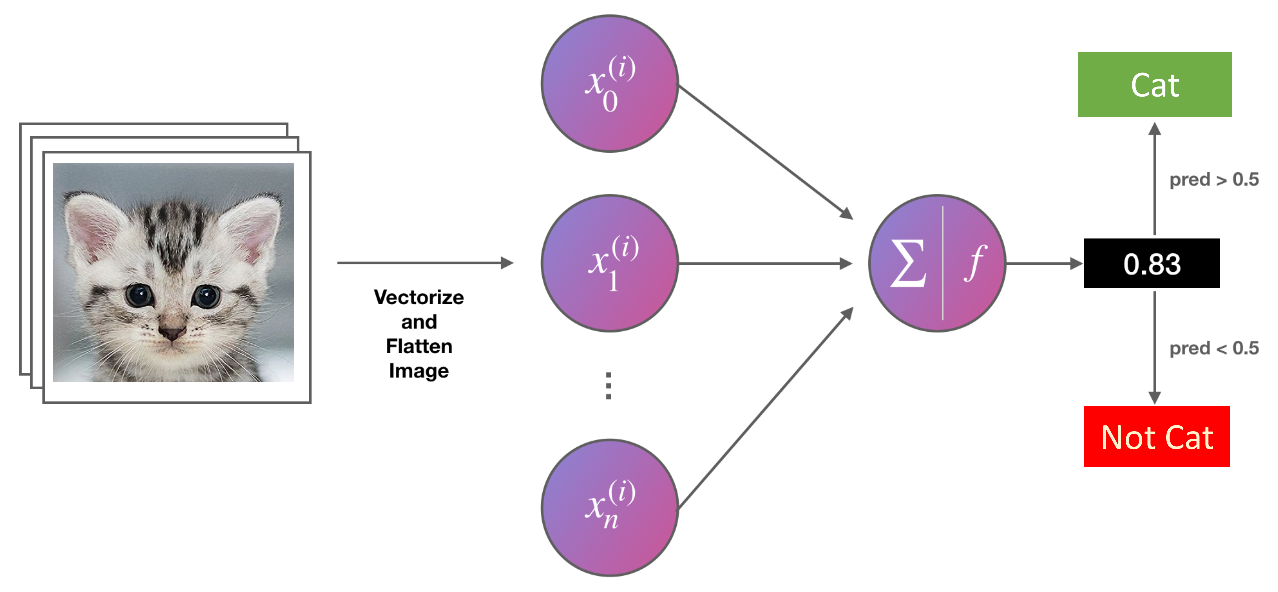
Lecture 6: Logistic Regression & PyTorch for Deep Learning



[Haiping Lu](#)

YouTube Playlist: https://www.youtube.com/c/HaipingLu/

COM4059/6059: MLAI20@The University of Sheffield

Week 6 Contents / Objectives

- Machine Learning Recap
- Motivation for Logistic Regression
- Logistic Regression
- Computational Graph
- PyTorch: A Deep Learning Library

