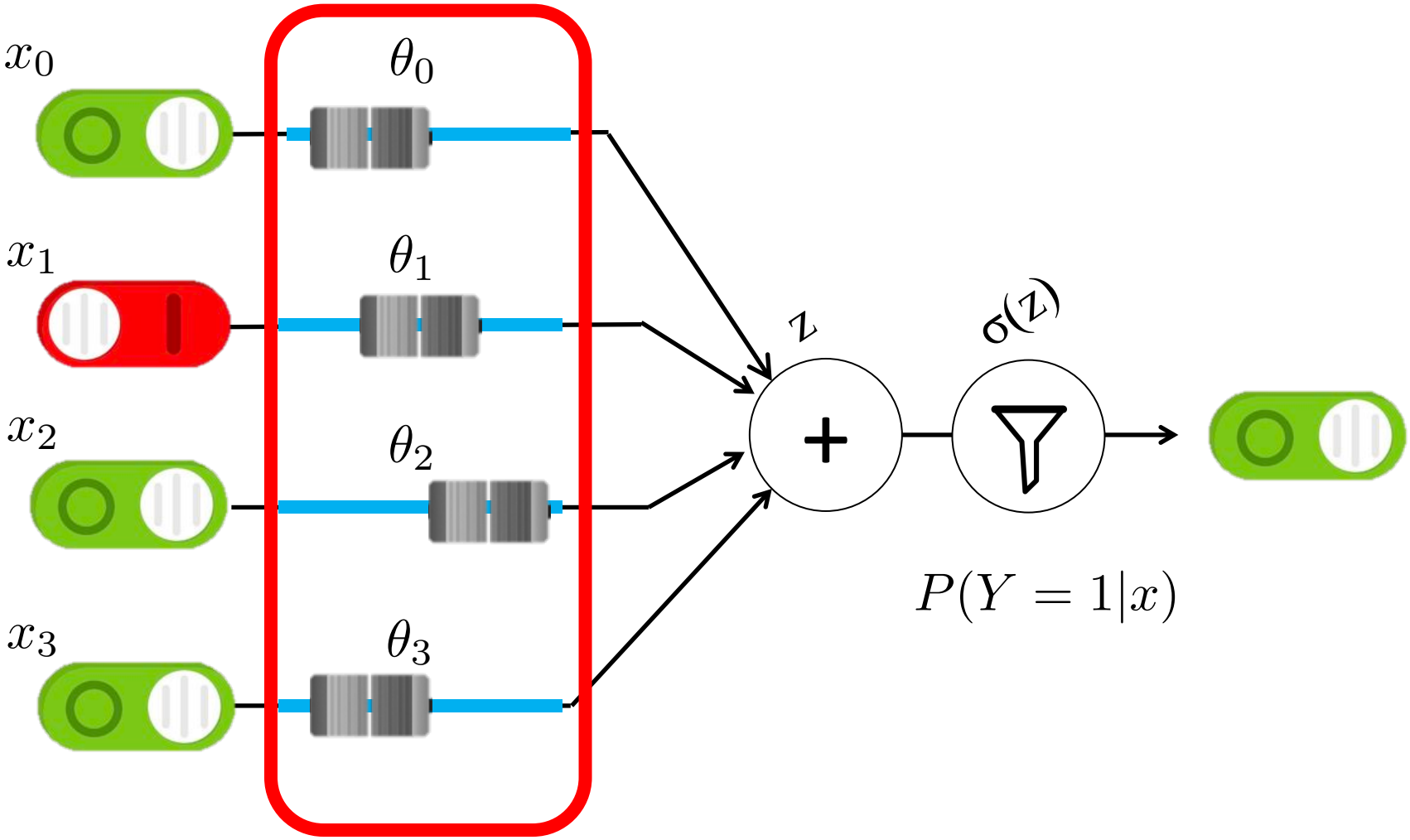
$$P(Y = 1|\mathbf{X} = \mathbf{x}) = \sigma\left(\sum_i \theta_i x_i\right)$$

Inputs



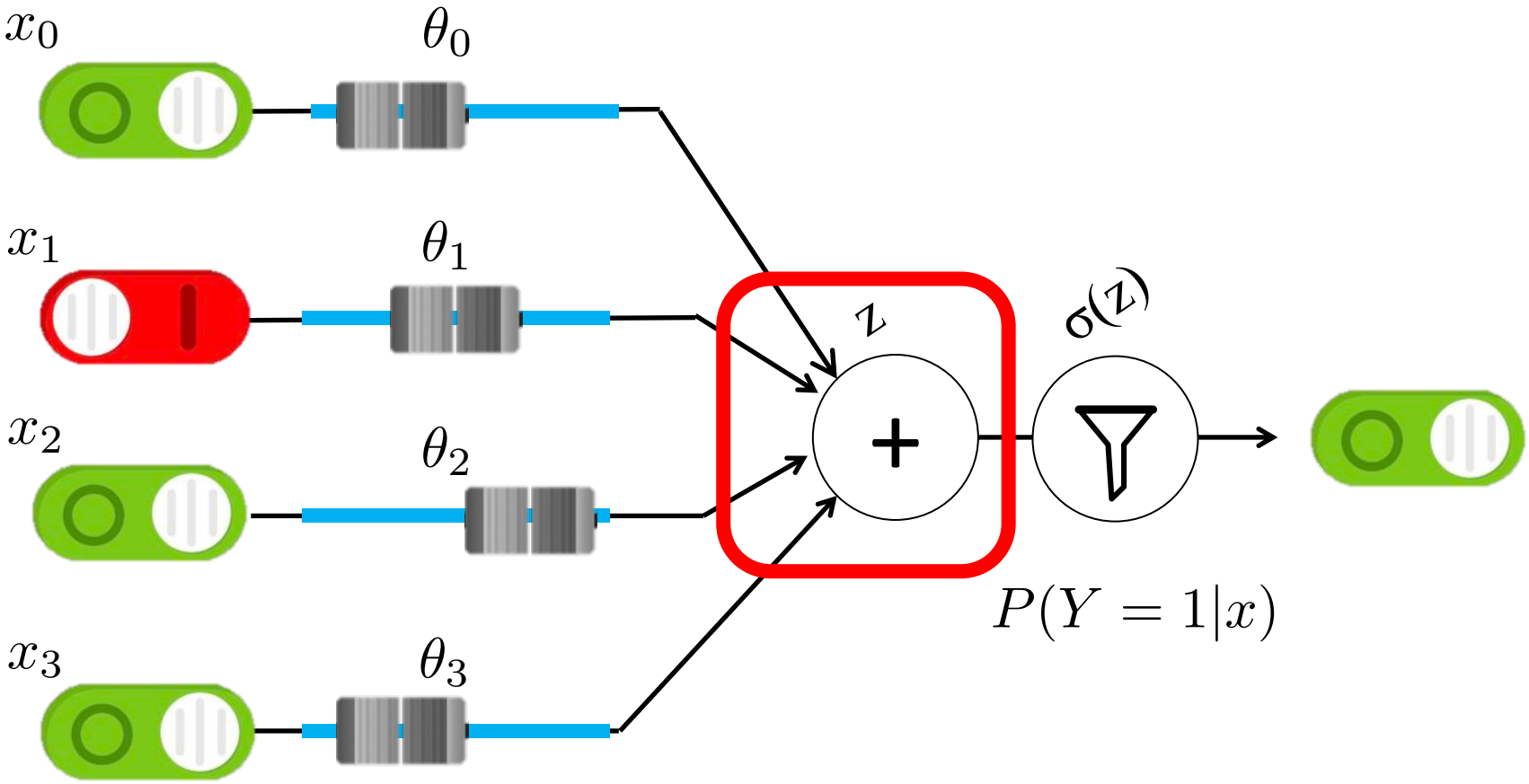
$$P(Y = 1|\mathbf{X} = \mathbf{x}) = \sigma\left(\sum_i \theta_i x_i\right)$$

Weights



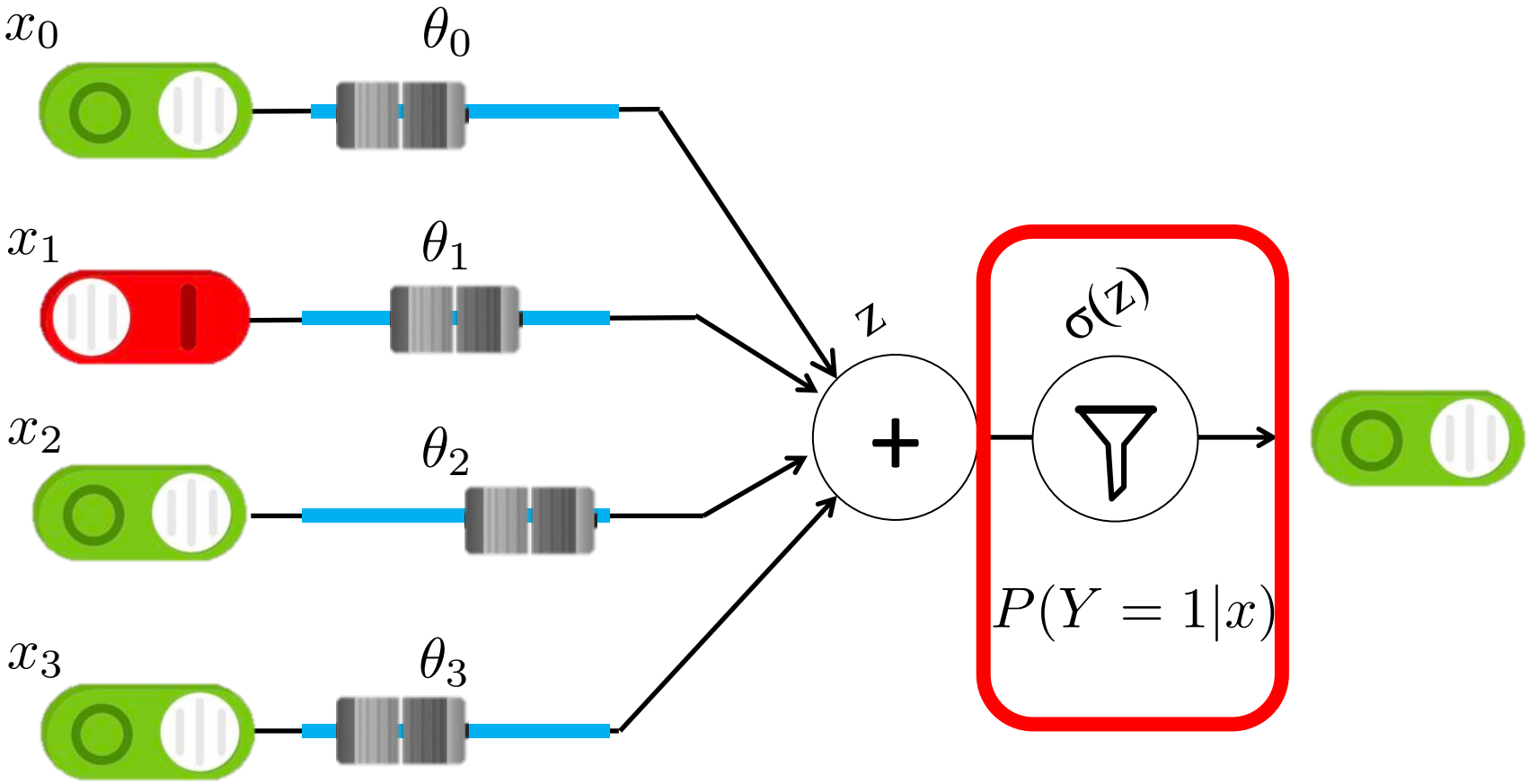
$$P(Y = 1|\mathbf{X} = \mathbf{x}) = \sigma\left(\sum_i \theta_i x_i\right)$$

