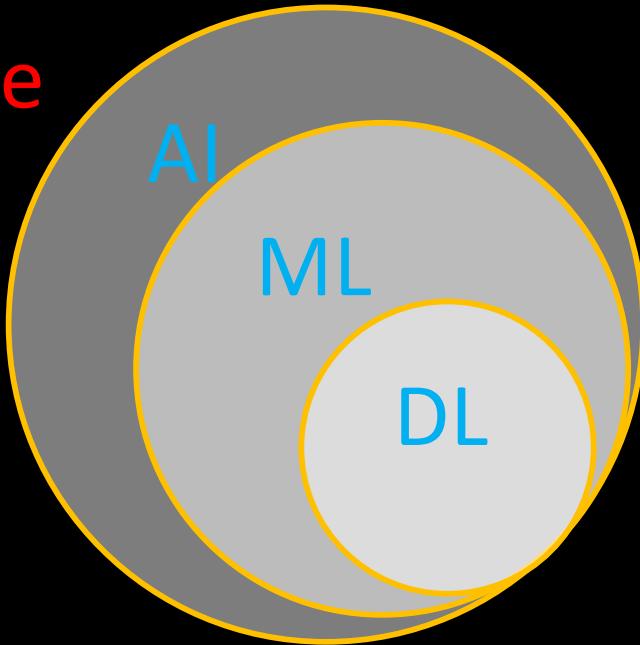


AI (Goal):  
Artificial intelligence

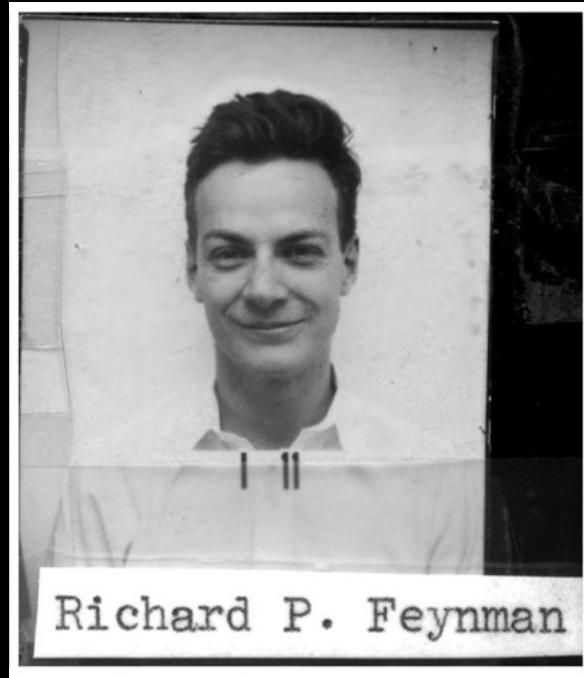


ML:  
machine learning

DL:  
deep learning



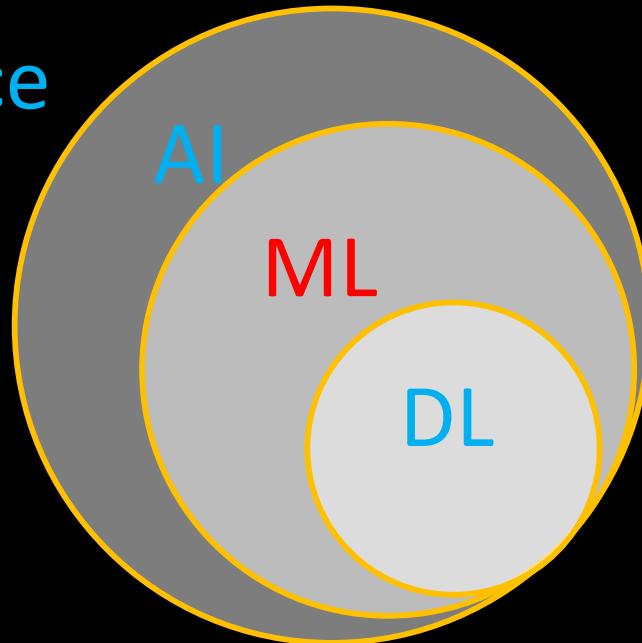
1. “human-level” intelligence has a diverse definition
2. AI may reach human level intelligence, but probably are not doing it in a “humane” way



AI (Goal):  
Artificial intelligence

ML:  
machine learning

DL:  
deep learning



ML: machine learning

(collection of methods) to develop  
algorithms automatically by learning  
from data

## Option 1: Manual-Crafted Rule Based



Truck

Wheels > 4

Truck = (Wheels > 4)  
and / or  
**A Good Rule**  
(Height > 2m)



Truck

Height > 2m

Truck = (Color == red)

**A Bad Rule**



Truck?

Color = red

Hand crafted (explicit rules)



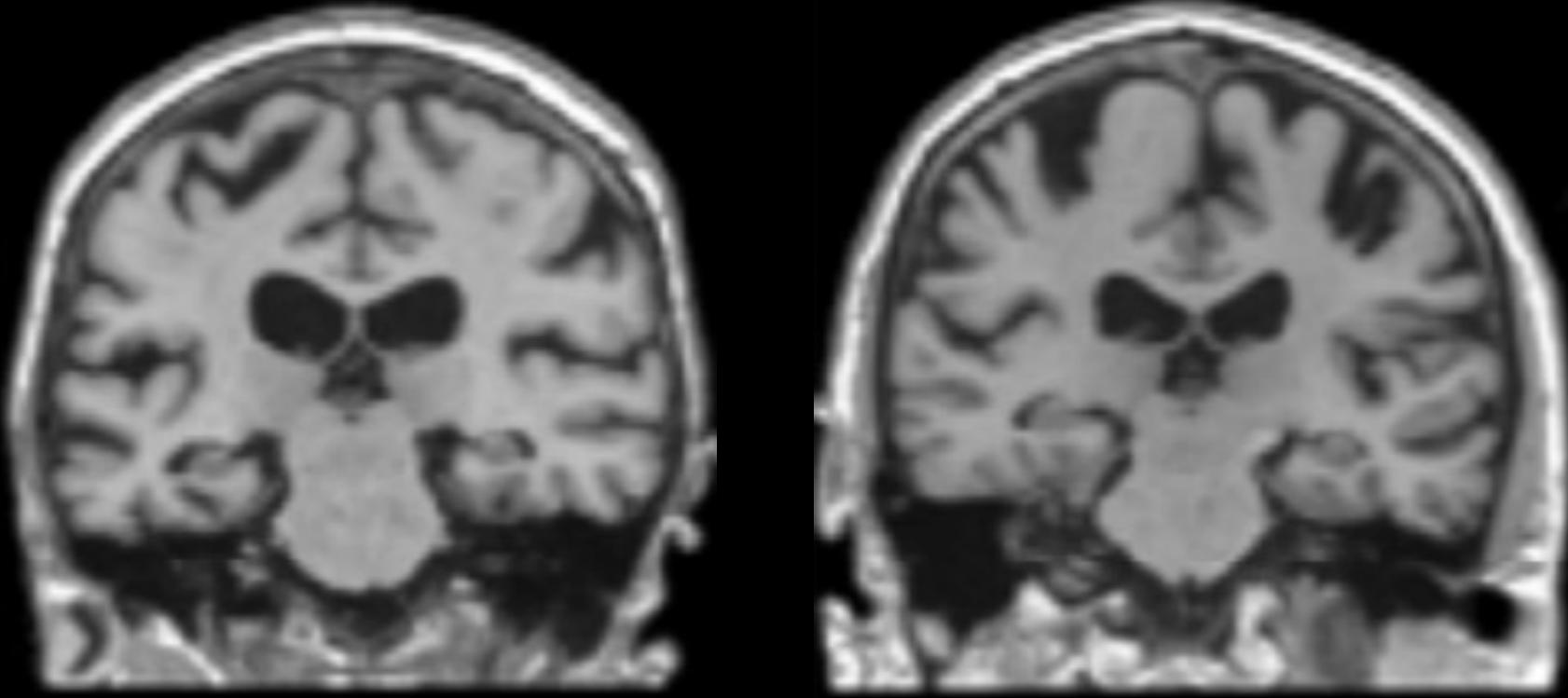
How to do define a function  
to detect tires?

get\_circle

get\_circle + is\_tire  
(black rims larger than....)

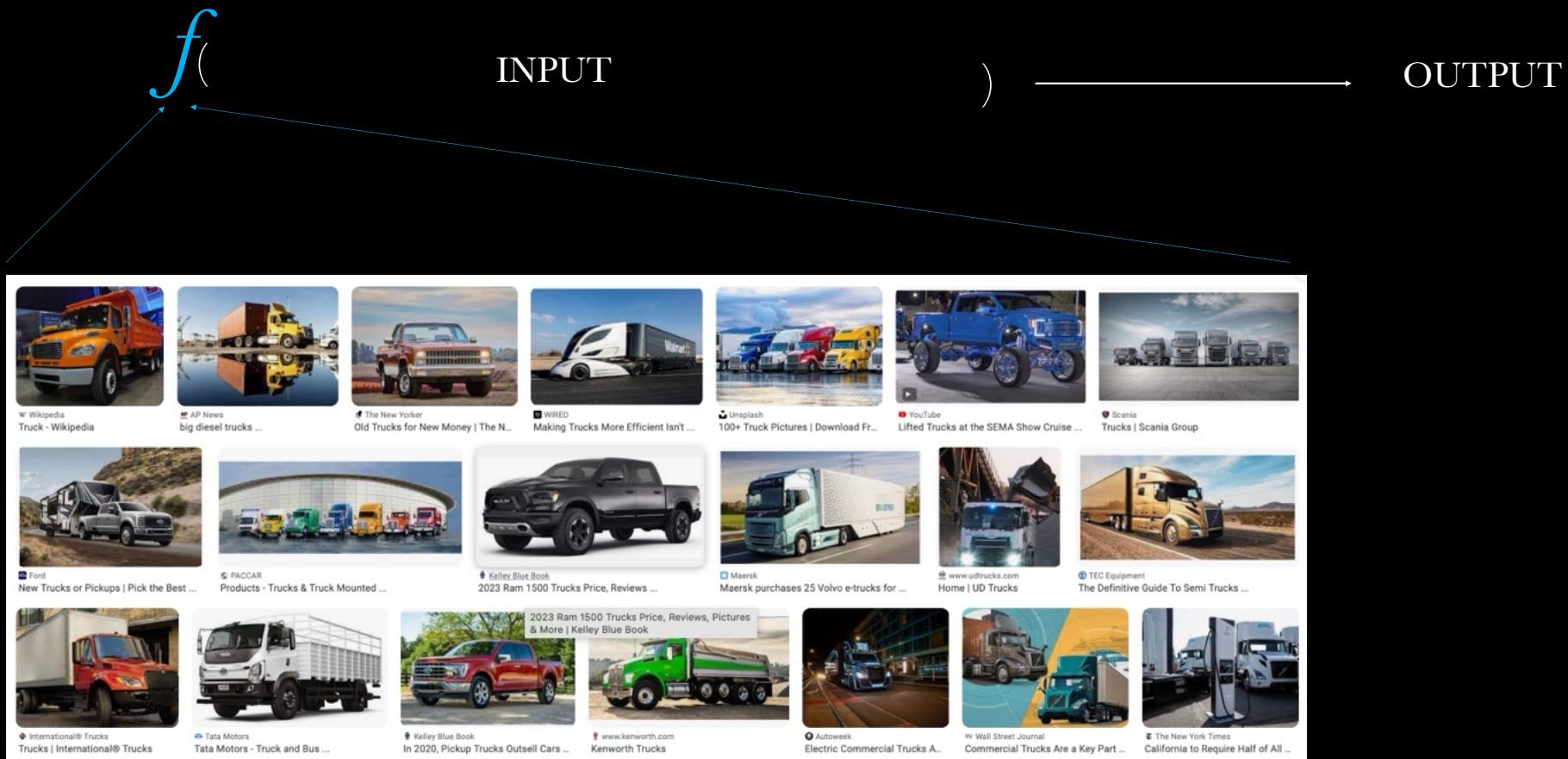


get\_circle + is\_tire +  
tires\_belong\_to\_the\_same\_car....



Complicated, real-life problems can't simply  
be resolved by rules

## Option 2: let the model to learn from data: Machine Learning



Model + Data + ways for the model to improve itself

## Machine learning:

Learning a model that don't have explicit rules,  
instead the model is derived implicitly from  
observations (data)

when,

Rules are hard to be implemented  
&  
We don't know the rules clearly.

## Look for Function(**s**)

$f$  ( INPUT )  $\longrightarrow$  OUTPUT

Visuals, audios, text...

Labels, predictions,  
decisions...

Look for Function(**s**)

$f$  ( INPUT )  $\longrightarrow$  OUTPUT  
“Magic”

(turn out it's neural networks)

# Machine Learning: Look for Function( $\mathbf{s}$ )

Classification



Class  
(what kind of bird)

Detection



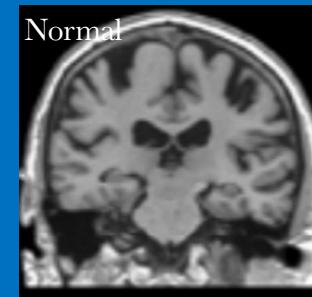
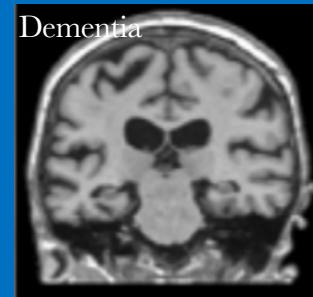
Class (people lamp),  
Box location,  
Box size

Segmentation



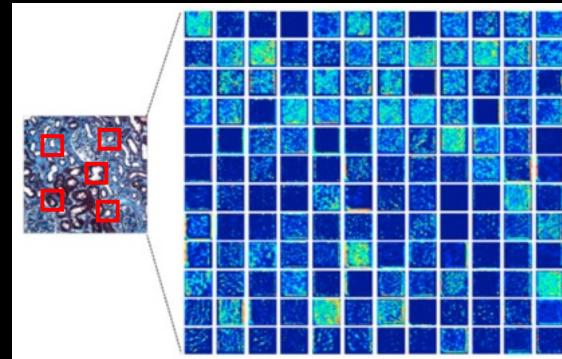
# Deep Learning in Medicine

## Classification



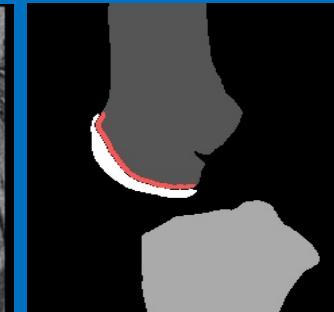
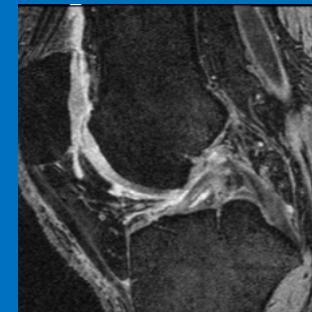
Dementia  
Prediction