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- **Machine Learning Recap**
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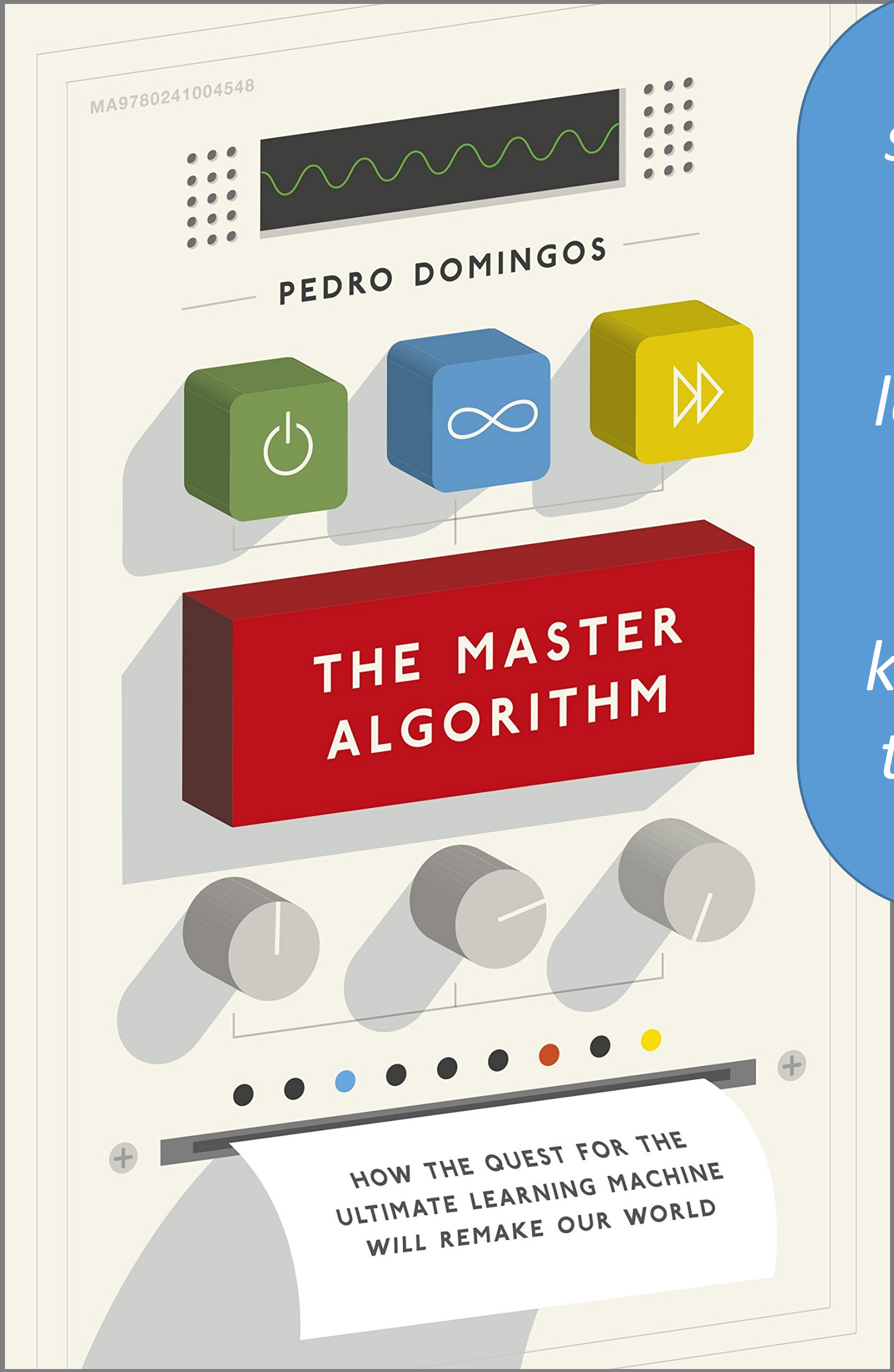

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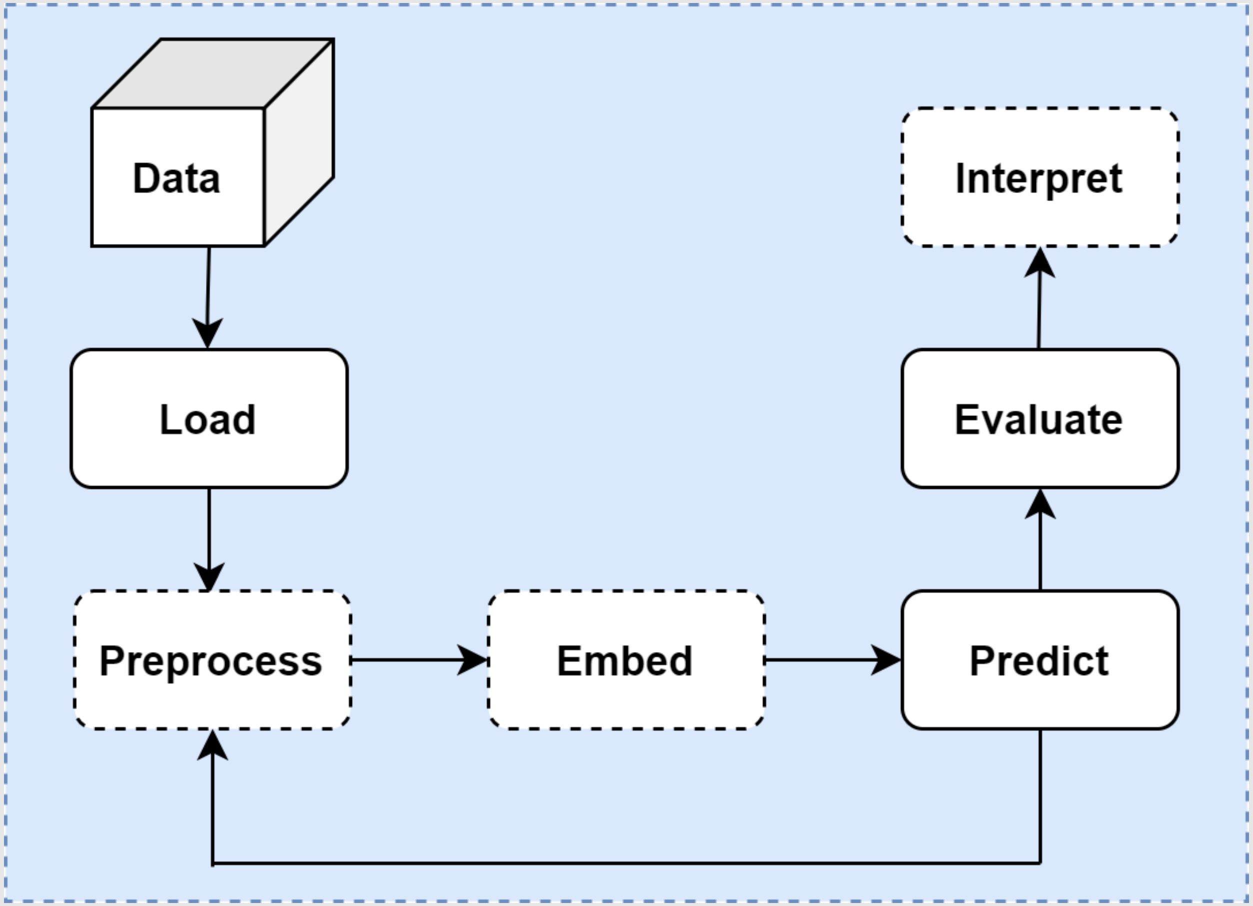
PEDRO DOMINGOS