Weighed Sum



$$P(Y = 1|\mathbf{X} = \mathbf{x}) = \sigma\Big(\sum_i \theta_i x_i\Big)$$

Squashing Function



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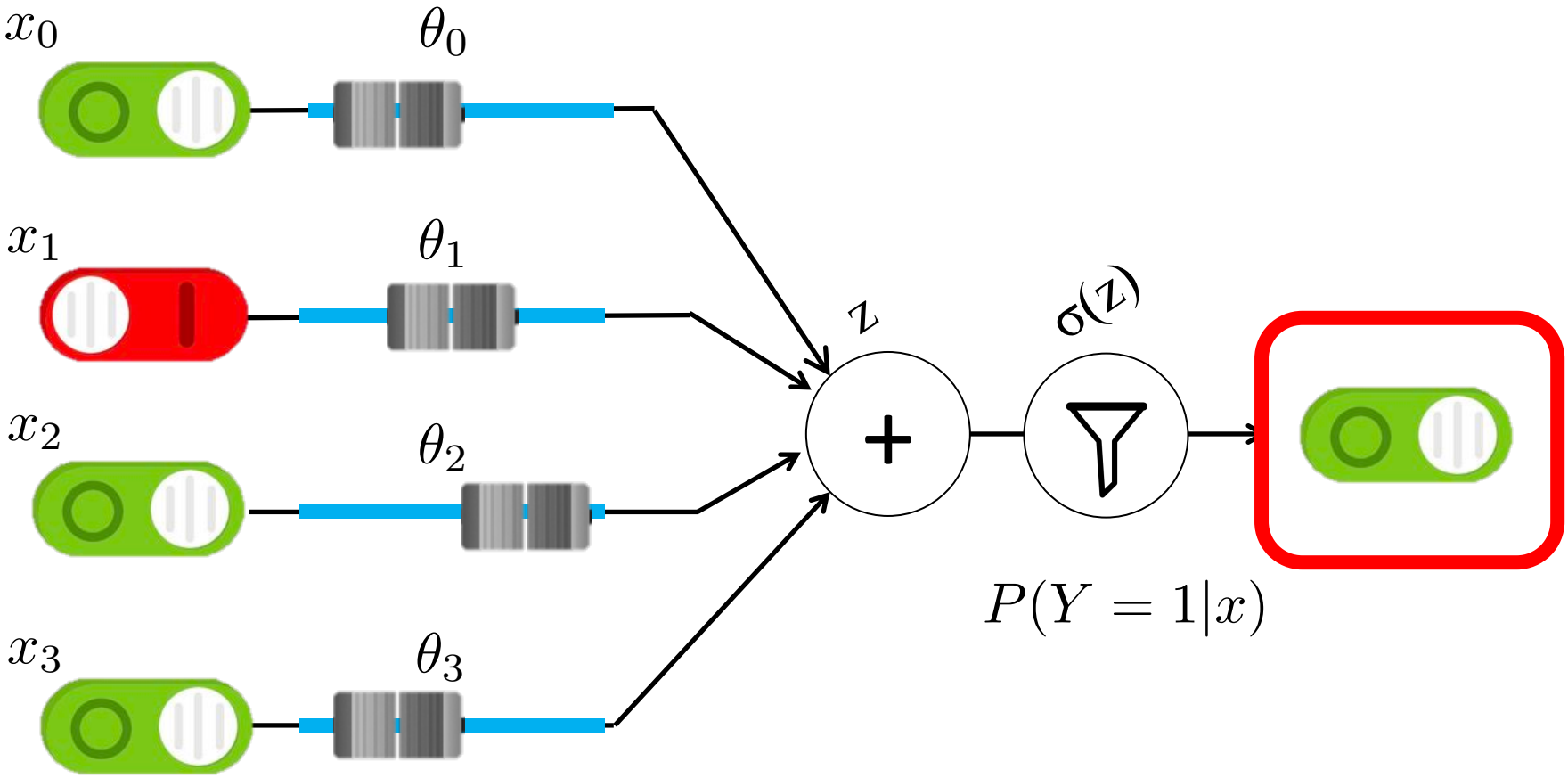
Prediction



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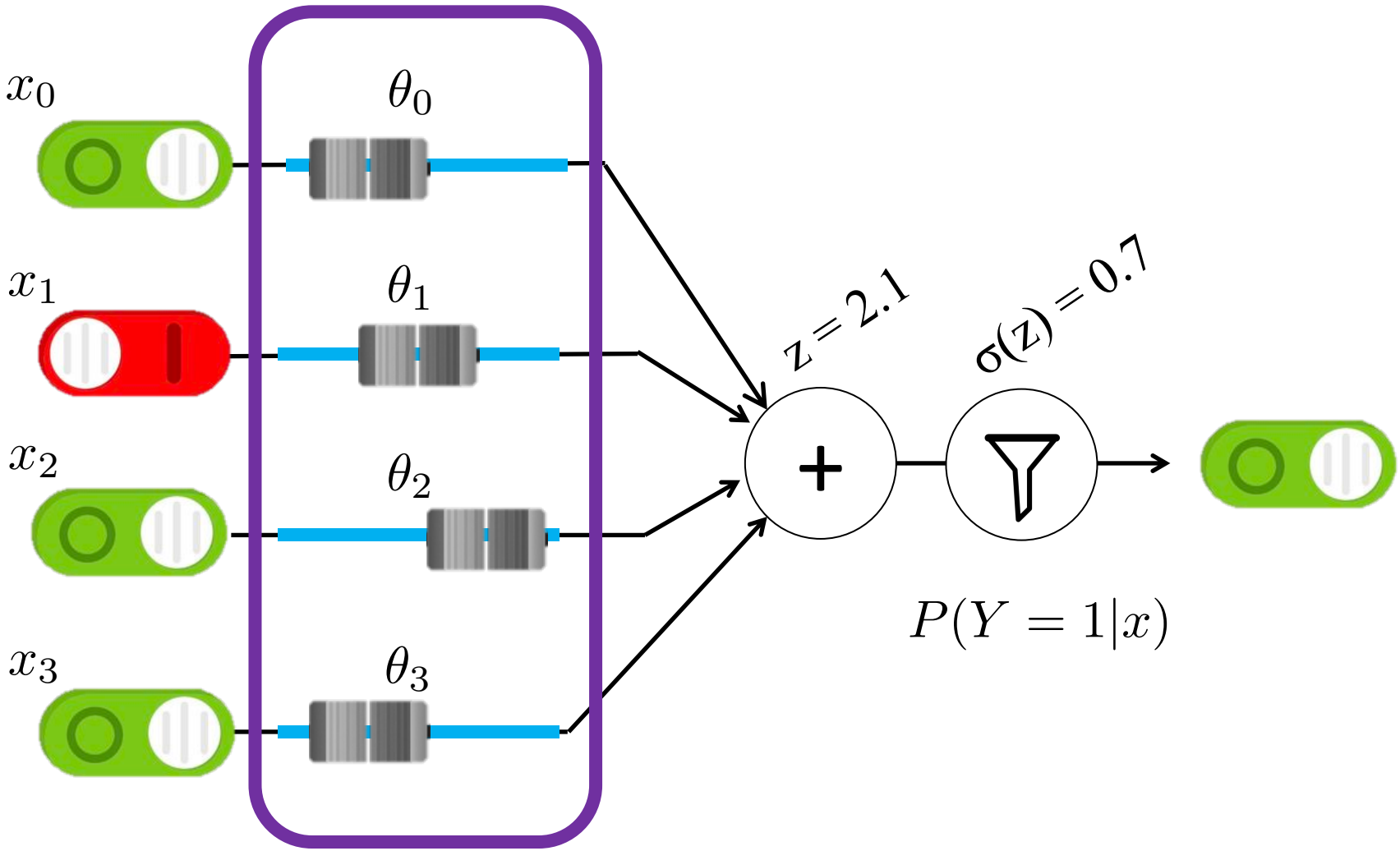
Parameters Affect Prediction