## Detection



Hypocellularity  
Detection

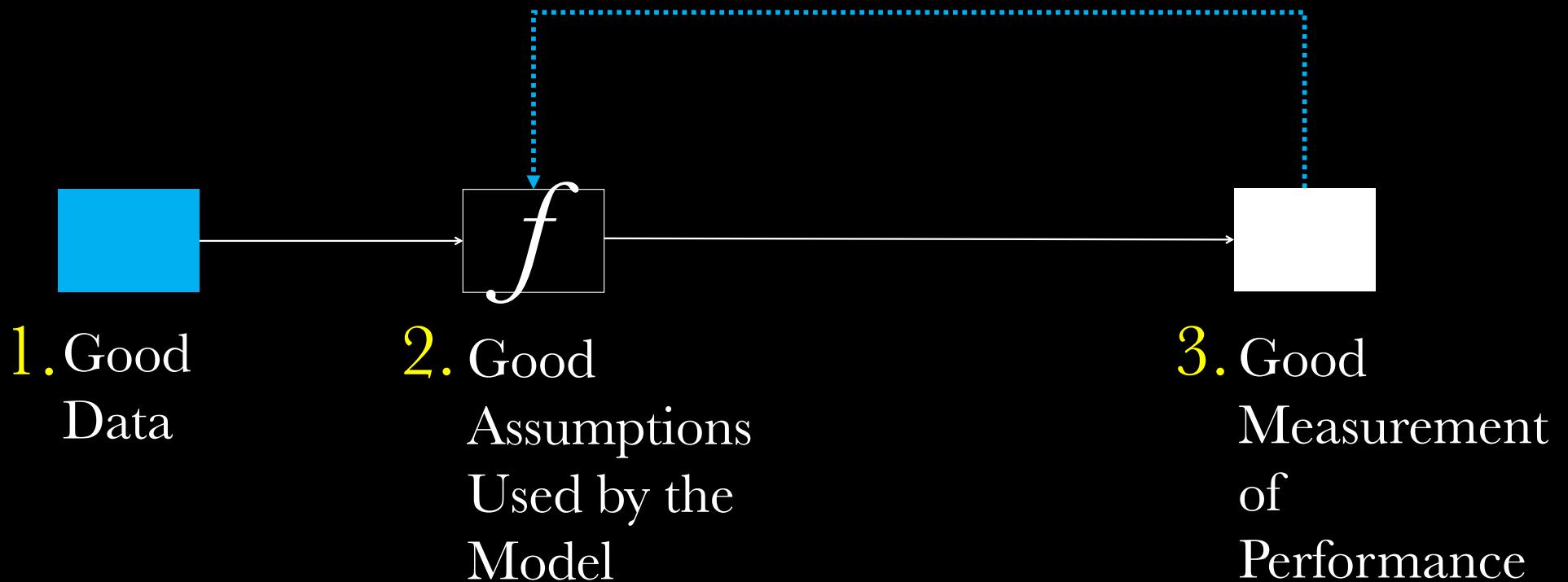
## Segmentation



knee anatomical  
segmentation

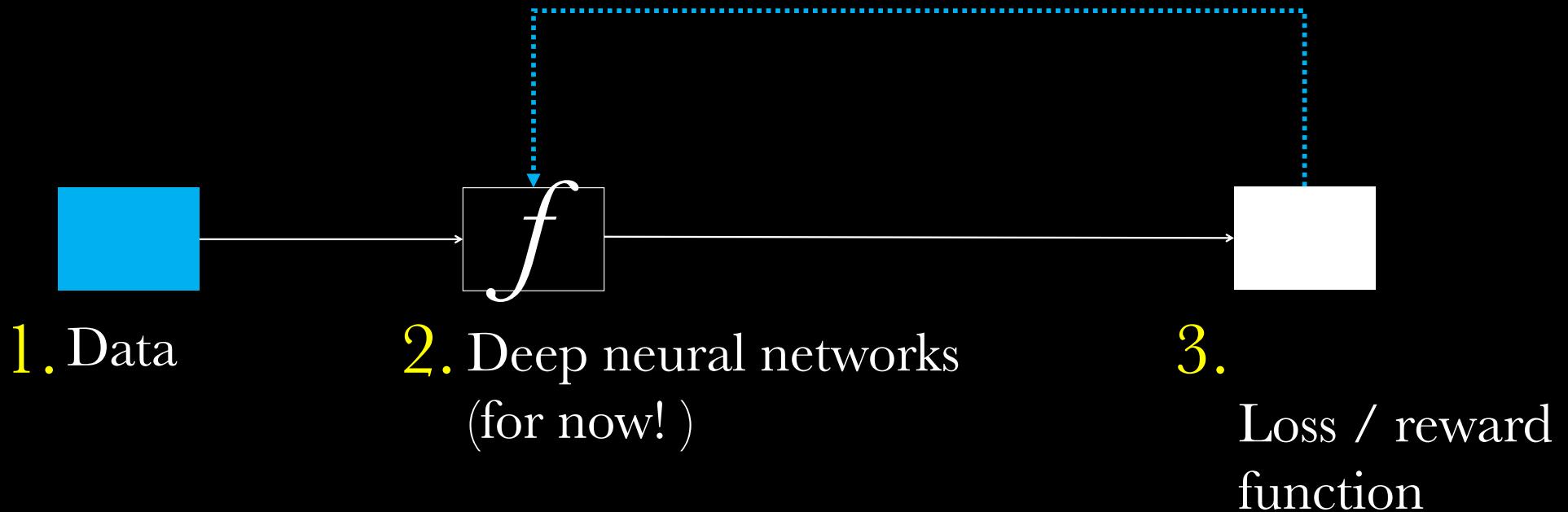
# Four Horseman of ML

4. Ability for the model to improve itself



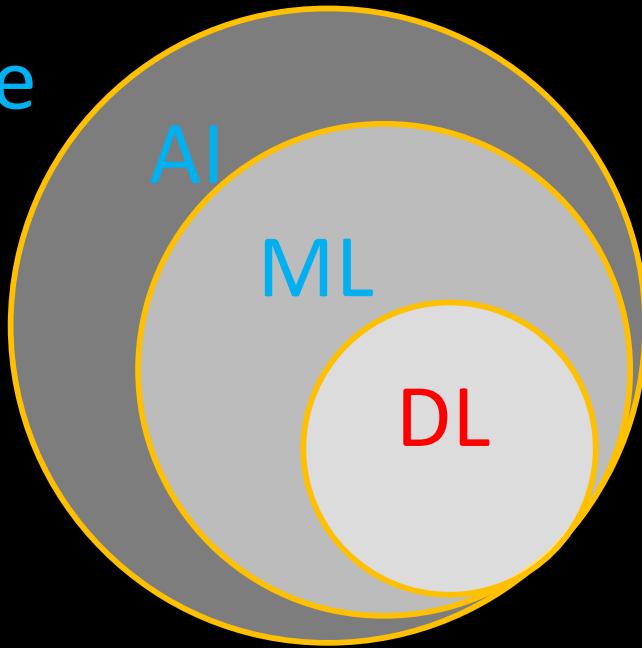
# Four Horseman of ML

## 4. Optimization



AI (Goal):  
artificial intelligence

ML:  
machine learning



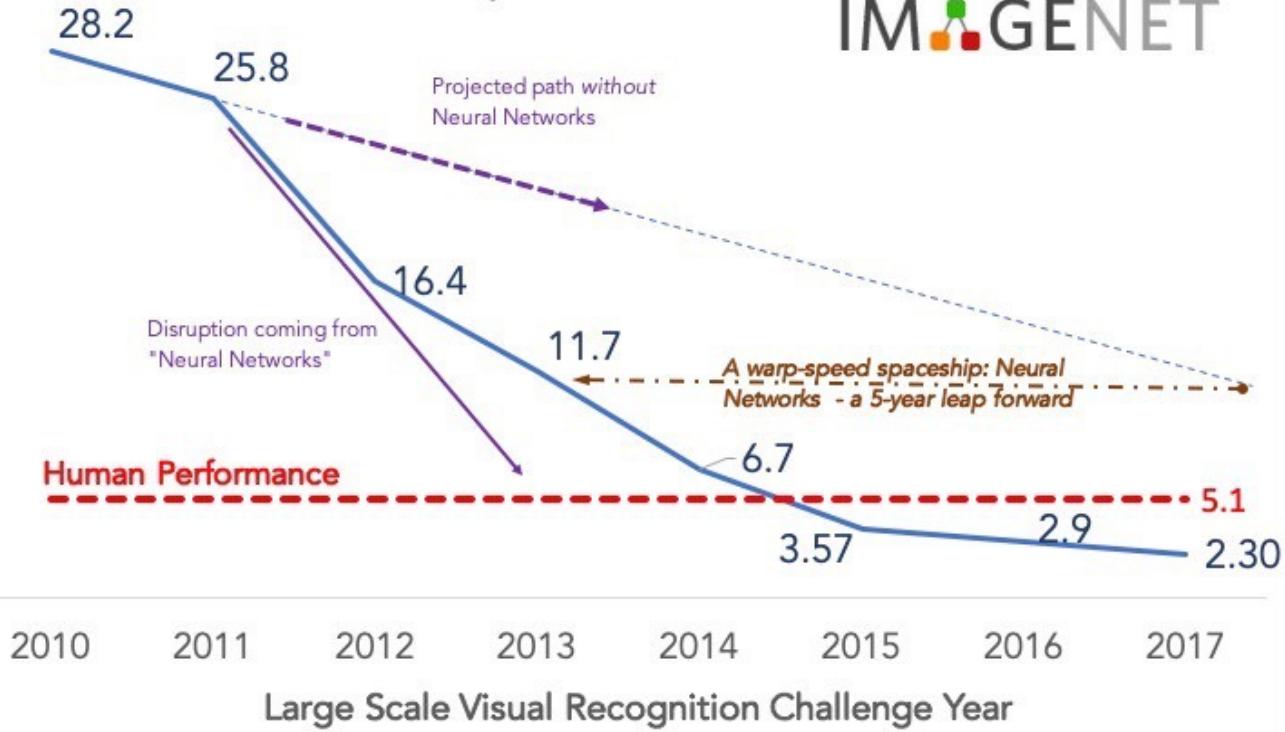
Deep Learning (DL):  
Specifically, the models using deep neural networks

## Accuracy of object detection software against the human eye

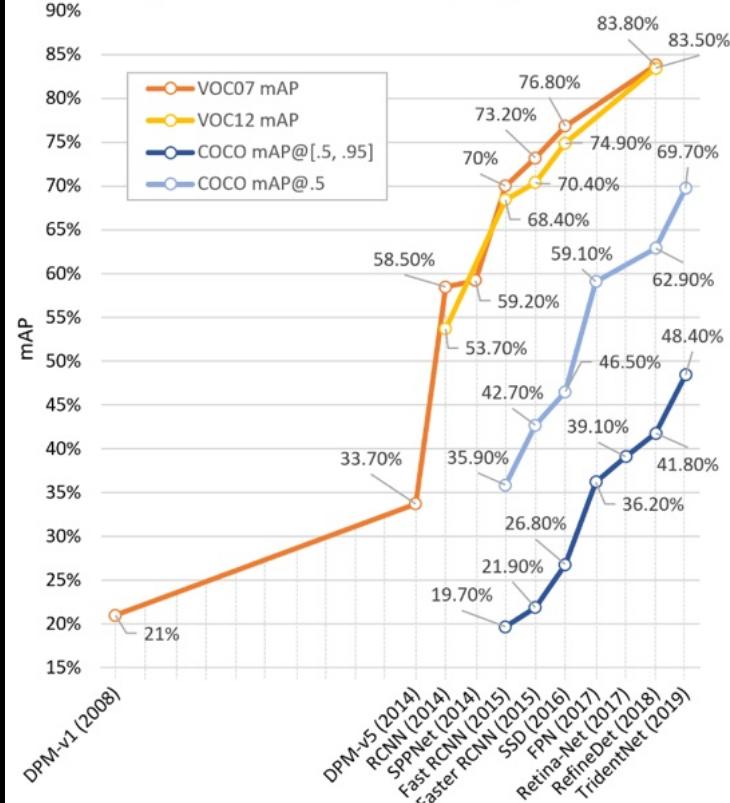
ImageNet (2010-2018)

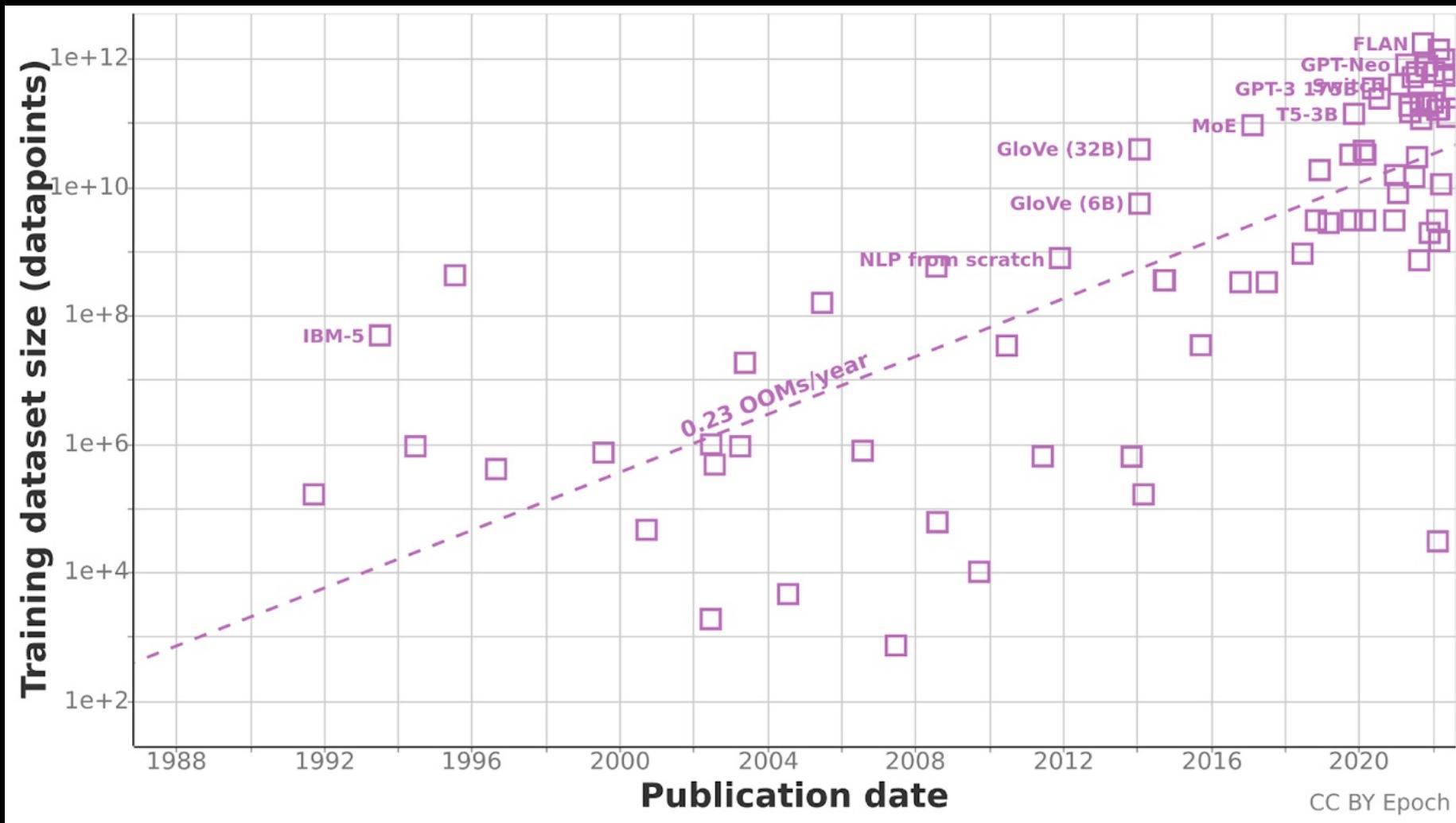


Percentage Error Rate %



## Object detection accuracy improvements





# Three Categories of AI Application in Medicine (or anything!)

Human  
Can't

AI  
Can



Human  
Can but Expensive

AI  
Equal quality but Automatic

Human  
Can but unavailable

AI  
Equal or Less but acceptable

# Most Simple ML:

## Linear & Logistic Regression

# **Regression vs Classification**

## **Regression:**

Predicts continuous outcomes by finding the best-fit line through data points.

## **Classification:**

Predicts the probability of an instance belonging to a particular class.