THE MASTER ALGORITHM

HOW THE QUEST FOR THE ULTIMATE LEARNING MACHINE WILL REMAKE OUR WORLD

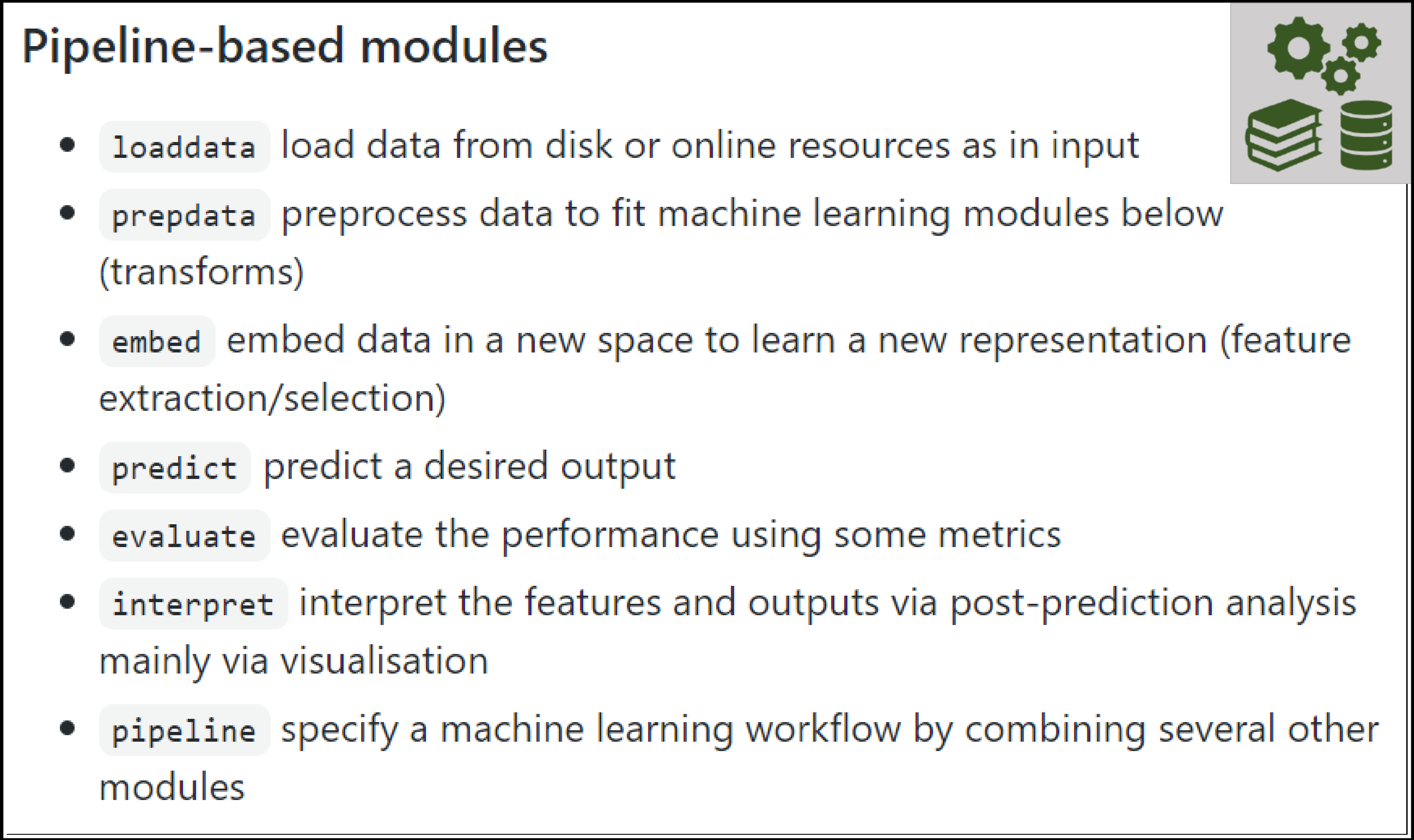
Learning algorithms are the seeds, data is the soil, and the learned programs are the grown plants. The machine-learning expert is like a farmer, sowing the seeds, irrigating and fertilizing the soil, and keeping an eye on the health of the crop but otherwise staying out of the way.