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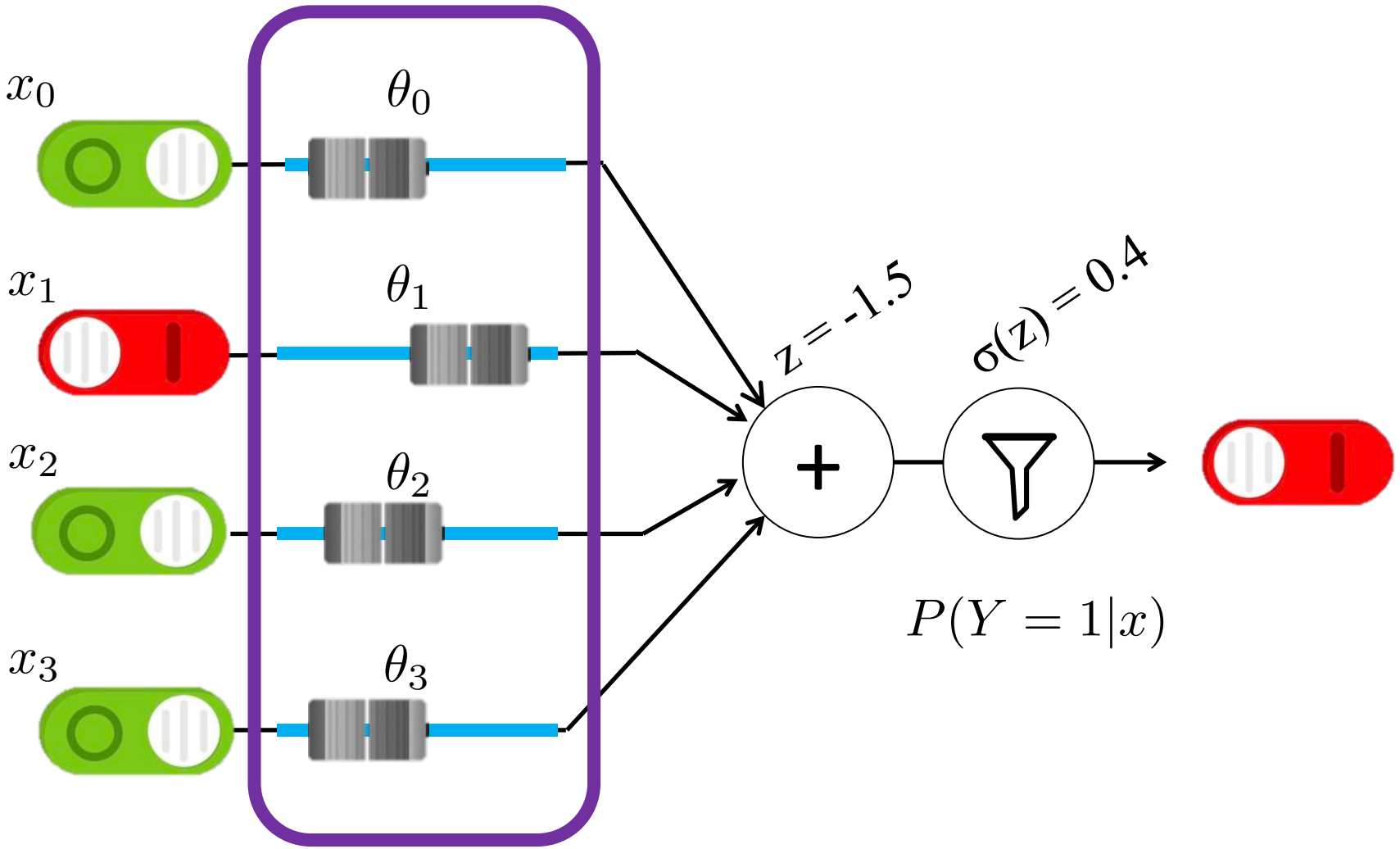

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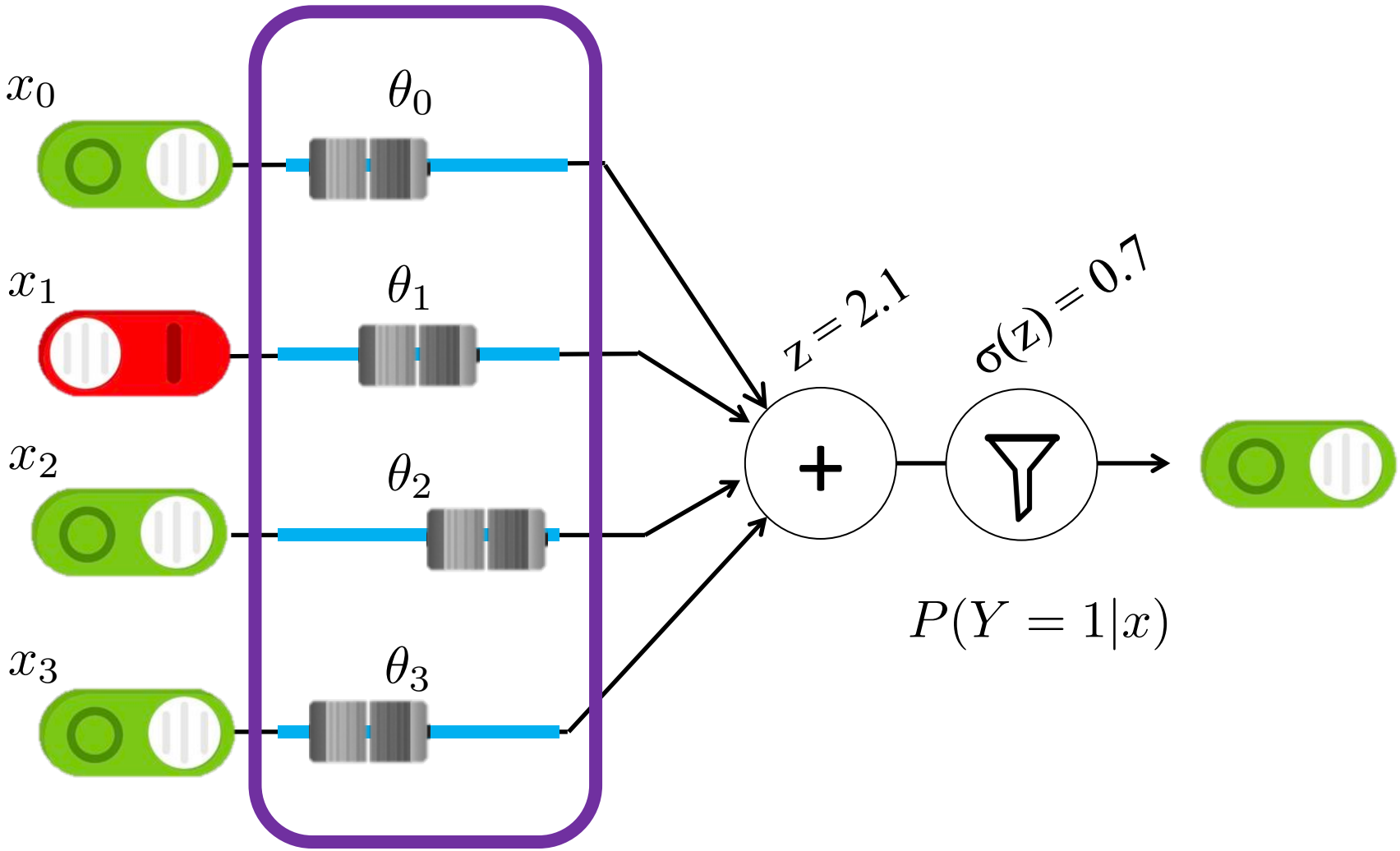

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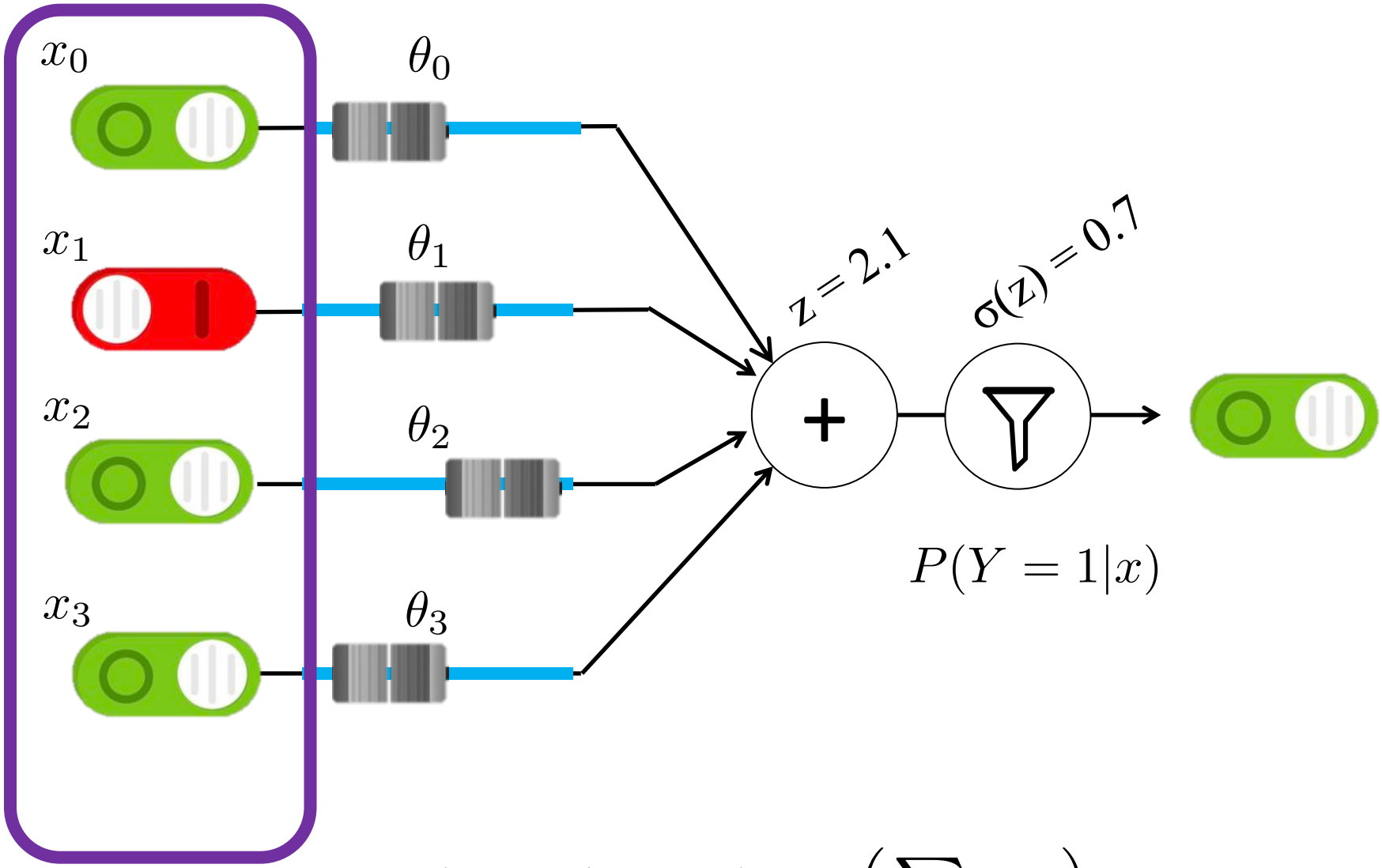
Different Predictions for Different Inputs