## **Regression:**

Predicting drug dosage <-> patient weight

Estimating bone density changes <-> X-ray

blood pressure <-> salt intake

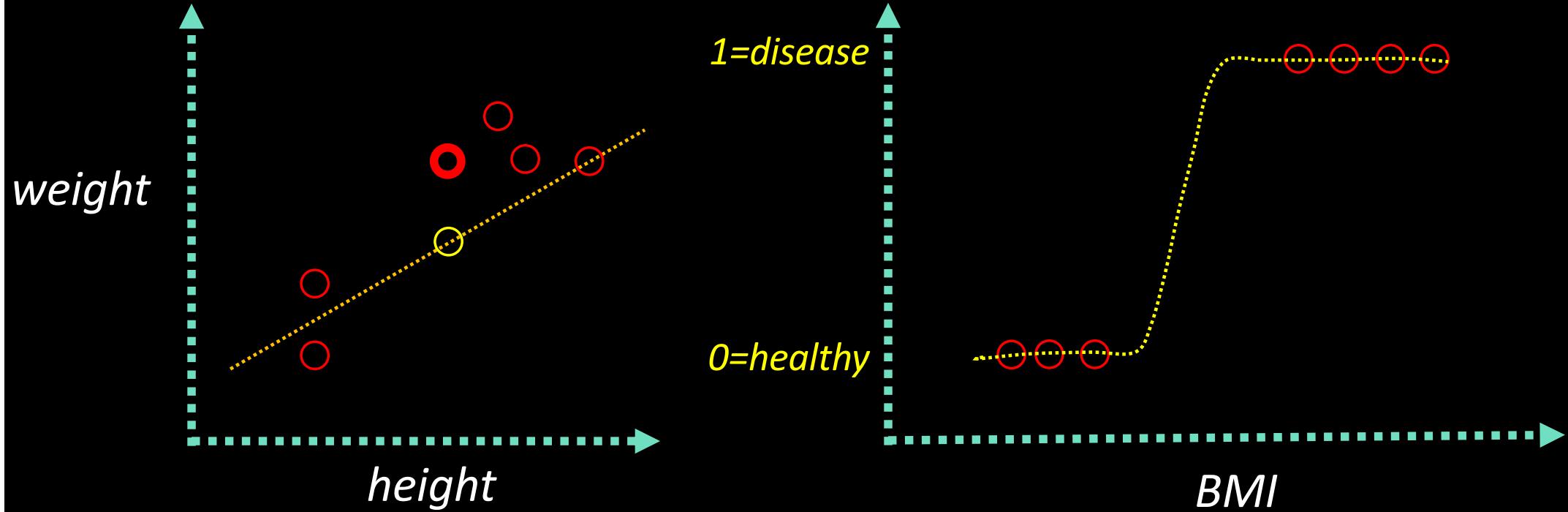
## **Classification:**

likelihood of heart disease <-> cholesterol levels

probability of remission in patients <-> treatment

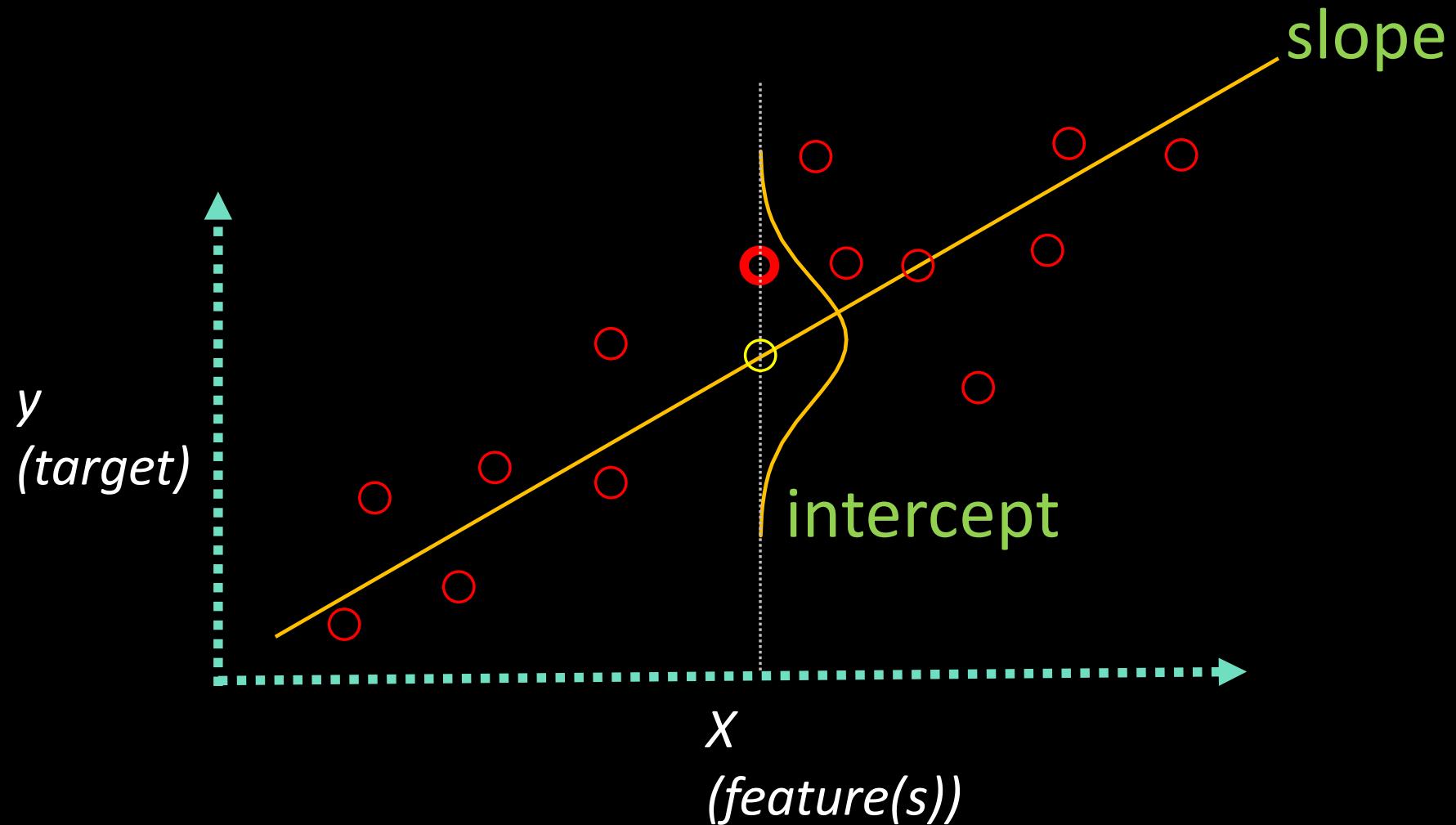
Classifying medical images <-> presence or absence of a tumor

# Regression vs Classification

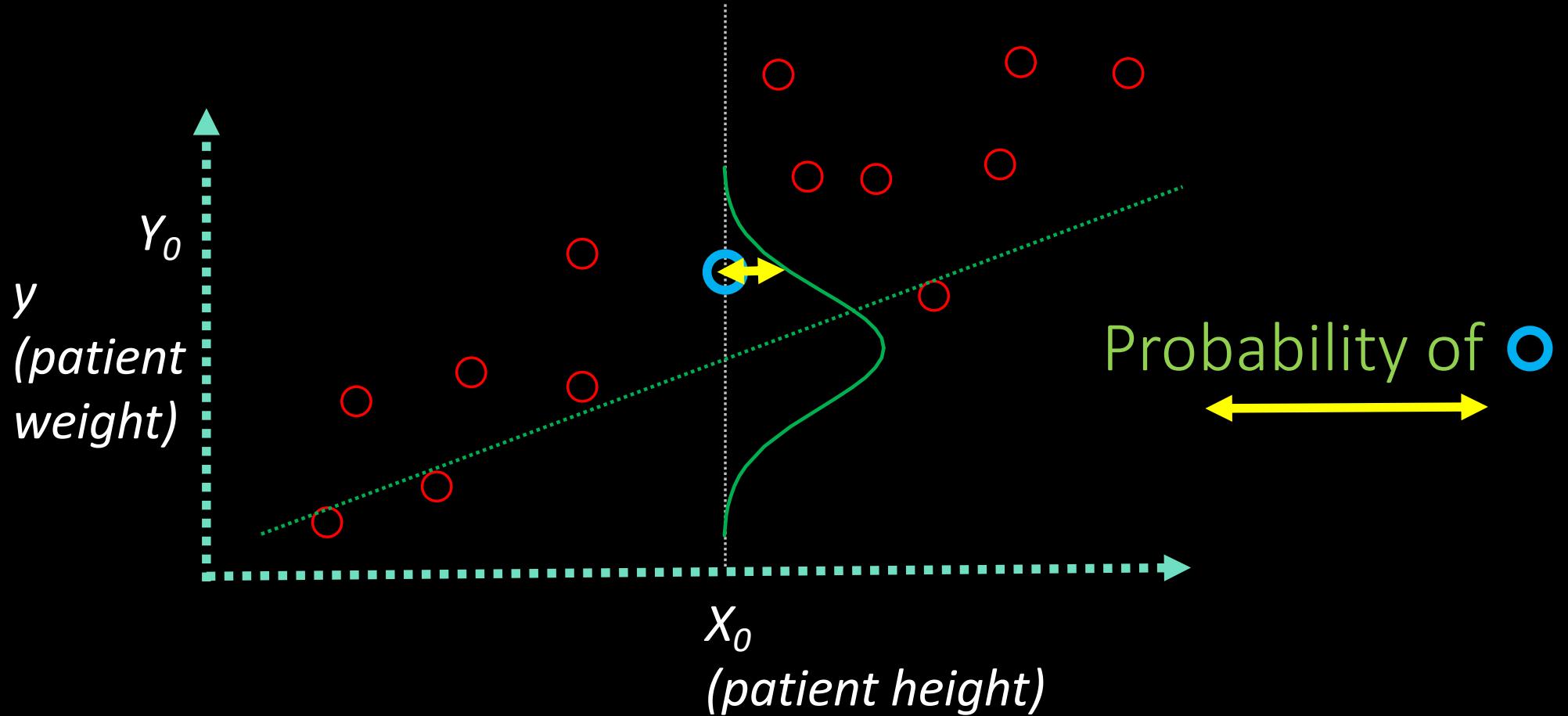


but why?

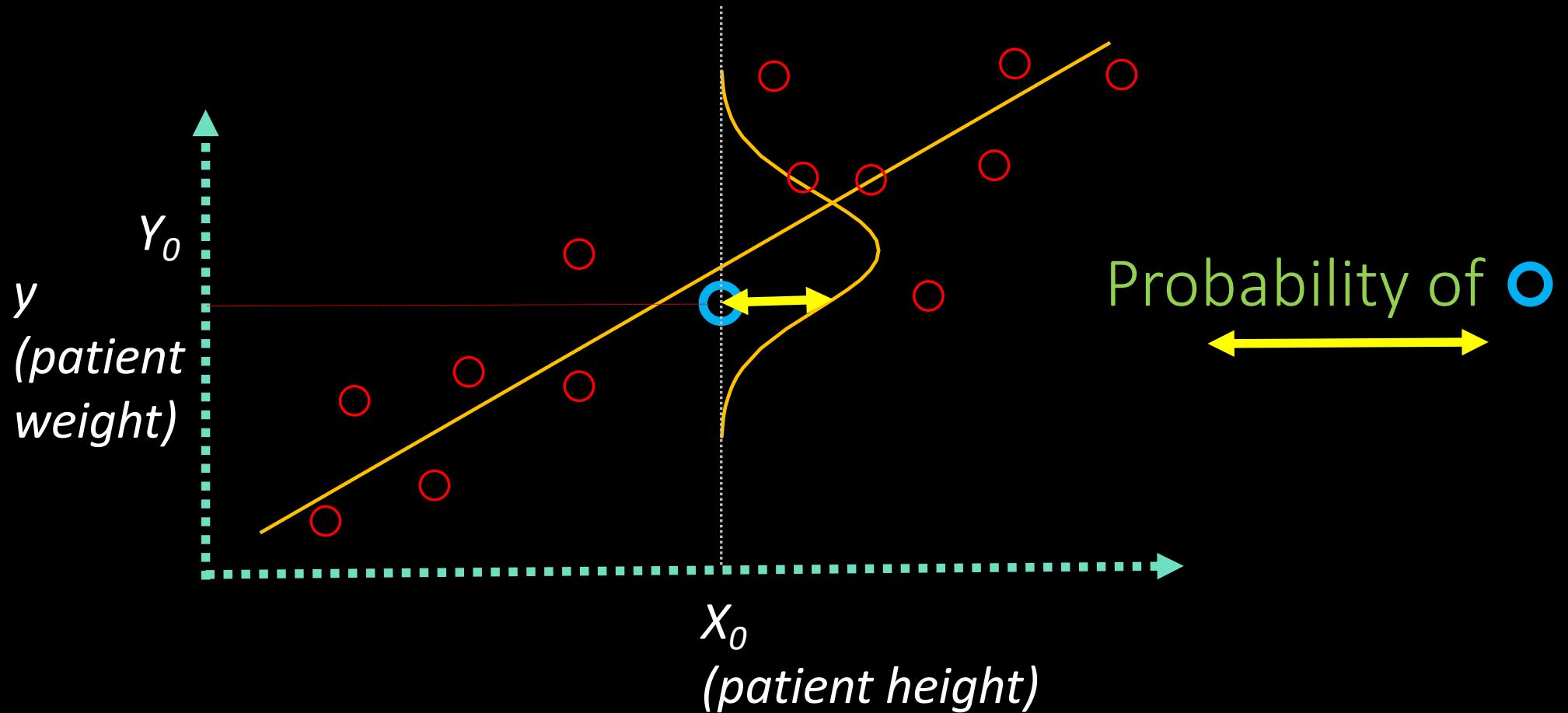
## What are the parameters?



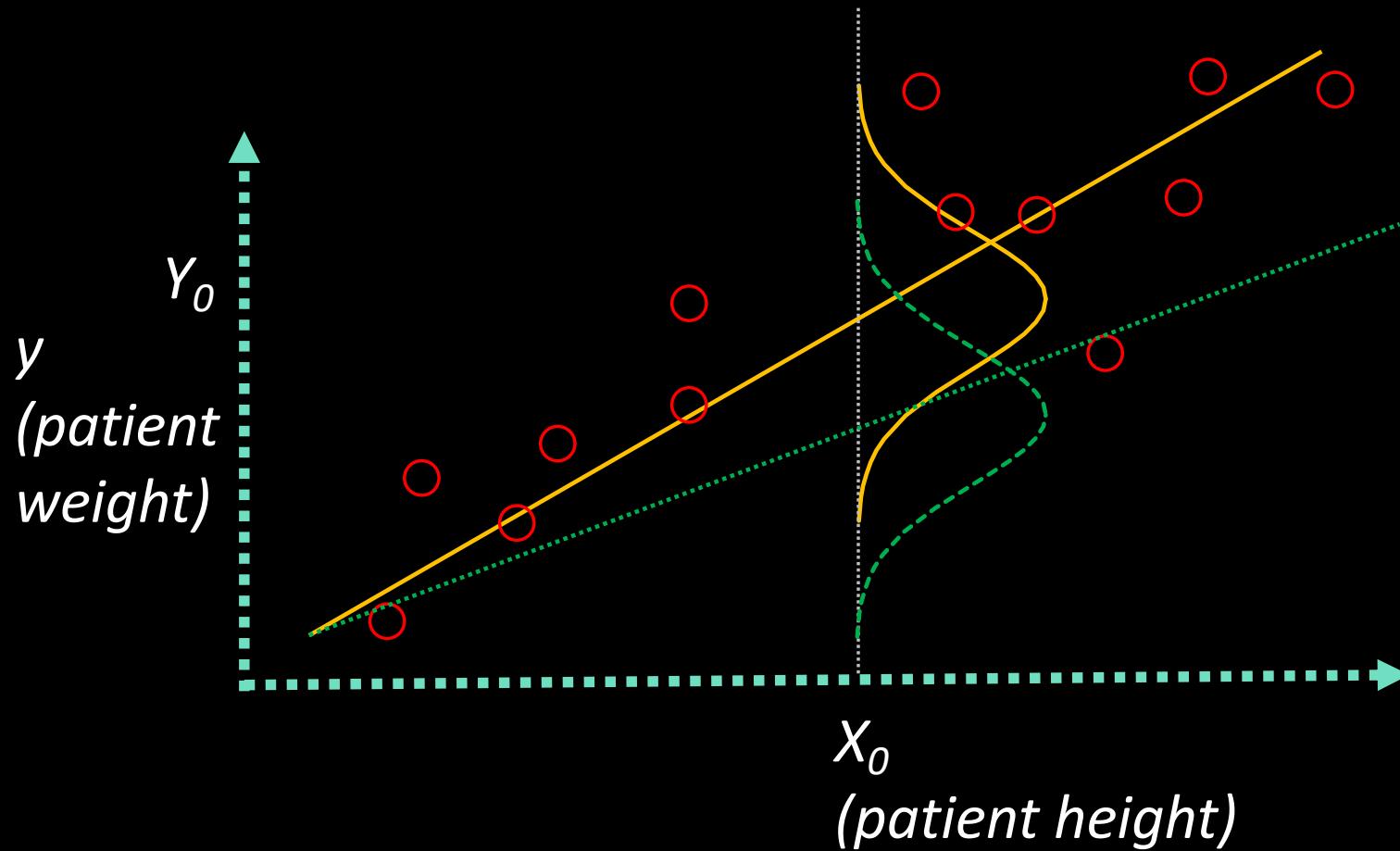
# What's the less probable model?



# What's the more probable model?



# Find the more probable model: Maximum likelihood estimation



## Maximum Likelihood Estimation (MLE)

$$\theta_{ML} = \underset{\theta}{\operatorname{argmax}} \ P(y|X; \theta)$$

It finds the parameter values that make the observed data most probable.

# Don't be scared by the math!

$$\theta_{ML} = \underset{\theta}{argmax} P(y|X; \theta)$$

$\theta$  means parameters

$argmax(*)$  Means adjusting the parameters until  
(\*) at its maximum

$P(y|X; \theta)$  Means the conditional probability:  
 $y$  appears given  $X$

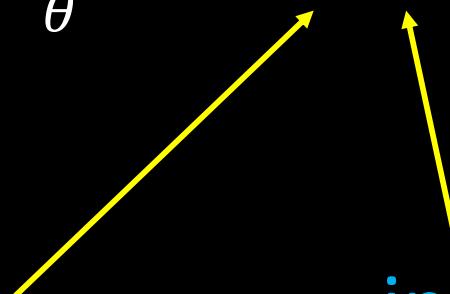
# Maximum Likelihood Estimation (MLE)

In the foundational of many ML models,  
including language models

$$\theta_{ML} = \underset{\theta}{argmax} \quad P(y|X; \theta) \quad y = M_{\theta}(X)$$

Output sentences

input sentences



# Maximum Likelihood Estimation (MLE)

Training a polite chatbot:

$$\theta_{ML} = \underset{\theta}{\operatorname{argmax}} \ P(\text{"I am fine, thank you"} | \text{"How are you"; } \theta)$$

Training a passive aggressive chatbot:

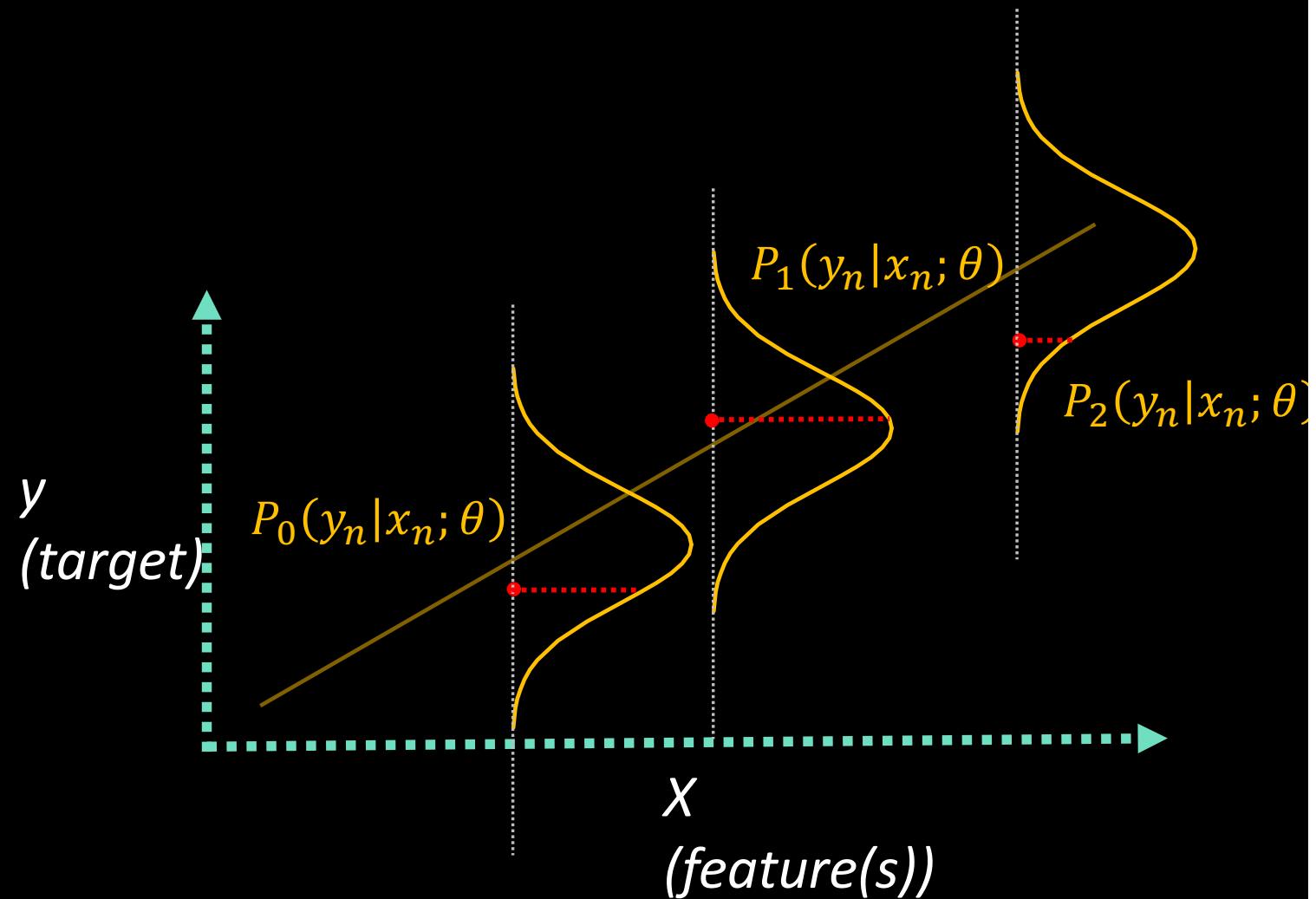
$$\theta_{ML} = \underset{\theta}{\operatorname{argmax}} \ P(\text{"Why do you care?"} | \text{"How are you"; } \theta)$$

How to evaluate  
many data  
points at once?

$$\prod_n P(y_n|x_n; \theta)$$

$$= P_0 * P_1 * P_2 \dots$$

Times them up  
together



Datapoints	1.	2.	3	4.	5
------------	----	----	---	----	---

*X : what's the capital of France, USA, Japan, UK, Germany*  
*Y: Paris DC Tokyo London Berlin*

Probabilities according to the bad model:

[0.171 0.110 0.06 0.03 0.01.....]

Probabilities according to the good model:

[0.498 0.598 0.398 0.598 0.698.....]

## Joint Probability

$$P(y_1|x_1; \theta) * P(y_2|x_2; \theta) \dots * P(y_n|x_n; \theta) = \prod_n P(y_n|x_n; \theta)$$

$$\prod_n P(y_n|x_n; \theta) \quad (0.1 * 0.1 * 0.1 * 0.1 \dots) \quad 0.000000001$$

VS

$$\sum_i \log P(y_n|x_n; \theta) \quad (-1 -1 -1 -1 -1 \dots) \quad -9$$

## Log Probability

# If you want to see the derivation

$$\sum_n \log P(y_n | x_n; \theta)$$

$$= n \sum \log\left(\frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y_n - wx_n - b)^2}{2\sigma^2}\right)\right)$$

Linear Regression picked from Normal Distribution

$$= -n * \log \frac{1}{\sqrt{2\pi\sigma^2}} - \sum_i \frac{(y_n - wx_n - b)^2}{2\sigma^2}$$

Assuming constant variance

$$\operatorname{argmax}(\sum_i \log P(y_n | x_n; \theta)) = \operatorname{argmin}(\sum_n (y_n - wx_n - b)^2)$$

$$= \operatorname{argmin}(\sum_n (\textcolor{red}{y_n} - \hat{y})^2)$$

Mean Square Error (MSE)

Linear Regression is optimized by  
minimize mean square error (MSE)

(but you actually just need:)

**Regression by just called a library (Scipy)**

```
from sklearn.linear_model import Regression
```

```
Regr = Regression()
```

```
Regr.fit(x_train, y_train)
```

## Mini-proposal ground rules

1. 80% of the scores (mid term + final), try your best!
2. Your group will work on the same topic before the midterm, but can work on individual sub-topics for final
3. Submit your group's overall topic and student ID to the TA before end of the class

Examples:

Group: how AI can help mental health patients:

Individual:

1. Can chatbot help to detect anxiety from social network
2. Can facial expression analysis track seasonal depression

Group: Can AI help improving the diagnosis accuracy of medical imaging

Individual:

1. Can neural networks detect lesions from low-dose CT
2. Can deep learning predict the prognosis of dementia from MRI

It's ok to select the same sub-topic!  
(particularly if all of you like it a lot)

But each one should submit their own writing in the final

If you have specific type of writing in mind  
(grant proposal / paper manuscript)

You can also bring to the class for additional review / support

# Mini-proposal (why give me money?)

1. How people have done it  
& why it's not enough

2. Why is this an  
important problem

3. Why / How  
I can do it (with AI)

4. What's the  
expected result?

# Mini-proposal (why should I be funded?)

1.How people have done it  
& why it's not enough

Literature Review

2.Why is this an  
important problem

Problem Statement

3.Why / How  
I can do it

Proposed Method

4.What's the  
expected result?

Deliverables

# AI Literature Gathering & Review

## AI tool ground rules:

We are not pretending to be "AI salesman"

We don't suggest or recommend any paid AI tools

We suggest using any generic LLM (ChatGPT / Claude) rather than "specialized" tools

X

Best AI Tool For  
Research

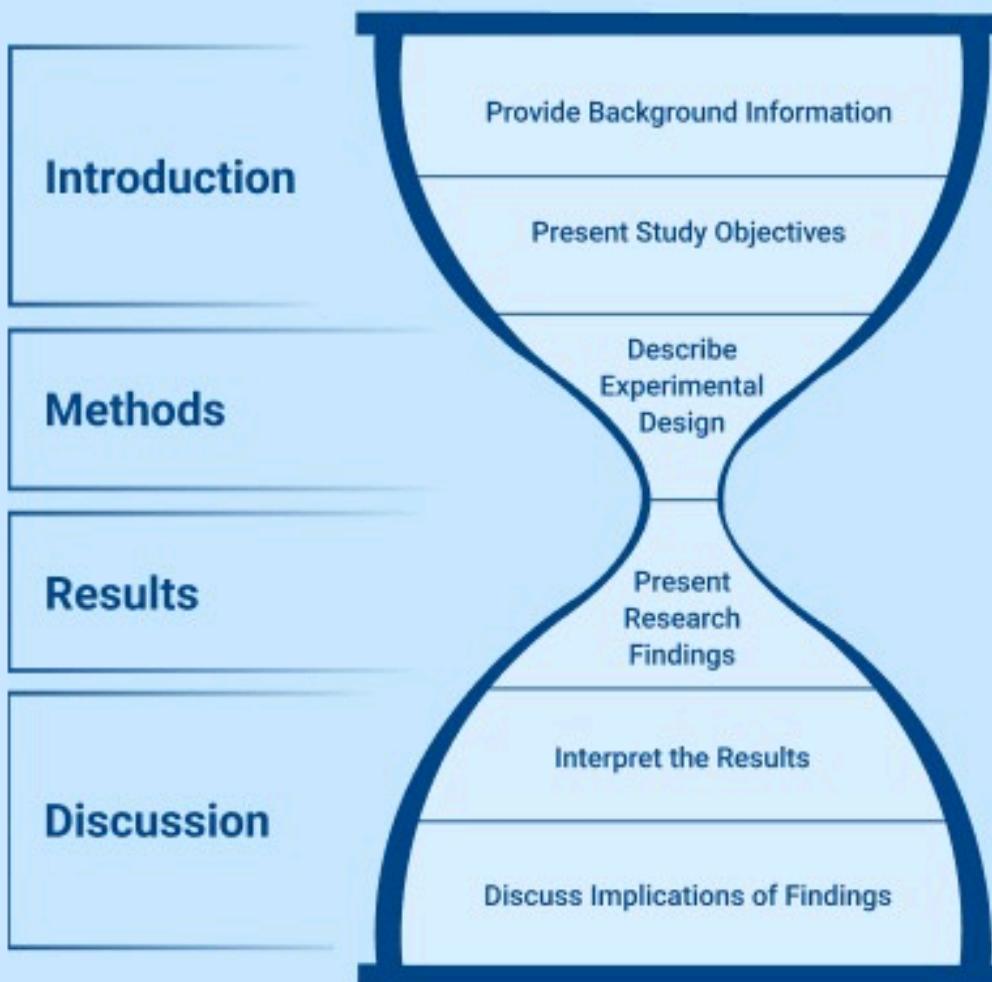
X

Best “prompt”  
or magical word

X

“Total  
Automation”

## Scientific Research Paper Basics



In which step(s) does “creativity” come in?

Idea  
of a scene



Background  
information

“Research  
Gap”

Experiment  
Design /  
Conduct

Result/  
Implication

Background information → “Research Gap” → Experiment Design / Conduct → Result/Implication

Your  
Input

The ones  
You curated  
  
(from all the  
papers)

The one  
you identified  
  
(from all the  
questions)

You design it

You explain it

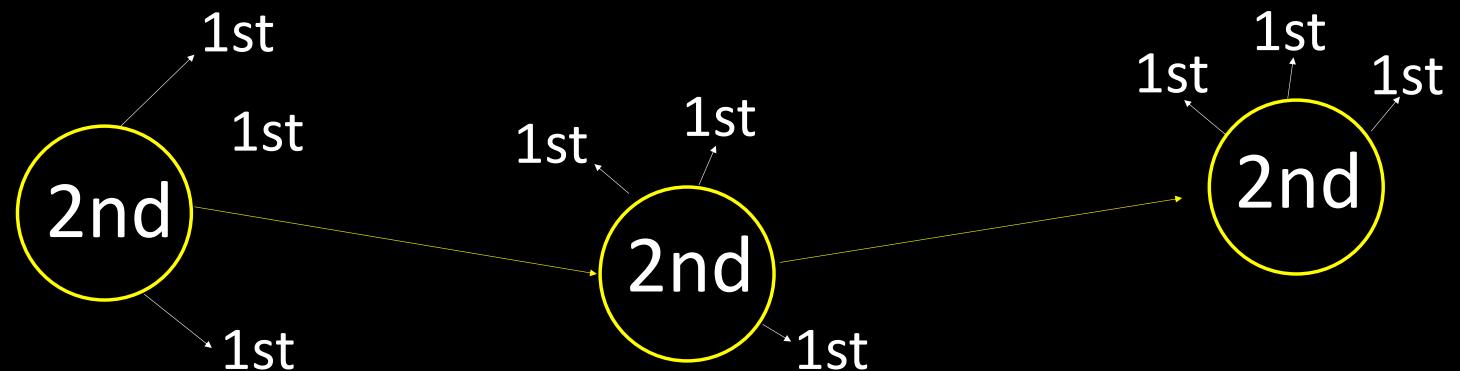
# Types of literatures:

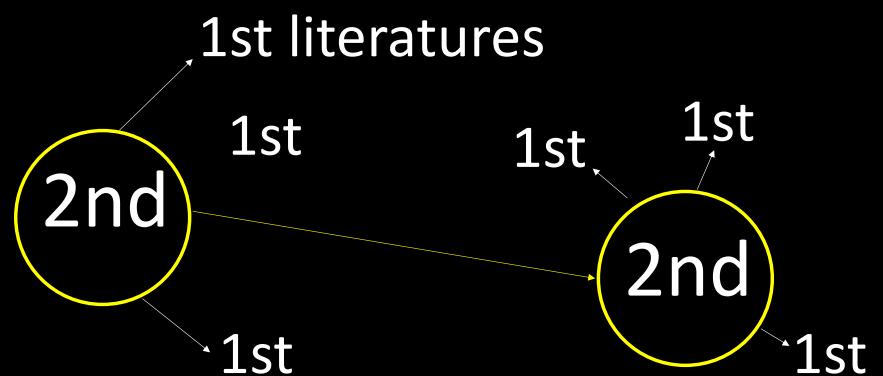
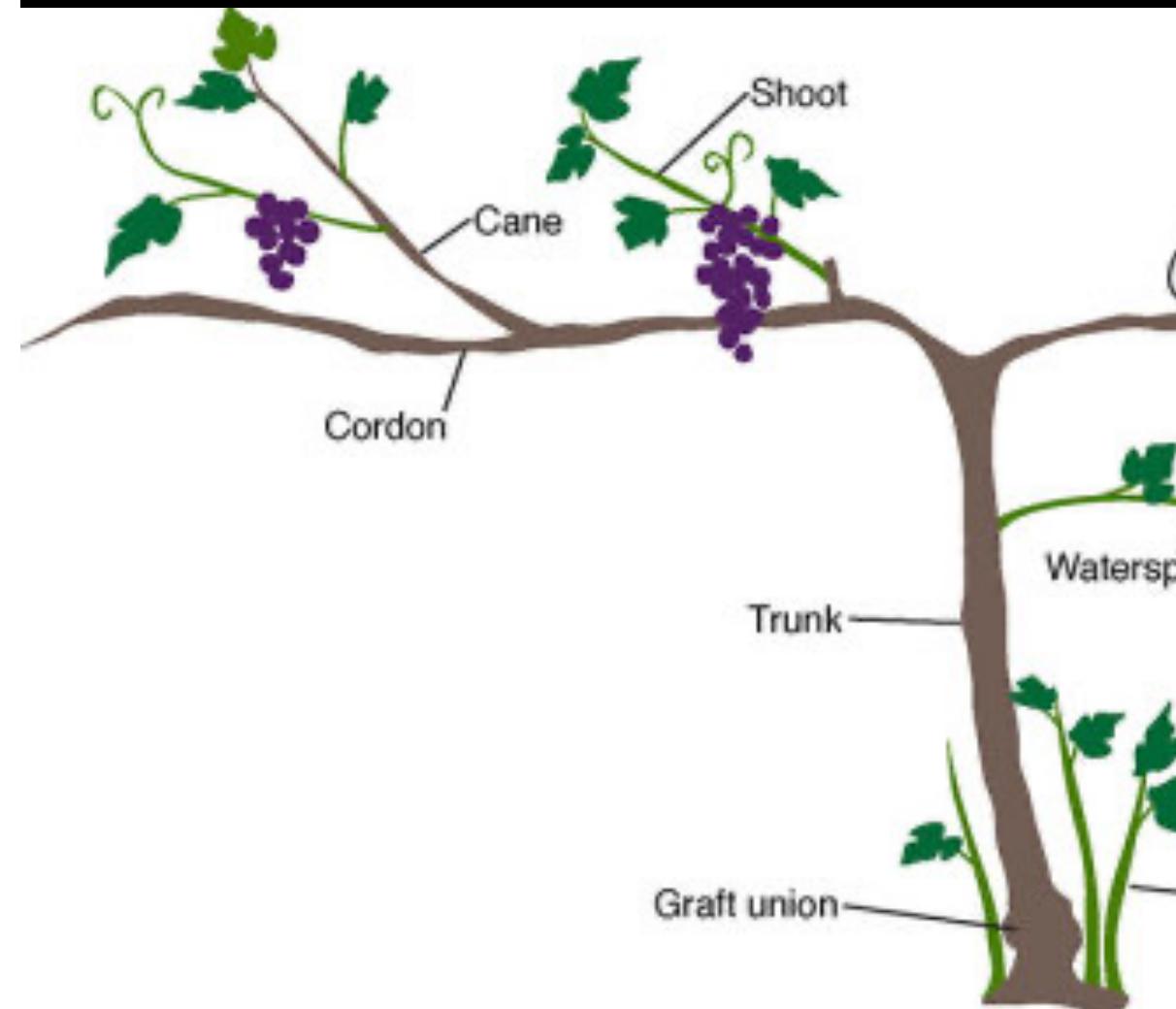
Primary literatures:

original experiments, trials studies

Secondary literatures:

review papers, meta-analyses





1. Each find  
**one** review  
paper

2. Skim  
abstract,  
conclusion,  
introduction

3. Answer the questions to  
each other:

Scope of this review?

What's main  
concept &  
arguments?

Background knowledge  
you're missing?

How is the related to my  
interest?

4. Vote for 1,2?  
review paper

5. Find the best  
original articles

Under the group topic, each member should find "1" good and distinct review paper from the same topic

Under the group topic, each member should find "1" good and distinct **review paper** from the same topic

H find good review paper of AI in dentistry

Hunting for cutting-edge review papers on AI in dentistry



I'll search for recent review papers on AI applications in dentistry to find you some high-quality academic sources.

***Discovery!***

## **Artificial Intelligence in Dentistry: Chances and Challenges**

F. Schwendicke<sup>1</sup>, W. Samek<sup>2</sup>, and J. Krois<sup>1</sup>

***Critical Reviews in Oral Biology & Medicine***

## **Application of Artificial Intelligence in Dentistry**

T. Shan<sup>1</sup>, F.R. Tay<sup>2</sup>, and L. Gu<sup>1</sup>

# Strategic Reading for Review Papers

1. Prioritize abstracts and introductions
2. Skim for key concepts and arguments

Review Article | [Open access](#) | Published: 14 March 2023

## AlphaFold2 and its applications in the fields of biology and medicine

Zhenyu Yang, Xiaoxi Zeng , Yi Zhao  & Runsheng Chen 

*Signal Transduction and Targeted Therapy* 8, Article number: 115 (2023) | [Cite this article](#)

103k Accesses | 361 Citations | 150 Altmetric | [Metrics](#)

### Abstract

AlphaFold2 (AF2) is an artificial intelligence (AI) system developed by DeepMind that can predict three-dimensional (3D) structures of proteins from amino acid sequences with atomic-level accuracy. Protein structure prediction is one of the most challenging problems in computational biology and chemistry, and has puzzled scientists for 50 years. The advent of

### Concluding remarks

The excellent performance of AF2 in predicting protein structure together with the release of structures of more than 200 million proteins predicted by AF2 is reshaping structural biology. AF2 will certainly have a significant impact on researches that need protein structure information, and could be applied in many fields such as drug discovery, protein design,

### Introduction

In December of 2020, AlphaFold2 (AF2),<sup>1</sup> a machine-learning based model to predict protein structures developed by DeepMind, won the championship in the 14th Critical Assessment of Structure prediction (CASP14).<sup>2</sup> One and a half years later, DeepMind and the EMBL's European Bioinformatics Institute (EMBL-EBI) released structures of more than 200 million proteins predicted by AF2,<sup>3</sup> which cover almost all the known proteins on the planet (protein universe). These two events have drawn great attention to AF2 in the science community. AF2 represents a milestone advance in protein structure prediction. It is considered as the greatest contribution of artificial intelligence (AI) to the scientific field and one of the most

What's scope of this review?

What's main concept & arguments?

How is it related to my interest?

Background knowledge you're missing?

# AI for lung cancer detection

Is it solved? (No)

Why (research gap)?

Model Design &  
Performance

Accuracy,  
efficiency....

Workflow  
Integration

Modality..regulation..

Clinical  
Implication

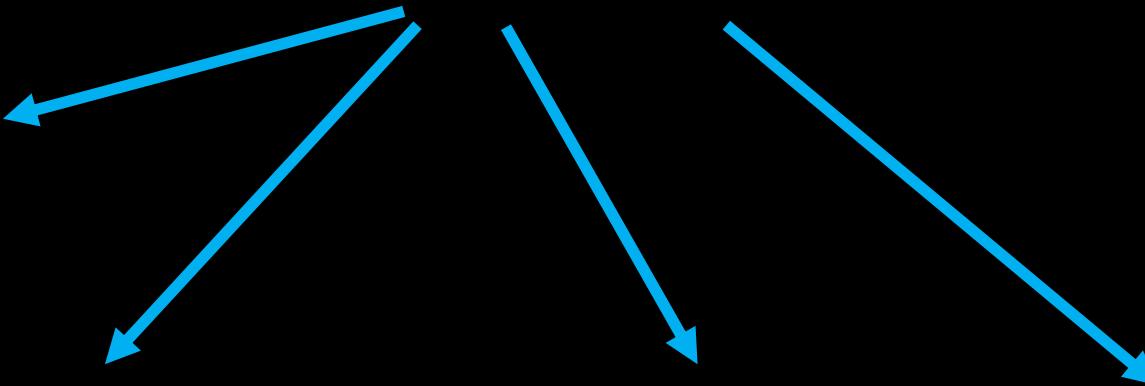
FP/FN...

Population

Bias

All local...

Financial  
Implication  
Who's paying...

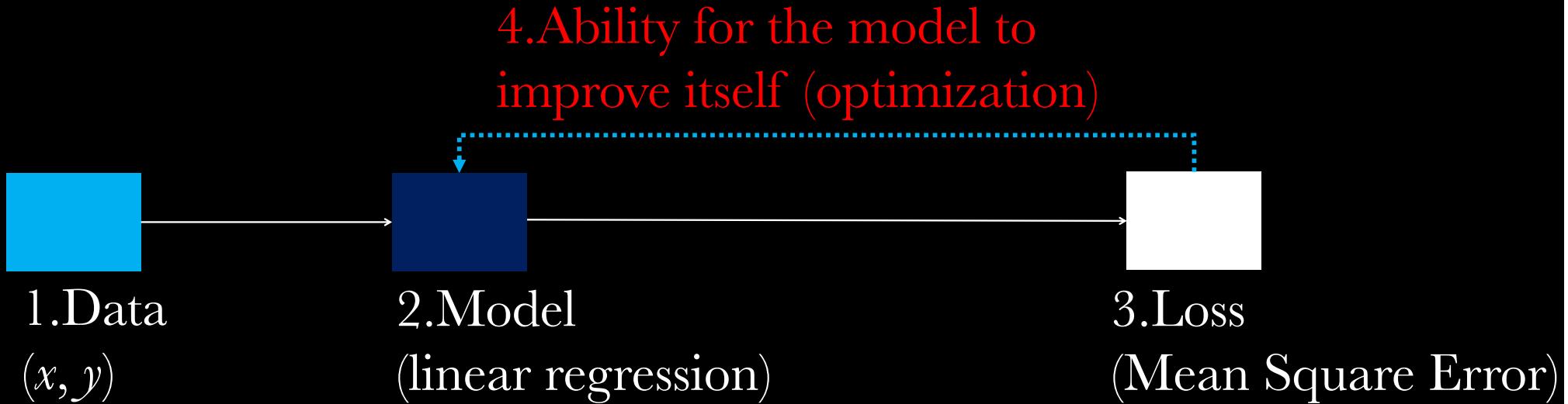


**Now you will select primary literature from the review paper(s)**

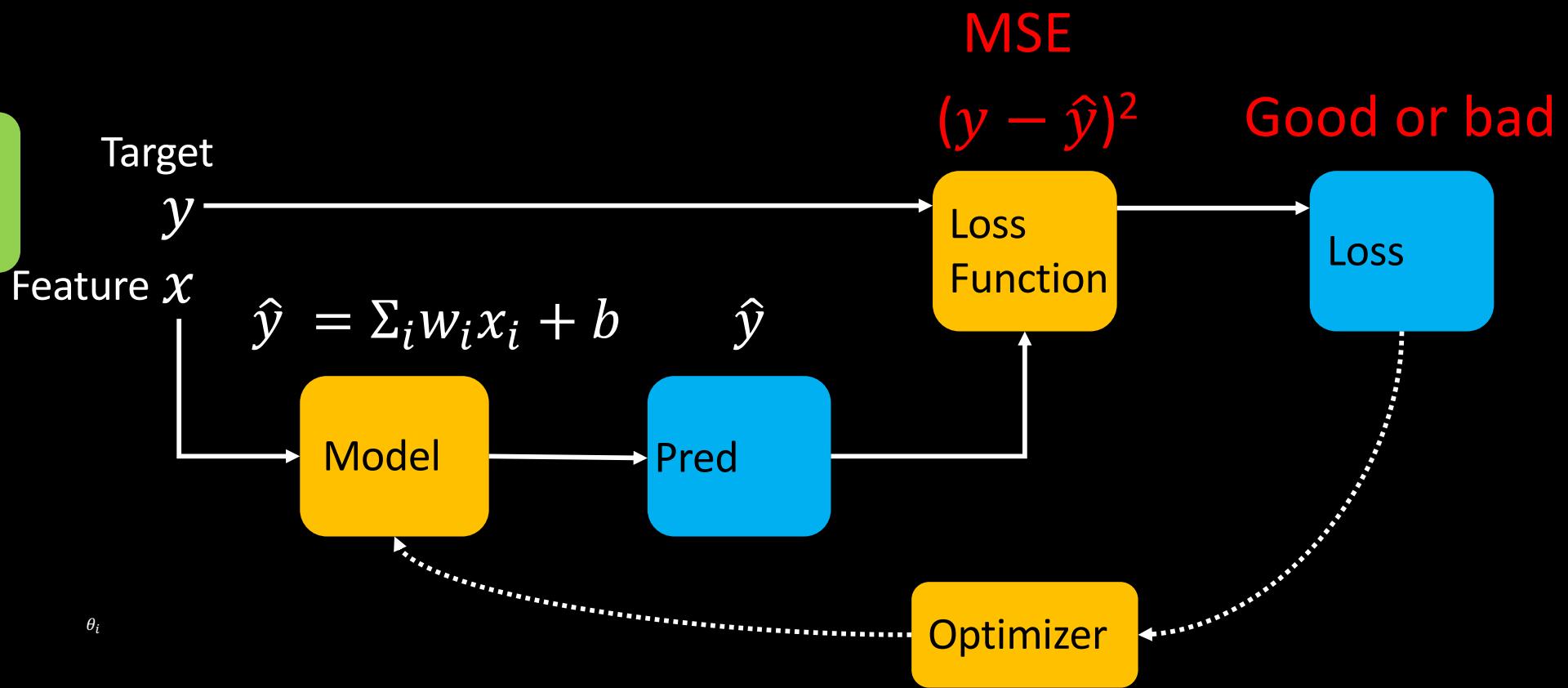
Each one will pick their own list (~10)