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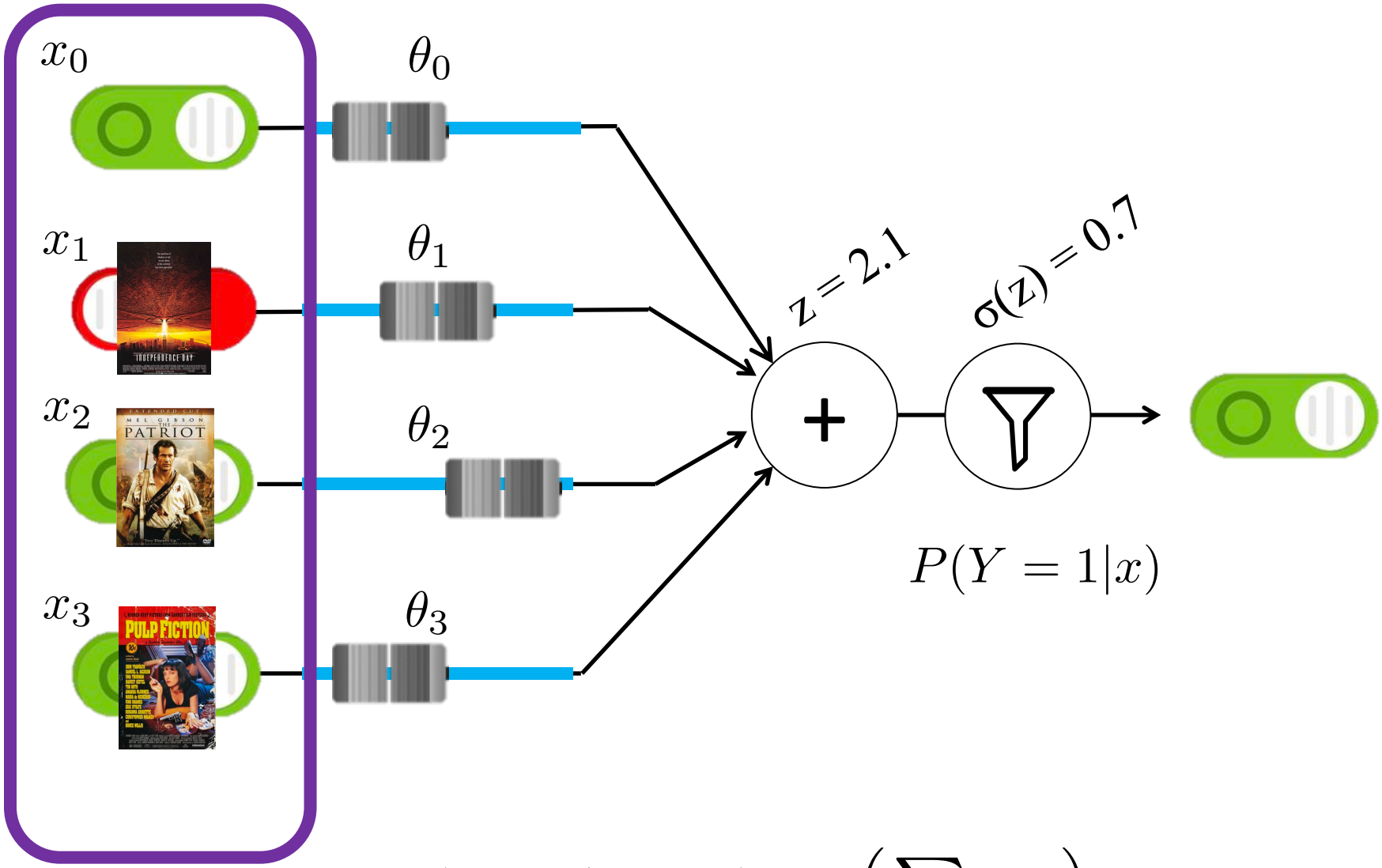
Different Predictions for Different Inputs



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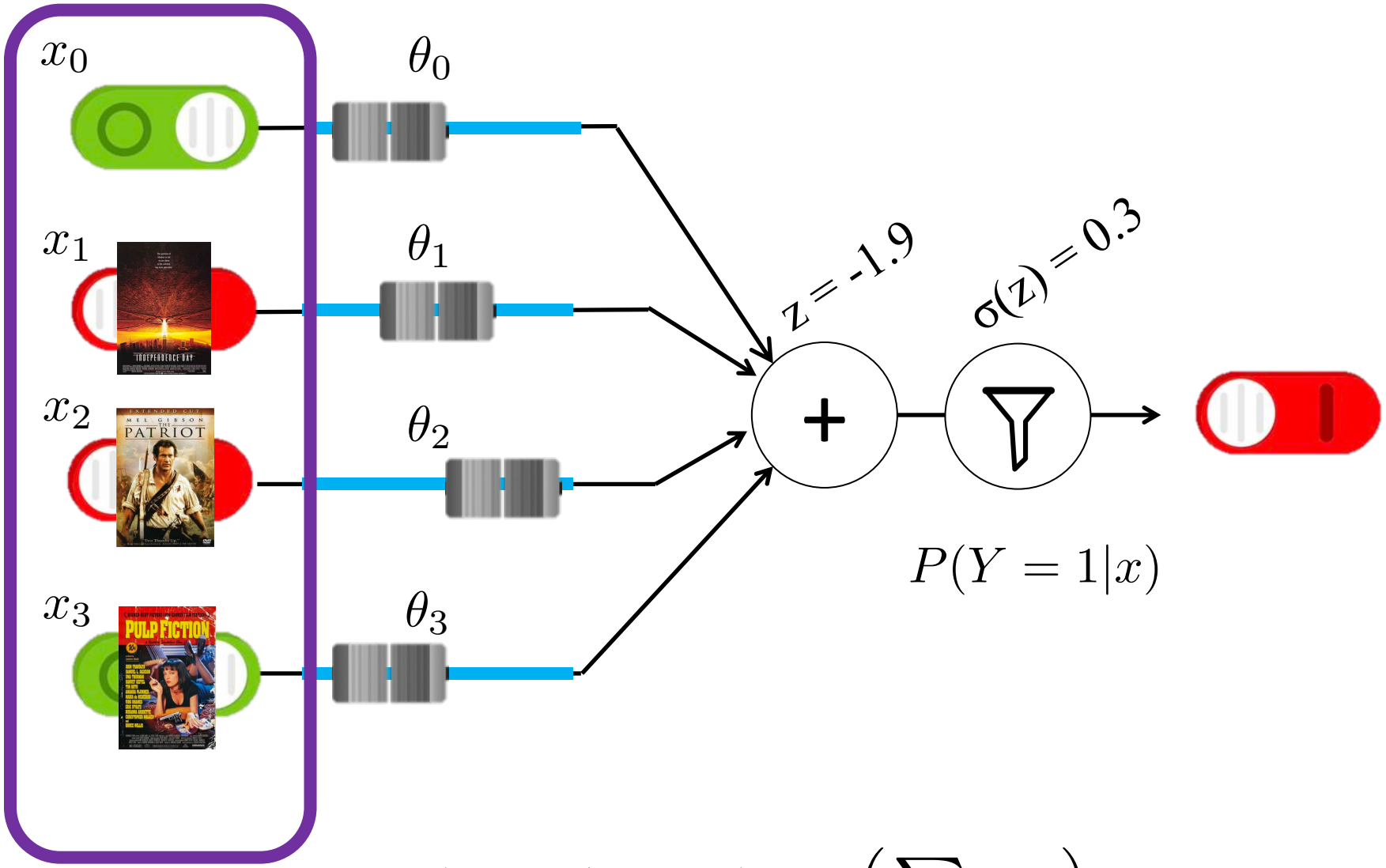
Different Predictions for Different Inputs



$$P(Y = 1|\mathbf{X} = \mathbf{x}) = \sigma\left(\sum_i \theta_i x_i\right)$$

Logistic Regression Assumption

- Model *conditional* likelihood P(Y | **X**) directly
  - Model this probability with *logistic* function:

$$P(Y = 1|\mathbf{X}) = \sigma(z) \text{ where } z = \theta_0 + \sum_{i=1}^{m} \theta_i x_i$$

  - For simplicity define $x_0 = 1$ so $z = \theta^T \mathbf{x}$
  - Since $\mathrm{P}(Y = 0 \mid \mathbf{X}) + \mathrm{P}(Y = 1 \mid \mathbf{X}) = 1$:

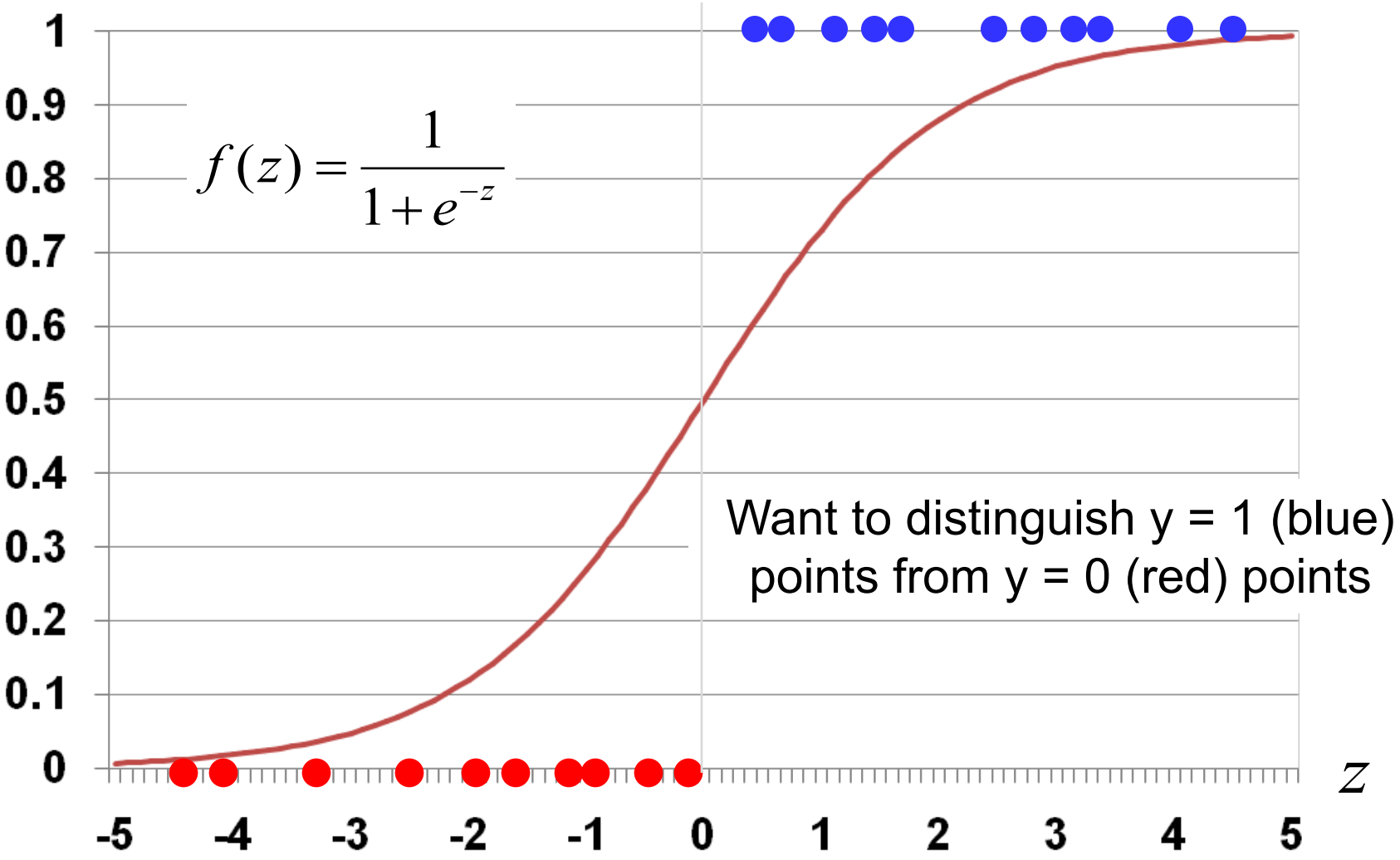
$$P(Y = 1|X = \mathbf{x}) = \sigma(\theta^T \mathbf{x})$$