You should be able to explain to me why

## Behind the Scene Regr.fit(x\_train, y\_train) Of linear regression

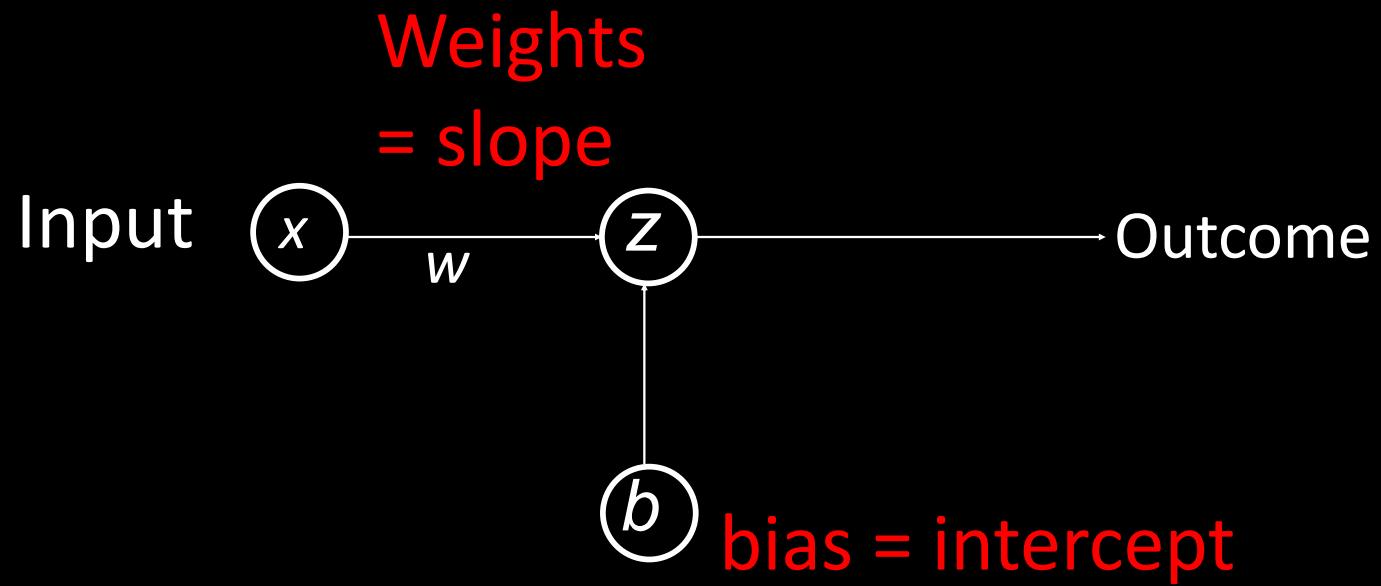


## Flow Chart for Linear Regression



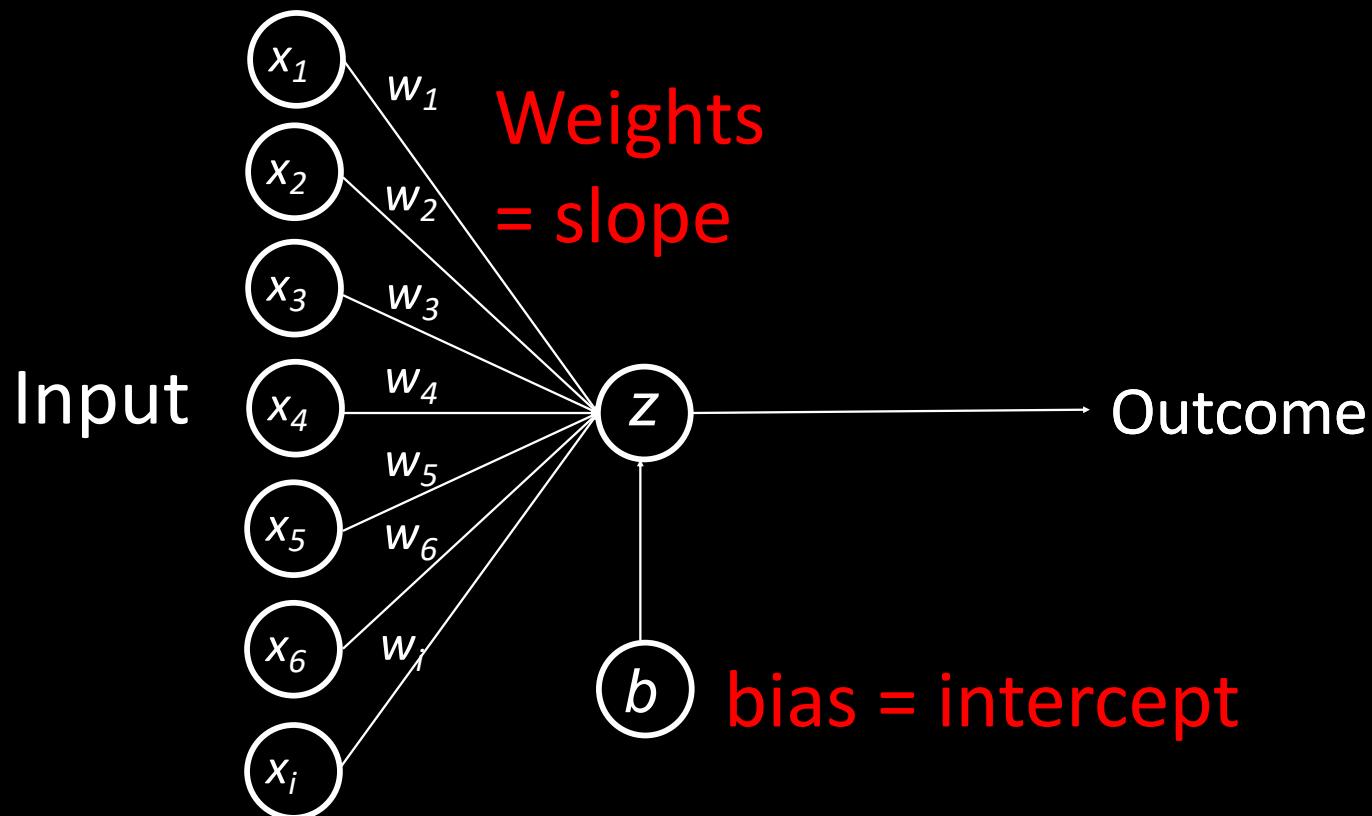
# Graph of Linear Regression

$$y = WX + b$$

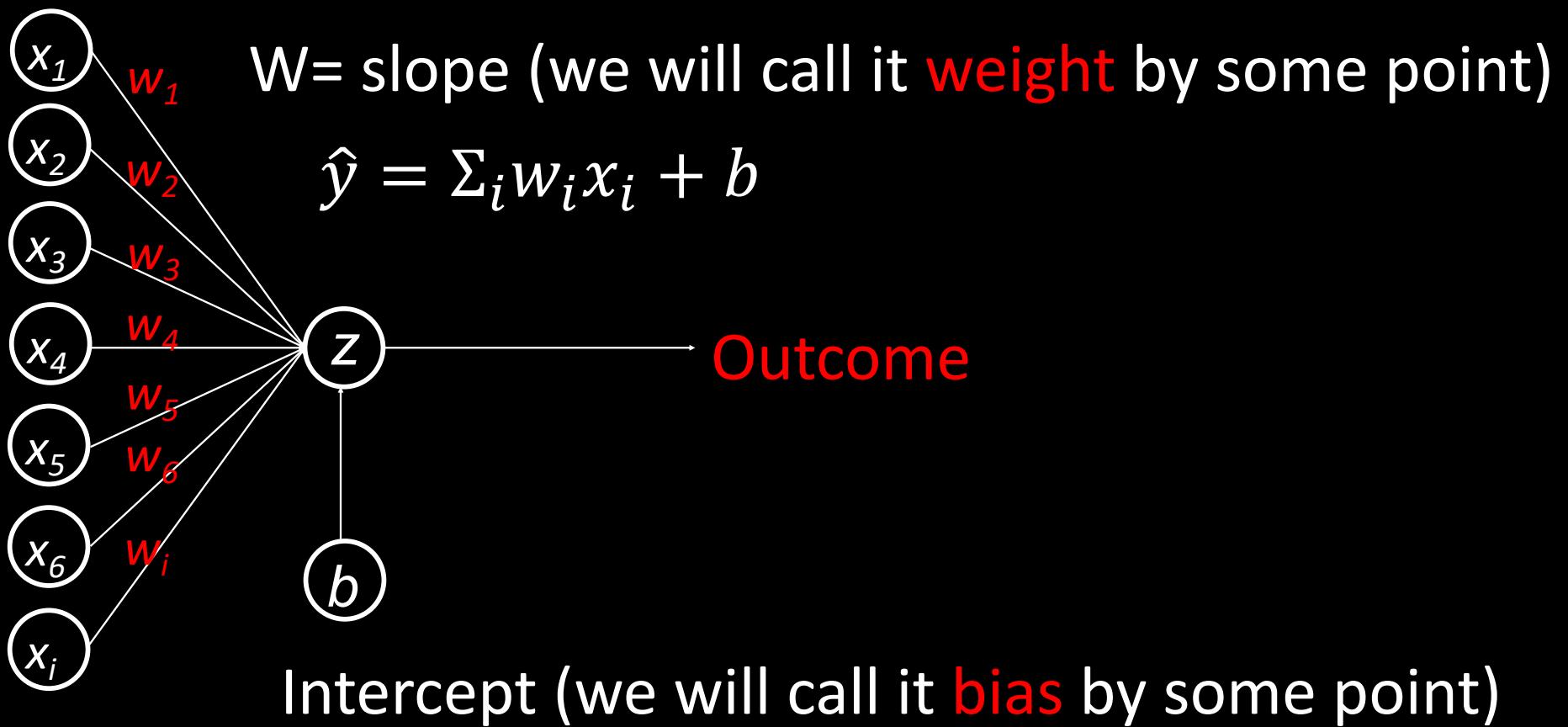


# Graph of Linear Regression

$$y = w_1x_1 + w_2x_2 + \dots + b$$



If we re-draw it into a graph.....



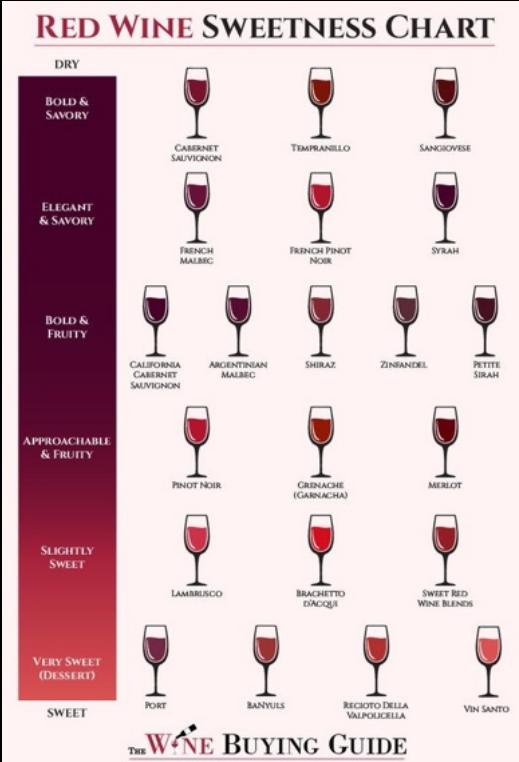
# Classification: Logistic Regression

Human has a tendency (or need) to categorize things for our own perception

Table 2. Examples of the training data set (values are normalized between 0 and 1)

Fruit image	Input of the network		Output
	Mean	Variance	
	0.43	0.11	'Extra'
	0.22	0.05	'Type 1'
	0.27	0.23	'Type 2'
	0.26	0.31	'Rejected'
	0.28	0.29	'Rejected'

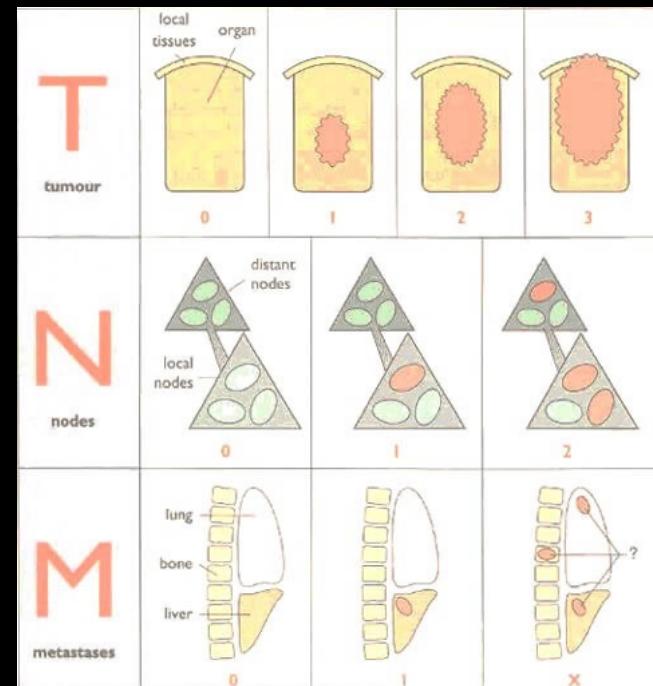
St. Cerc. St. CICBIA 2016 17 (1)



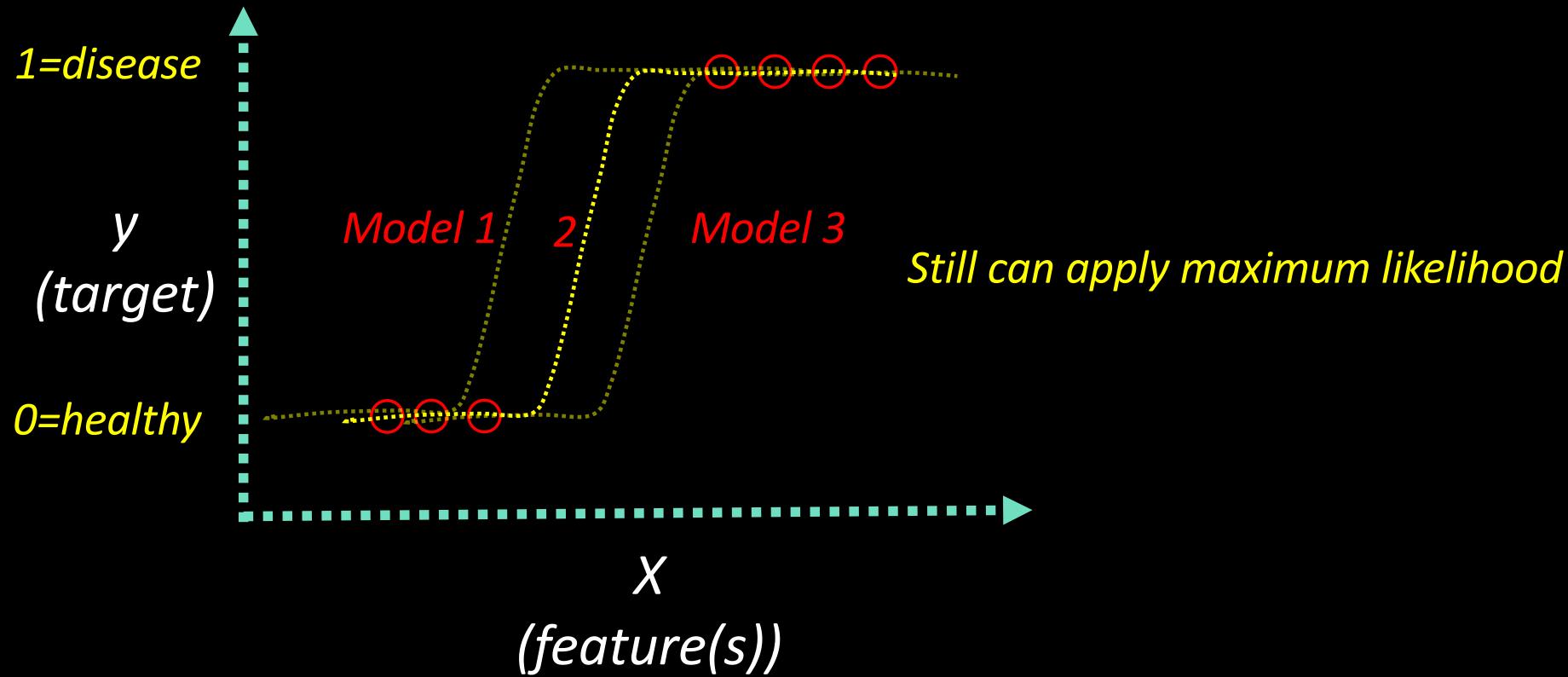
2023 Federal Tax Brackets			
TAX BRACKET/RATE	SINGLE	MARRIED FILING JOINTLY	HEAD OF HOUSEHOLD
10%	\$0 - \$11,000	\$0 - \$22,000	\$0 - \$15,700
12%	\$11,001 - \$44,725	\$22,001 - \$89,450	\$15,701 - \$59,850
22%	\$44,726 - \$95,375	\$89,451 - \$190,750	\$59,851 - \$95,350
24%	\$95,376 - \$182,100	\$190,751 - \$364,200	\$95,351 - \$182,100
32%	\$182,101 - \$231,250	\$364,201 - \$462,500	\$182,101 - \$231,250
35%	\$231,251 - \$578,125	\$462,501 - \$693,750	\$231,251 - \$578,100
37%	\$578,126+	\$693,751+	\$578,101+

THE COLLEGE INVESTOR

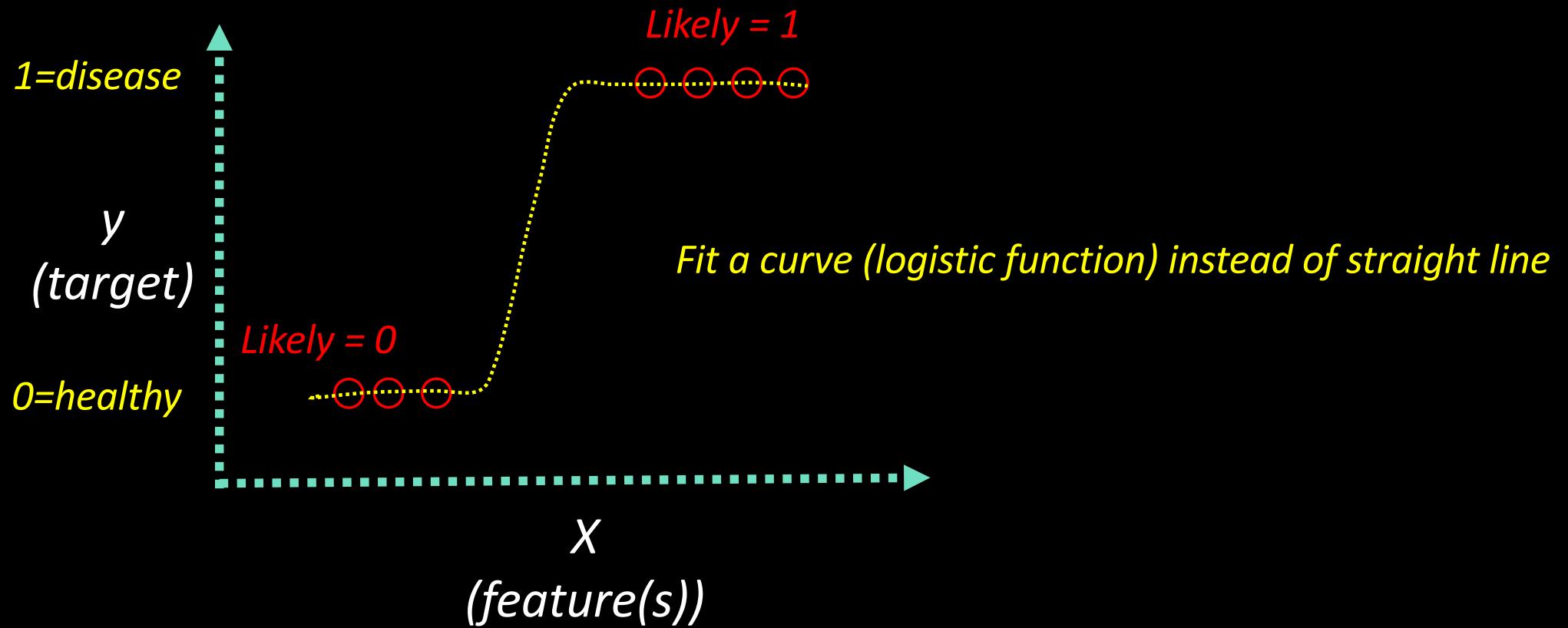
Source: TheCollegeInvestor.com



# Logistic Regression: Predicts categorical outcomes



# Logistic Regression: Predicts categorical outcomes



## Chance of wolf (=1)



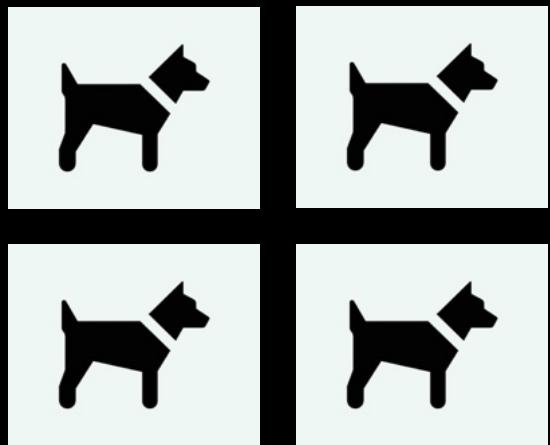
0 (very sure)

0.2 (not sure)

0.7 (not sure)

1 (very sure)

Clean cut



Clean cut

ambiguous

$y$   
*(Output Probability)*

$P=0.5$

$P=0$

$P=0.2$

$P=0.7$

$P=1.0$



$X$   
*feature(s)*

*y*  
*(Output Probability)*

$P=0.5$

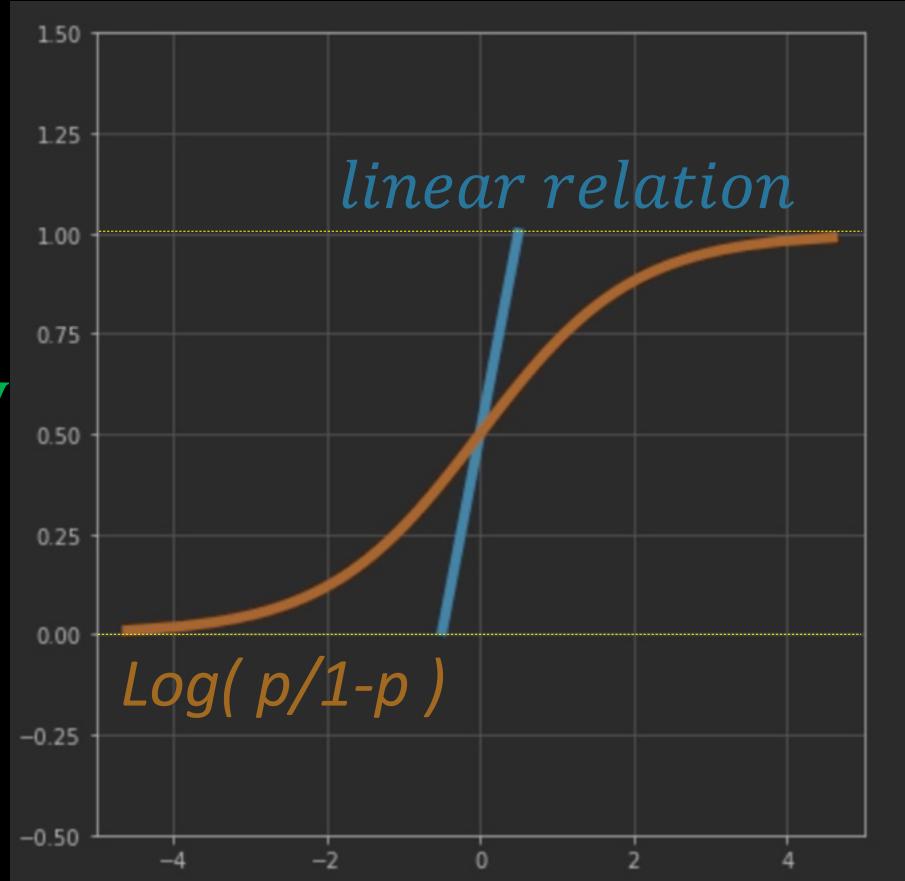
*X*  
*feature(s)*

$P \geq 0.5$  *Class=1*

$P < 0.5$  *Class=0*



Probability  
0-1



feature –  $\infty \sim \infty$

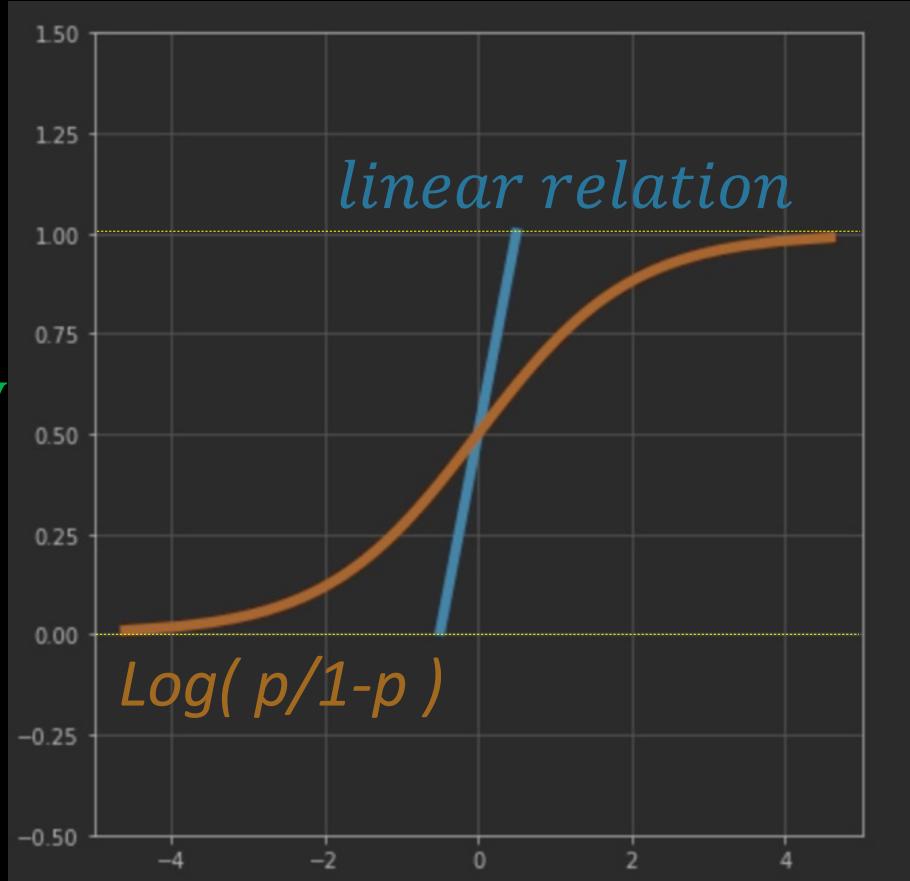
How to predict probability?

Remember we got  
output of range

$-\infty \sim \infty$

From regression

Probability  
0-1



feature —  $-\infty \sim \infty$

Probability  $p$   $0 \sim 1$

Odd Ratio  $\frac{p}{1-p}$   $0 \sim \infty$

*Logit*  $\log\left(\frac{p}{1-p}\right)$   $-\infty \sim \infty$

*same range!*

linear regression  $\sum_i w_i x_i + b$   $-\infty \sim \infty$

Now we can just do regression to logit!

	No. of case patients	No. of control subjects	Odds ratio	95% confidence interval	P for trend*
Nonsmokers	117	1750	1.0	Referent	
Duration of tobacco use, y					
0.1–20.0	3	33	1.3	0.4–4.5	
20.1–32.0	7	33	3.4	1.4–8.0	
32.1–44.0	21	33	13.3	7.2–24.9	
≥44.1	30	30	19.1	10.4–35.1	<.0001
Average consumption of tobacco, g/day					
0.1–3.5	2	10	2.2	0.5–10.4	
3.6–5.0	22	54	7.9	4.3–14.3	
5.1–10.7	6	18	4.8	1.9–12.6	
≥10.8	31	47	12.4	7.2–21.4	.1
Cumulative consumption of tobacco, g/day × y					
1–71	3	31	1.3	0.4–4.4	
72–157	13	34	7.6	3.8–15.4	
158–382	15	32	8.0	4.0–15.7	
≥383	30	32	18.3	10.2–32.8	.0006
Age at start of tobacco use, y					
≤19	27	48	9.6	5.6–16.7	
20–26	20	52	6.3	3.5–11.2	
≥27	14	29	8.2	4.1–16.3	.4

\*Test for linear trend, two-sided *P* value (considered statistically significant for *P*<.05).

Now we are mapping the output of regression:

$$\sum_i w_i x_i + b \quad -\infty \sim \infty$$

to

To logit  
 $\text{Logit } \log\left(\frac{p}{1-p}\right) -\infty \sim \infty$

$$p = \frac{1}{1+exp-(\sum_i w_i x_i + b)} = \text{Sigmoid}(w_i x_i + b) = S(\beta X)$$

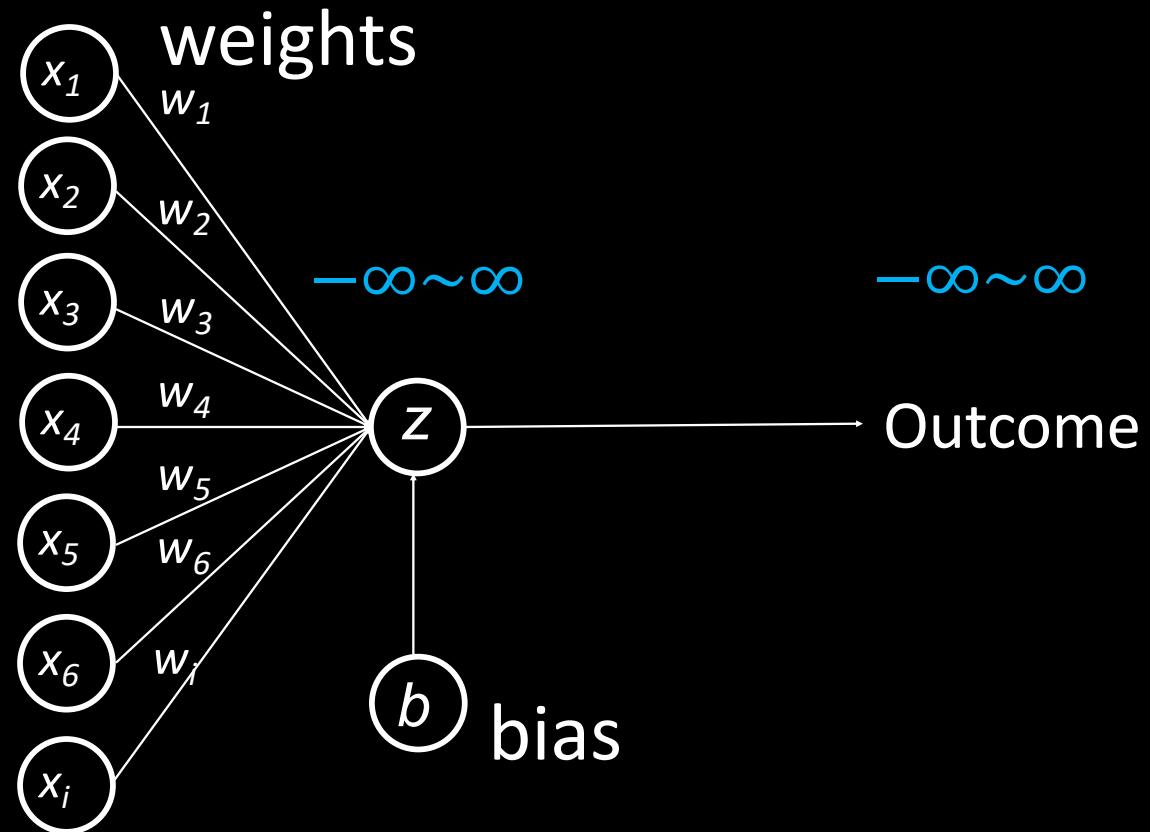
Just  
Logistic  
Regression

$$p = \frac{1}{1 + \exp - (\sum_i w_i x_i + b)} = \text{Sigmoid}(w_i x_i + b) = S(\beta X)$$