$$P(Y = 0|X = \mathbf{x}) = 1 - \sigma(\theta^T \mathbf{x})$$

Recall:
Sigmoid function

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

The Sigmoid Function



Note: inflection point at z = 0. $f(0) = 0.5$

What is in a Name

Regression Algorithms

Linear Regression 

Classification Algorithms

Naïve Bayes 

Logistic Regression 

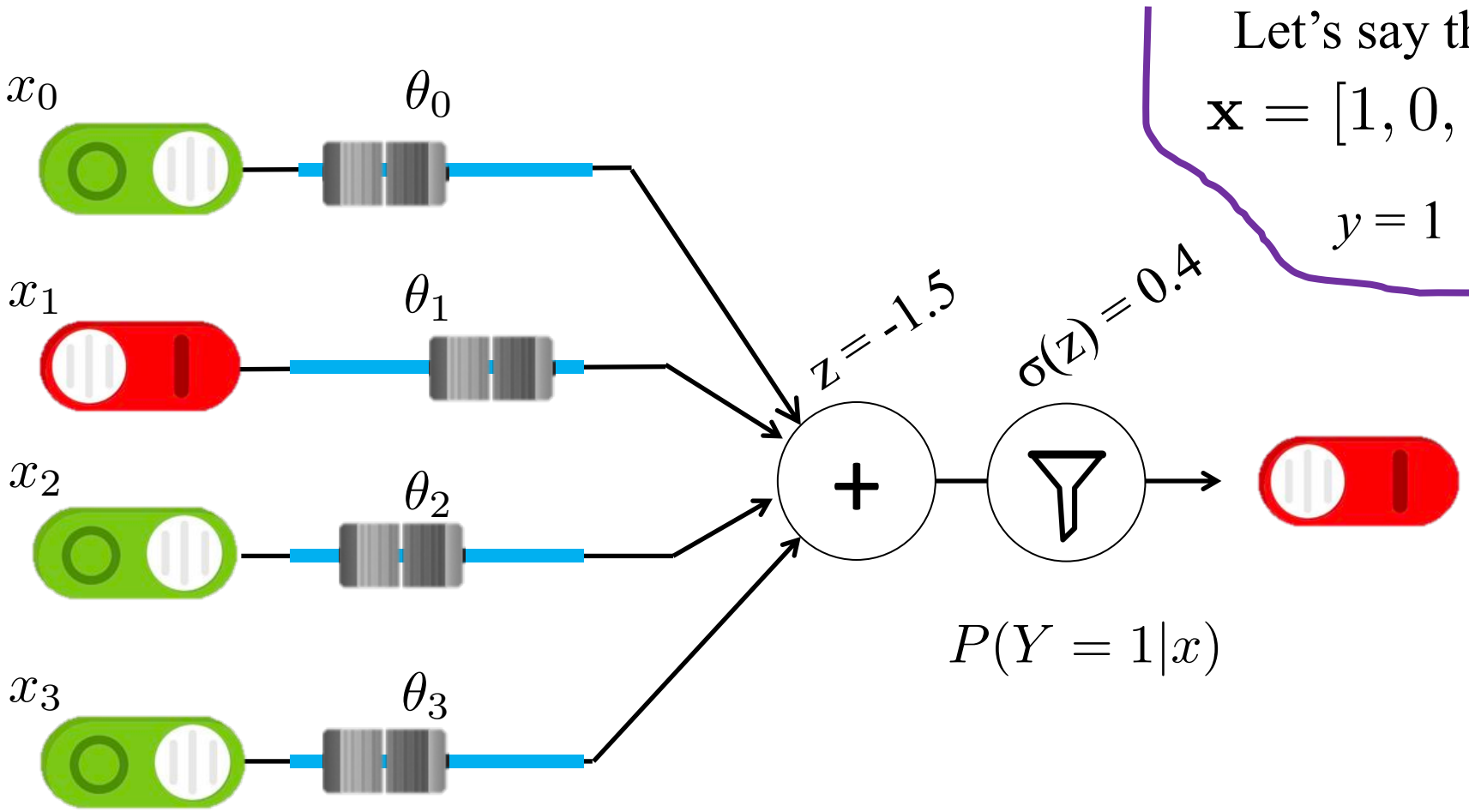
Awesome classifier, terrible name

If Chris could rename it he would call it: Sigmoidal Classification

What makes for a “smart” logistic regression algorithm?

Logistic regression gets its ***intelligence*** from its thetas (aka its parameters)

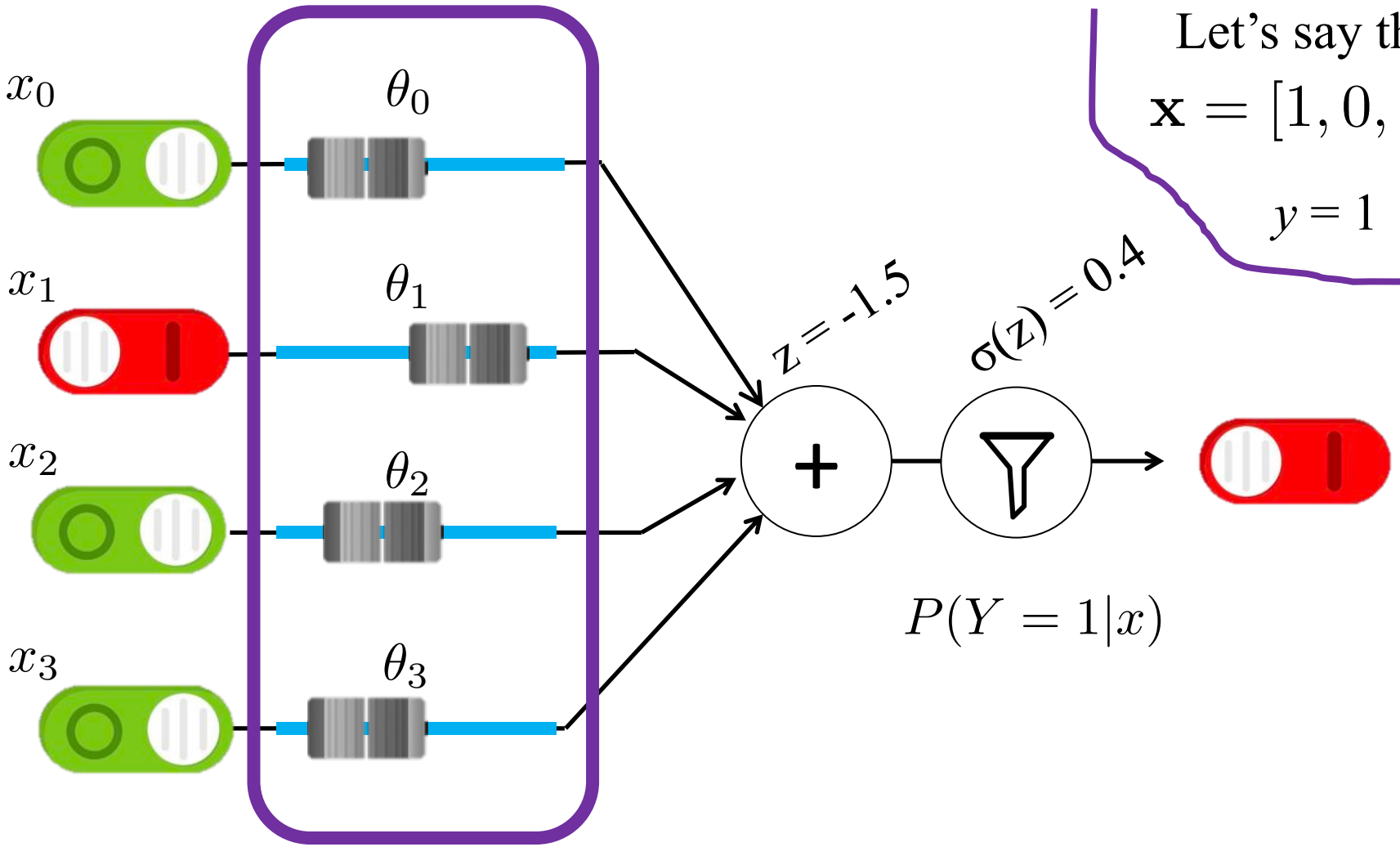
How Do We Learn Parameters?



$$P(Y = 1|\mathbf{X} = \mathbf{x}) = \sigma\left(\sum_i \theta_i x_i\right) = 0.4$$

Data looks unlikely

How Do We Learn Parameters?



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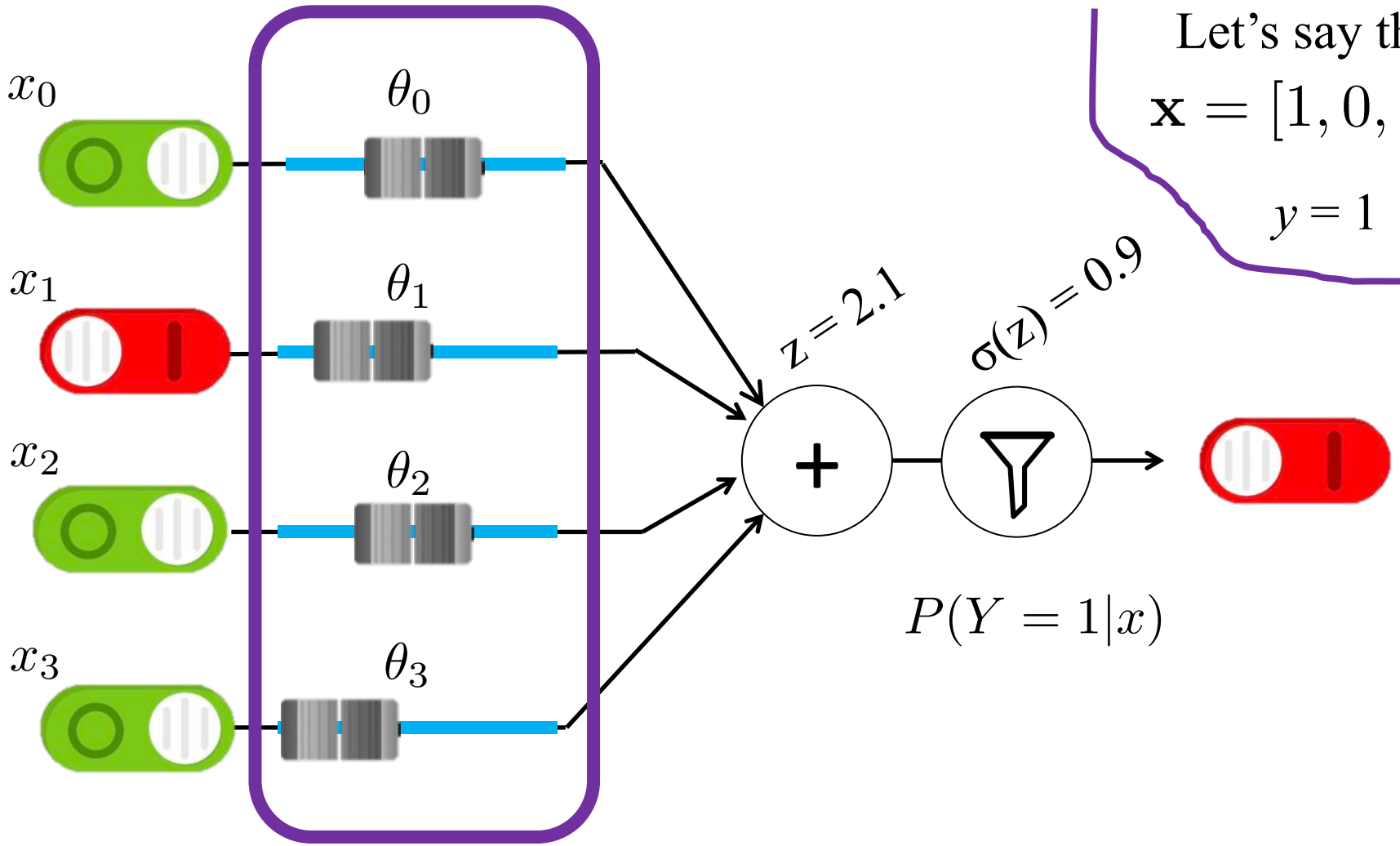
Data looks unlikely

How Do We Learn Parameters?

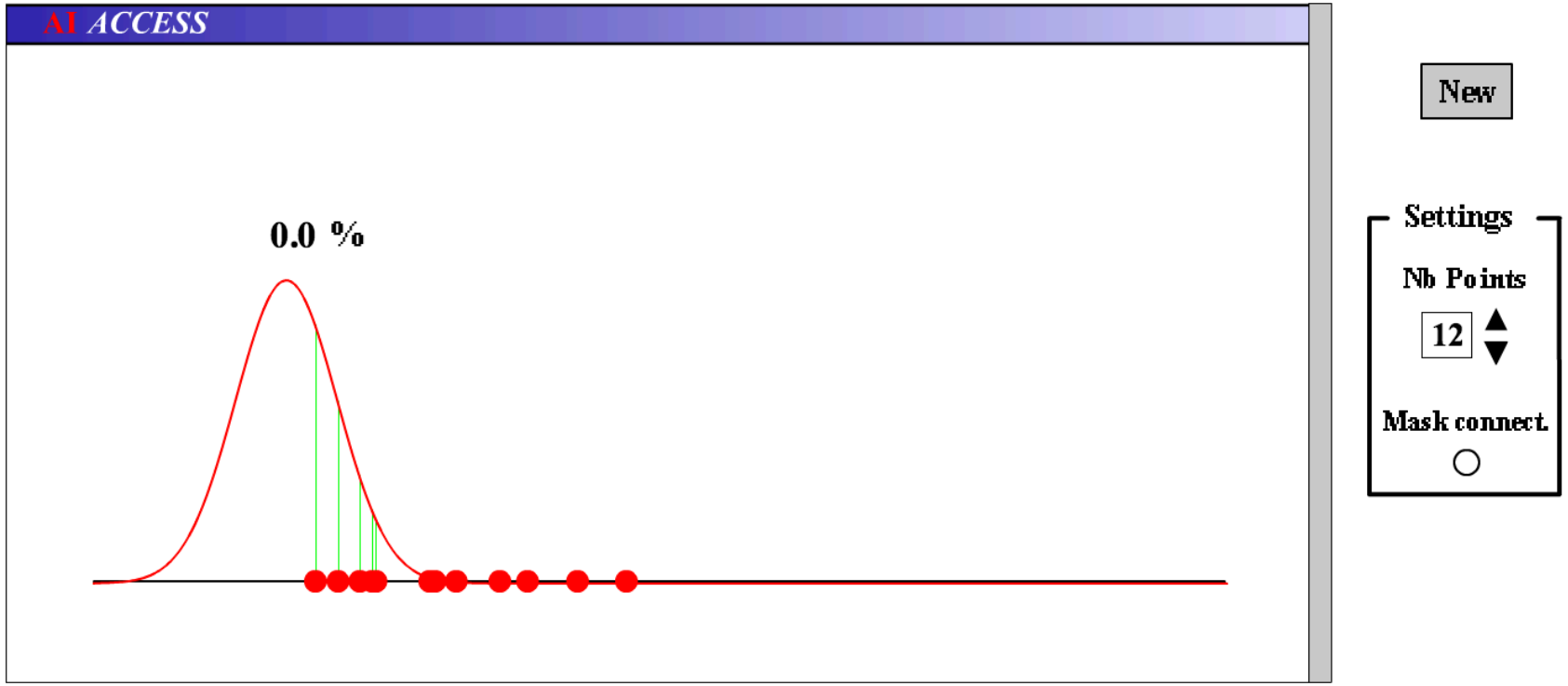


$$P(Y = 1|\mathbf{X} = \mathbf{x}) = \sigma\left(\sum_i \theta_i x_i\right) = 0.9$$

Data is much more likely!

Maximum Likelihood Estimation

Likelihood of Data from a Normal



Remember this?

Math for Logistic Regression

1 Make logistic regression assumption

$$P(Y = 1|X = \mathbf{x}) = \sigma(\theta^T \mathbf{x})$$
$$P(Y = 0|X = \mathbf{x}) = 1 - \sigma(\theta^T \mathbf{x})$$

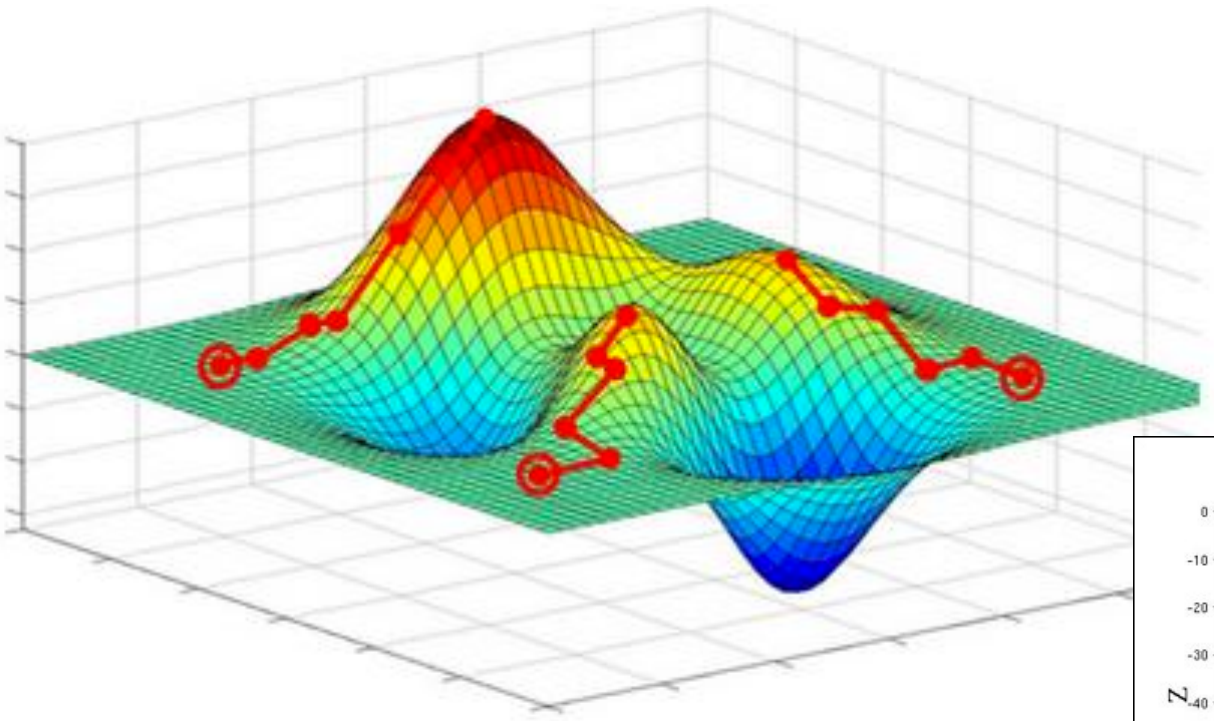
2 Calculate the log likelihood for all data

$$LL(\theta) = \sum_{i=0}^{n} y^{(i)} \log \sigma(\theta^T \mathbf{x}^{(i)}) + (1 - y^{(i)}) \log[1 - \sigma(\theta^T \mathbf{x}^{(i)})]$$