$$P = S(\beta X)$$

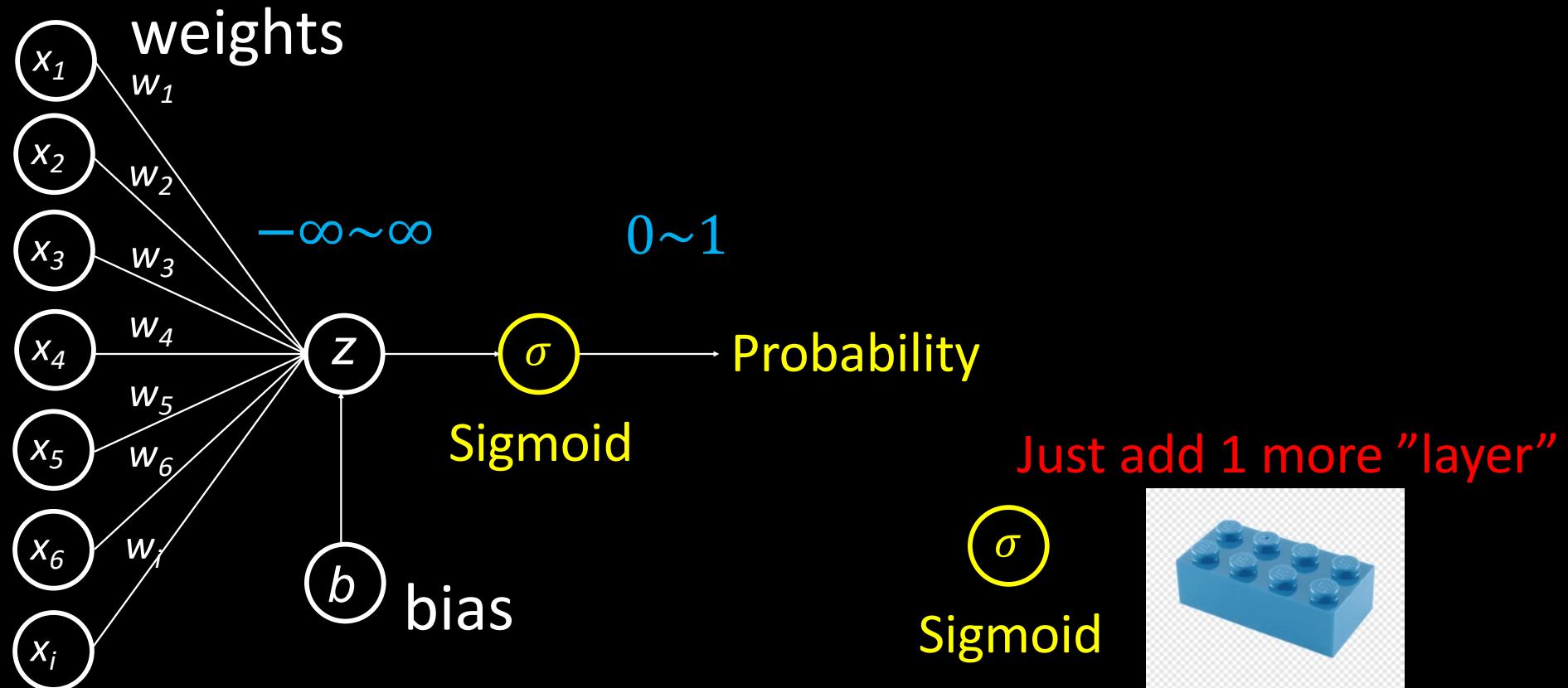
Logistic Regression = Regression  
Between  
Probability and Sigmoid of  
(weighted features)

# Graph of Linear Regression



# Graph of Logistic Regression

$$p = \frac{1}{1 + \exp(-(\sum_i w_i x_i + b))} = \text{Sigmoid}(\sum_i w_i x_i + b) = S(WX)$$



# Loss Function for Classification

(need to way to say good or bad)

$P=1$

Probability  
of  
 $P=1$

$P=0$



Wrong

Right



Wrong

Right

$P=1$



*Probability of  $P=0$*

$P=0$



*Probability of  $P=1$*



*How right are we?*

$P=1$



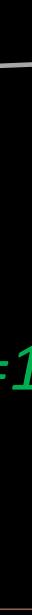
*Probability of  $P=0$*



$P=0$



*Probability of  $P=1$*

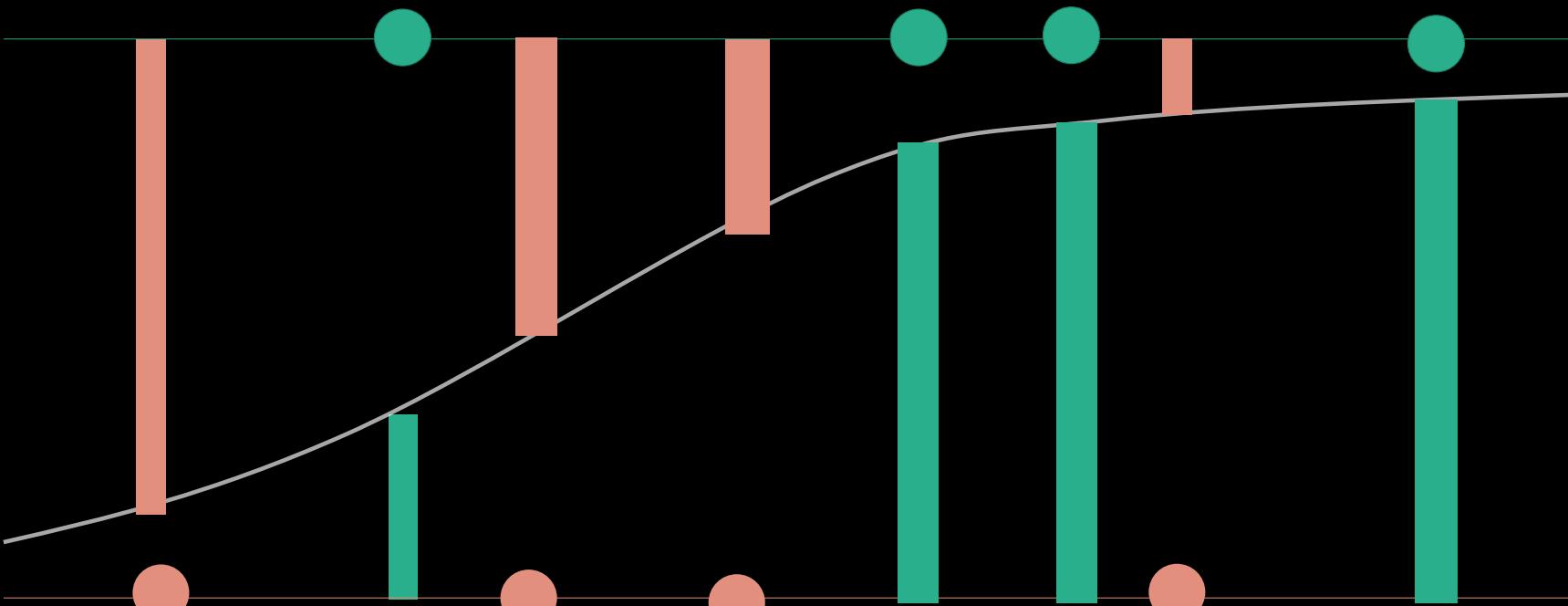


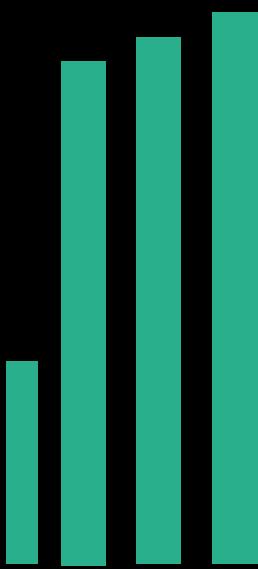
*How right we are?*

*Probability of all the cases=* $p_0 * p_1 * p_2 * p_3 * p_4$

$P=1$

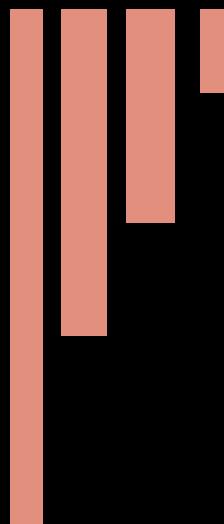
$P=0$





*Probability of all the cases*

$$(+)\ p_0 * p_1 * p_2 * \dots \dots$$



$$(-)\ p_0 * p_1 * p_2 * \dots \dots$$

Remember  $\log(\text{Prob.})$

$$\prod_n P(y_n|x_n; \theta)$$

VS

$$\sum_i \log P(y_n|x_n; \theta)$$

## Binary Cross Entropy (BCE) loss

$y = 1$

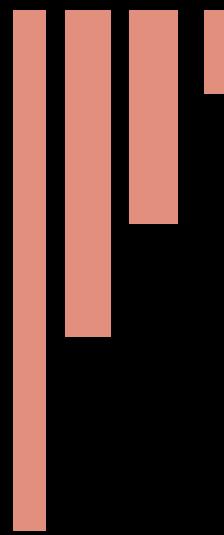
$y = 0$

$$BCE = - \sum_n \begin{cases} 1 & y \cdot \log(p(\hat{y})) \\ 1 & (1 - y) \cdot \log(p(1 - \hat{y})) \end{cases}$$

*All the probs  
predicted  $y = 1$   
correctly*

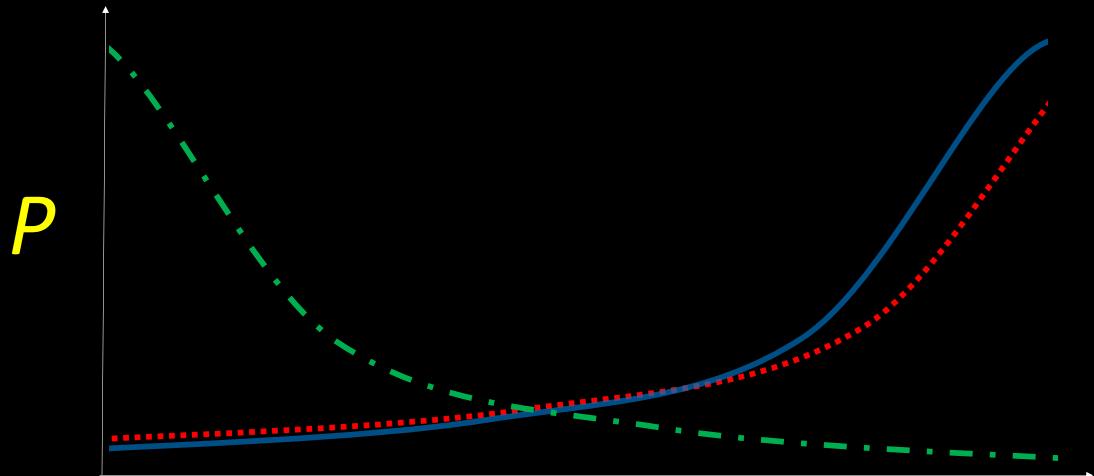


*All the probs  
predicted  $y = 0$   
correctly*



Again, this is based on Maximum Likelihood Estimation (MLE)

$$\theta_{ML} = \operatorname{argmax}_{\theta} P(y|X; \theta)$$



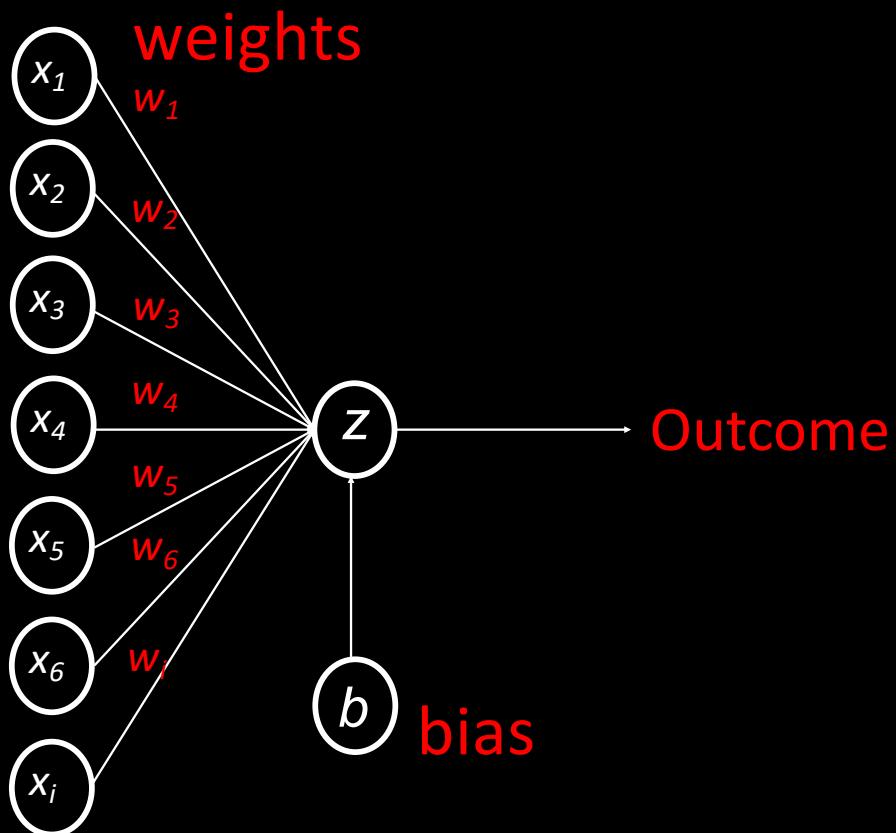
Q, Real Probability

$P(y|X; \theta)$ , good prediction

$P(y|X; \theta)$ , bad prediction

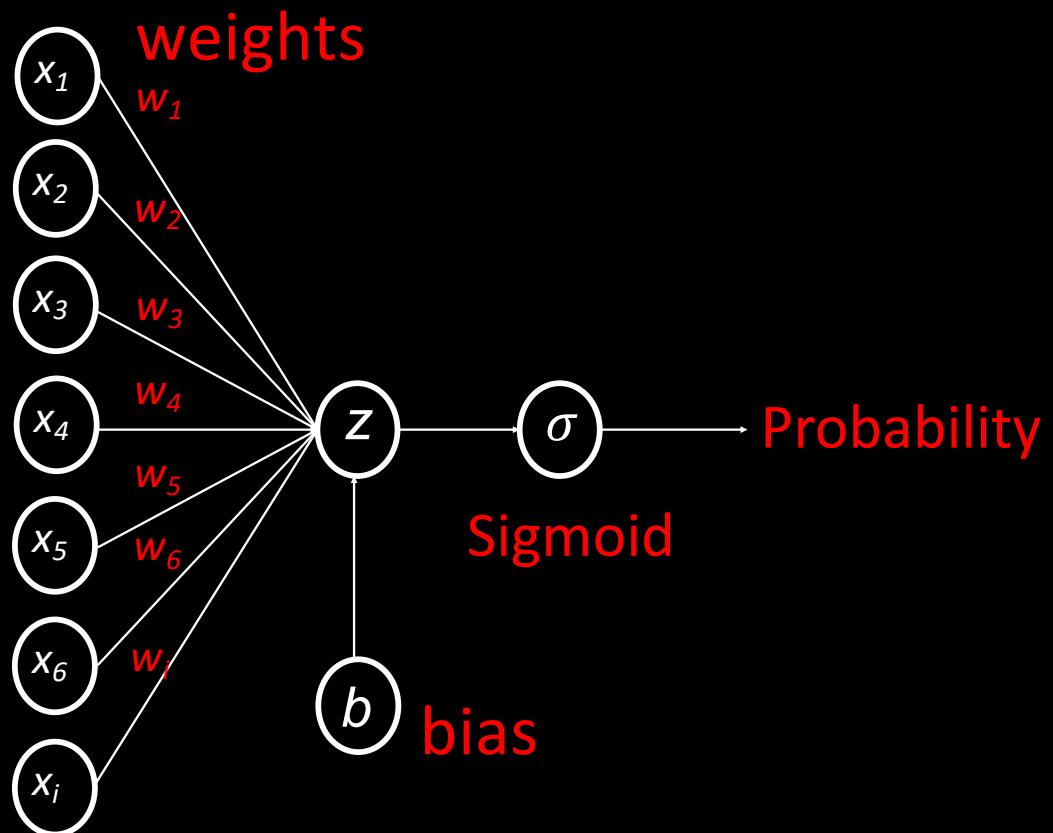
Cross Entropy:  
how different they are?

## Summary: Regression



Loss: Mean Square error

## Classification (logistic regression)



Loss: Cross Entropy