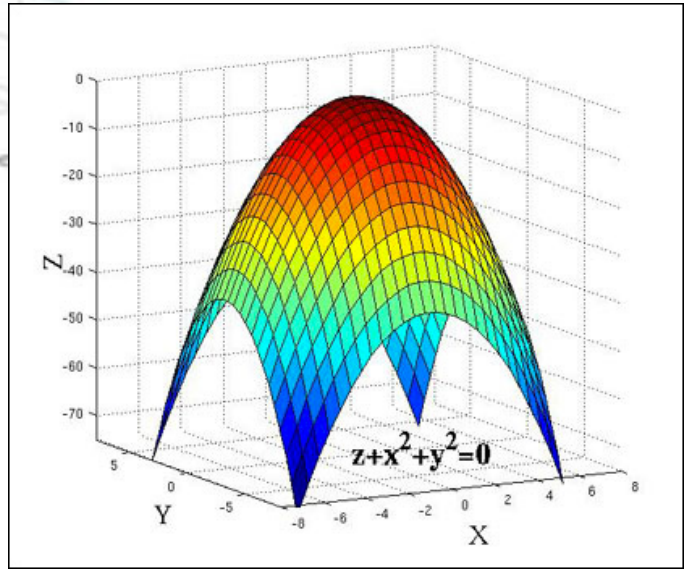
3 Get derivative of log likelihood with respect to thetas

$$\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=0}^{n} \left[y^{(i)} - \sigma(\theta^T \mathbf{x}^{(i)}) \right] x_j^{(i)}$$

Gradient Ascent



Logistic regression
LL function is
convex



Walk uphill and you will find a local maxima
(if your step size is small enough)

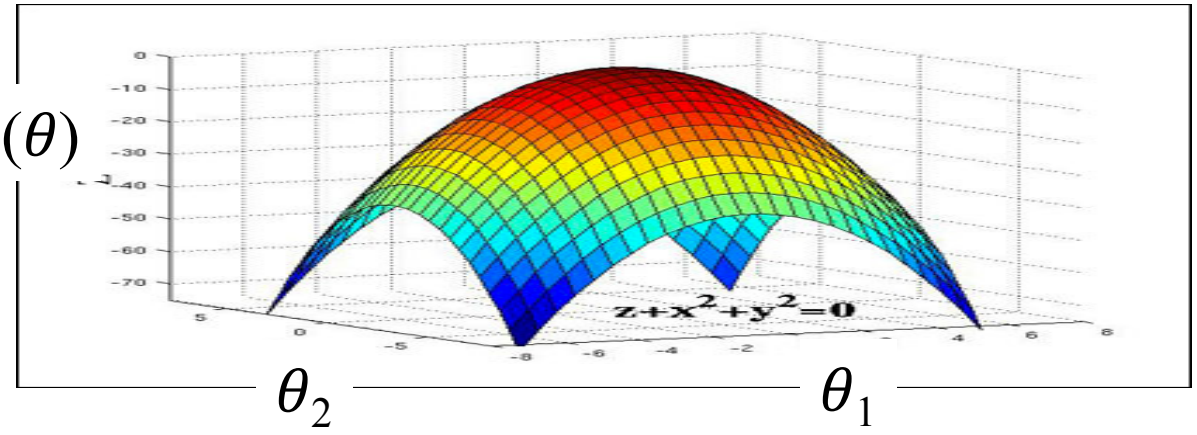
Gradient Ascent Step

$$\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=0}^{n} \left[y^{(i)} - \sigma(\theta^T \mathbf{x}^{(i)}) \right] x_j^{(i)}$$

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

$$= \theta_j^{\text{old}} + \eta \cdot \sum_{i=0}^{n} \left[y^{(i)} - \sigma(\theta^T \mathbf{x}^{(i)}) \right] x_j^{(i)}$$

Do this for all thetas!



Gradient ascent is your bread and butter algorithm for optimization (eg argmax)

Logistic Regression Training

Initialize: $\theta_j = 0$ **for all** $0 \leq j \leq m$

Calculate all θ_j

Logistic Regression Training

Initialize: $\theta_j = 0$ for all $0 \leq j \leq m$

Repeat many times:

gradient[j] = 0 for all $0 \leq j \leq m$

Calculate all gradient[j]*'s based on data*

θ_j += η * gradient[j] for all $0 \leq j \leq m$

Logistic Regression Training

Initialize: $\theta_j = 0$ for all $0 \le j \le m$

Repeat many times:

gradient[j] = 0 for all $0 \le j \le m$

For each training example (x, y):

For each parameter j:

Update gradient[j] *for current training example*

θ_j += η * gradient[j] for all $0 \le j \le m$

Logistic Regression Training

Initialize: $\theta_j = 0$ for all $0 \le j \le m$

Repeat many times:

gradient[j] = 0 for all $0 \le j \le m$

For each training example (x, y):

For each parameter j:

gradient[j] $+= x_j \left(y - \frac{1}{1 + e^{-\theta^{\mathrm{T}} \mathbf{x}}} \right)$

θ_j += η * gradient[j] for all $0 \le j \le m$

Don’t forget:

x_j is j-th input variable and $x_0 = 1$.

Allows for θ_0 to be an intercept.

Classification with Logistic Regression

- Training: determine parameters θ_j (for all $0 \leq j \leq m$)
  - After parameters θ_j have been learned, test classifier
- To test classifier, for each new (test) instance ***X***:
  - Compute: $p = P(Y = 1 \mid \boldsymbol{X}) = \dfrac{1}{1 + e^{-z}}$, where $z = \theta^T \mathbf{x}$
  - Classify instance as: $\hat{y} = \begin{cases} 1 & p > 0.5 \\ 0 & \text{otherwise} \end{cases}$
  - Note about evaluation set-up: parameters θ_j are **not** updated during "testing" phase

Chapter 2: How Come?

Logistic Regression

1 Make logistic regression assumption

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

$$P(Y = 0|X = \mathbf{x}) = 1 - \sigma(\theta^T \mathbf{x})$$

2 Calculate the log probability for all data

$$LL(\theta) = \sum_{i=0}^{n} y^{(i)} \log \sigma(\theta^T \mathbf{x}^{(i)}) + (1 - y^{(i)}) \log[1 - \sigma(\theta^T \mathbf{x}^{(i)})]$$

3 Get derivative of log probability with respect to thetas

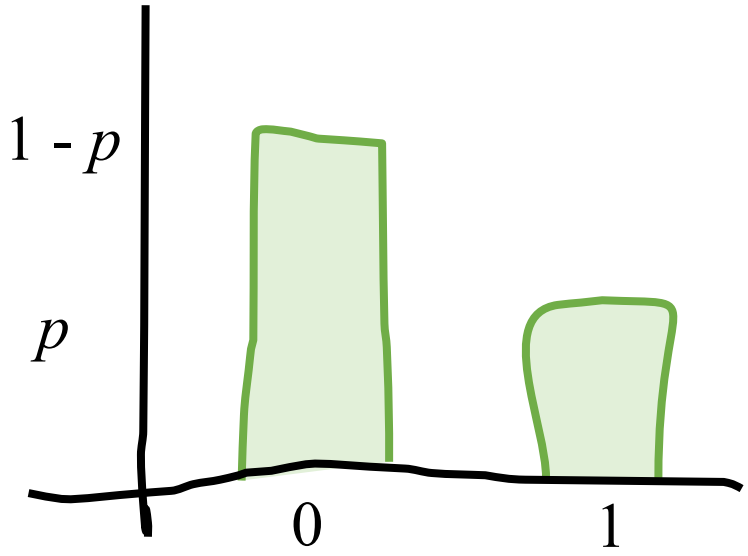
$$\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=0}^{n} \left[y^{(i)} - \sigma(\theta^T \mathbf{x}^{(i)}) \right] x_j^{(i)}$$

How did we get that LL function?

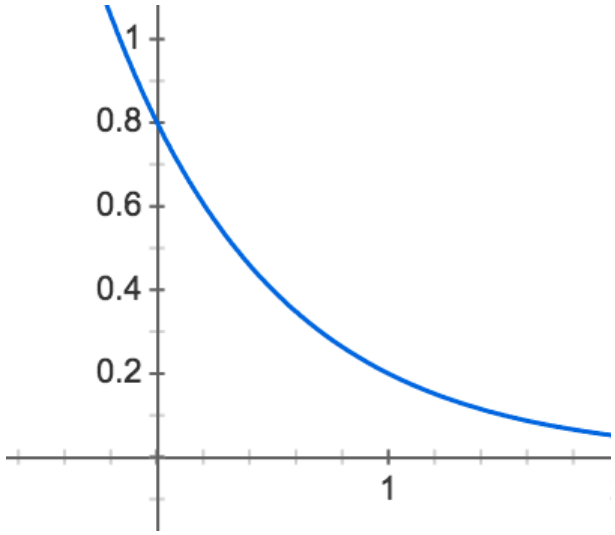
Recall: PMF of Bernoulli

- Y ~ Ber(*p*)
- Probability mass function: $P(Y = y)$

PMF of Bernoulli



PMF of Bernoulli (*p* = 0.2)



$$P(Y = y) = p^y(1-p)^{1-y}$$

$$P(Y = y) = 0.2^y(0.8)^{1-y}$$

Log Probability of Data

$$P(Y = 1|X = \mathbf{x}) = \sigma(\theta^T \mathbf{x})$$
$$P(Y = 0|X = \mathbf{x}) = 1 - \sigma(\theta^T \mathbf{x})$$

Implies

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

For IID data

$$L(\theta) = \prod_{i=1}^{n} P(Y = y^{(i)}|X = \mathbf{x}^{(i)})$$
$$= \prod_{i=1}^{n} \sigma(\theta^T \mathbf{x}^{(i)})^{y^{(i)}} \cdot \left[1 - \sigma(\theta^T \mathbf{x}^{(i)})\right]^{(1-y^{(i)})}$$

Take the log

$$LL(\theta) = \sum_{i=0}^{n} y^{(i)} \log \sigma(\theta^T \mathbf{x}^{(i)}) + (1 - y^{(i)}) \log[1 - \sigma(\theta^T \mathbf{x}^{(i)})]$$

How did we get that gradient?

Sigmoid has a Beautiful Slope

True fact about
sigmoid functions

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

Sigmoid has a Beautiful Slope

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

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

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

Chain rule!

where $z = \theta^T x$

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

Plug and chug

Sigmoid, you should be a ski hill

Gradient Update One Train Example

$$LL(\theta) = y \log \sigma(\theta^T \mathbf{x}) + (1-y) \log[1 - \sigma(\theta^T \mathbf{x})]$$

$$\begin{aligned}
\frac{\partial LL(\theta)}{\partial \theta_j} &= \frac{\partial}{\partial \theta_j} y \log \sigma(\theta^T \mathbf{x}) + \frac{\partial}{\partial \theta_j} (1-y) \log[1 - \sigma(\theta^T \mathbf{x}] \\
&= \left[\frac{y}{\sigma(\theta^T x)} - \frac{1-y}{1-\sigma(\theta^T x)} \right] \frac{\partial}{\partial \theta_j} \sigma(\theta^T x) \\
&= \left[\frac{y}{\sigma(\theta^T x)} - \frac{1-y}{1-\sigma(\theta^T x)} \right] \frac{\partial}{\partial \theta_j} \sigma(\theta^T x) \\
&= \left[\frac{y - \sigma(\theta^T x)}{\sigma(\theta^T x)[1-\sigma(\theta^T x)]} \right] \sigma(\theta^T x)[1-\sigma(\theta^T x)] x_j \\
&= \left[y - \sigma(\theta^T x) \right] x_j
\end{aligned}$$

Gradient Update Many Train Examples

$$LL(\theta) = \sum_{i=0}^{n} y^{(i)} \log \sigma(\theta^T \mathbf{x}^{(i)}) + (1 - y^{(i)}) \log[1 - \sigma(\theta^T \mathbf{x}^{(i)})]$$

$$\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=0}^{n} \frac{\partial}{\partial \theta_j} \left[y^{(i)} \log \sigma(\theta^T \mathbf{x}^{(i)}) + (1 - y^{(i)}) \log[1 - \sigma(\theta^T \mathbf{x}^{(i)}) \right]$$

$$\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=0}^{n} \left[y^{(i)} - \sigma(\theta^T \mathbf{x}^{(i)}) \right] x_j^{(i)}$$

final answer

Phew!

The Hard Way

$$LL(\theta) = y \log \sigma(\theta^T \mathbf{x}) + (1 - y) \log[1 - \sigma(\theta^T \mathbf{x})]$$

The Simple Way!

$$LL(\theta) = y \log \hat{y} + (1 - y) \log[1 - \hat{y}]$$

$$\text{Where} \quad \hat{y} = \sigma(\theta^T \mathbf{x})$$

$$\frac{\partial LL(\theta)}{\partial \theta_j} = \frac{\partial LL(\theta)}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial \theta_j}$$

$$= \frac{\partial LL(\theta)}{\partial \hat{y}} \hat{y}(1 - \hat{y}) x_j$$

$$= \left[\frac{y}{\hat{y}} + \frac{1 - y}{1 - \hat{y}}\right] \hat{y}(1 - \hat{y}) x_j$$

$$= (y - \hat{y}) x_j \quad = [y - \sigma(\theta^T \mathbf{x})] x_j$$

Boom!

Logistic Regression

1 Make logistic regression assumption

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

$$P(Y = 0|X = \mathbf{x}) = 1 - \sigma(\theta^T \mathbf{x})$$

2 Calculate the log probability for all data

$$LL(\theta) = \sum_{i=0}^{n} y^{(i)} \log \sigma(\theta^T \mathbf{x}^{(i)}) + (1 - y^{(i)}) \log[1 - \sigma(\theta^T \mathbf{x}^{(i)})]$$

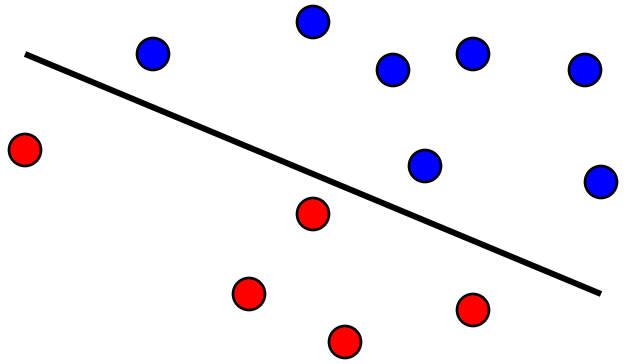
3 Get derivative of log probability with respect to thetas

$$\frac{\partial LL(\theta)}{\partial \theta_j} = \sum_{i=0}^{n} \left[y^{(i)} - \sigma(\theta^T \mathbf{x}^{(i)}) \right] x_j^{(i)}$$

Chapter 3: Philosophy

Discrimination Intuition

- Logistic regression is trying to fit a **line** that separates data instances where *y* = 1 from those where *y* = 0



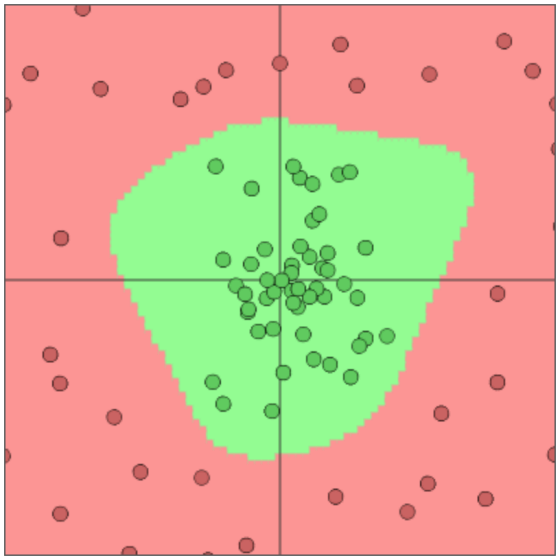
$$\theta^T \mathbf{x} = 0$$

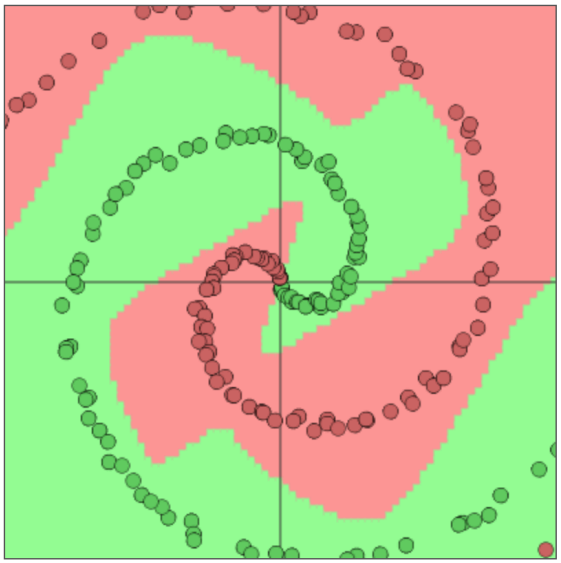
$$\theta_0 x_0 + \theta_1 x_1 + \cdots + \theta_m x_m = 0$$

- We call such data (or the functions generating the data) "**linearly separable**"
- Naïve bayes is linear too as there is no interaction between different features.

Some Data Not Linearly Seperable

- Some data sets/functions are not separable





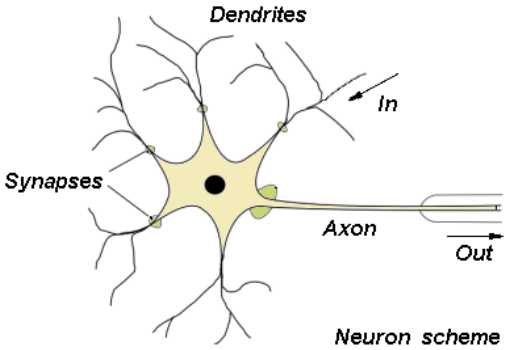
  - Not possible to draw a line that successfully separates all the $y = 1$ points (green) from the $y = 0$ points (red)
  - Despite this fact, logistic regression and Naive Bayes still often work well in practice

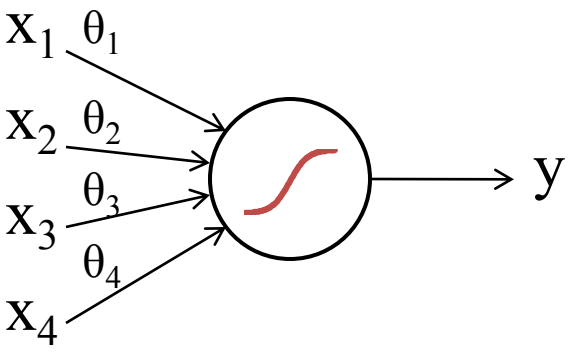
Choosing an Algorithm?

- Many trade-offs in choosing learning algorithm
  - Continuous input variables
    - Logistic Regression easily deals with continuous inputs
    - Naive Bayes needs to use some parametric form for continuous inputs (e.g., Gaussian) or “discretize” continuous values into ranges (e.g., temperature in range: <50, 50-60, 60-70, >70)
  - Discrete input variables
    - Naive Bayes naturally handles multi-valued discrete data by using multinomial distribution for $P(X_i \mid Y)$
    - Logistic Regression requires some sort of representation of multi-valued discrete data (e.g., one hot vector)
    - Say $X_i \in \{A, B, C\}$. Not necessarily a good idea to encode X_i as taking on input values 1, 2, or 3 corresponding to A, B, or C.

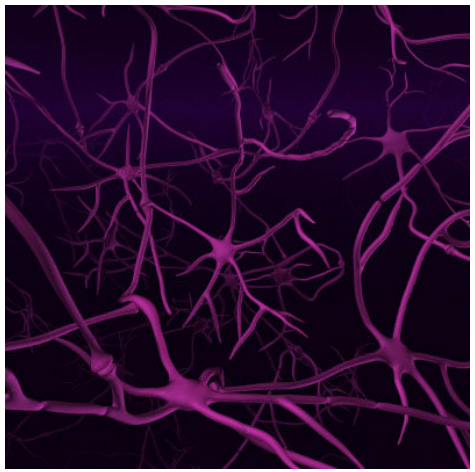
Biological Basis for Neural Networks

- A neuron

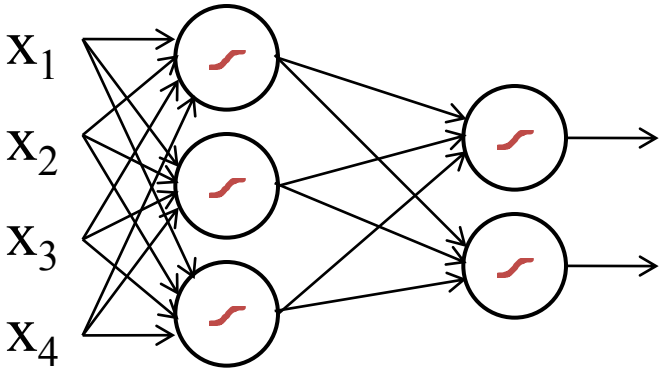




- Your brain



Actually, it's probably someone else's brain



Next up: Deep Learning!