Machine Learning Pipeline



- Example: a library defined in this pipeline→PyKale

PyKale: https://github.com/pykale/pykale



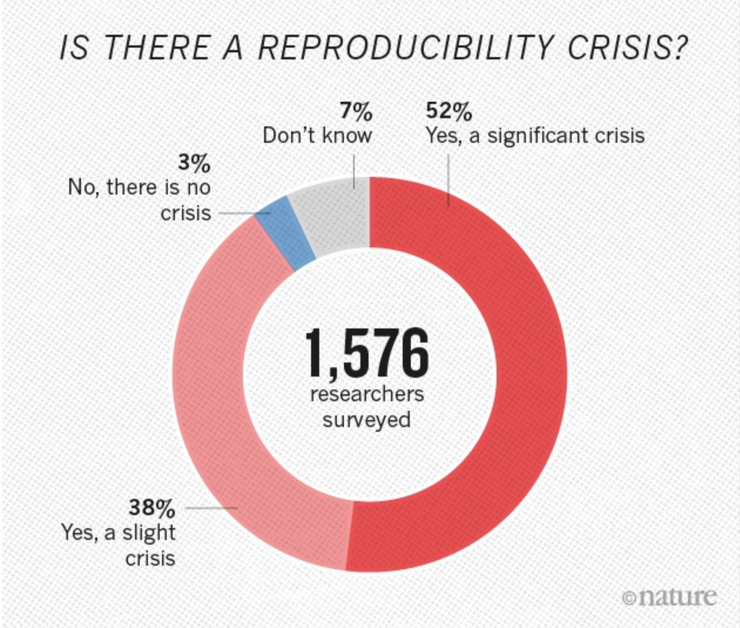
Pipeline-based modules

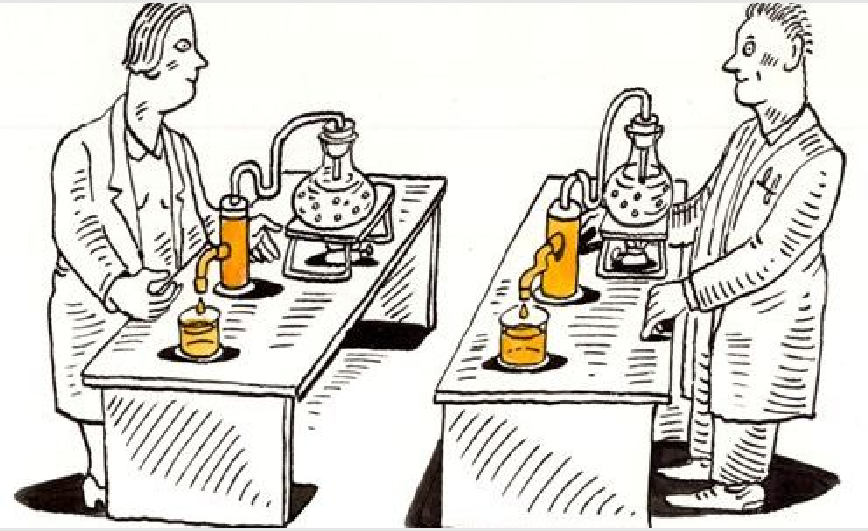
- `loaddata` load data from disk or online resources as in input
- `prepdata` preprocess data to fit machine learning modules below (transforms)
- `embed` embed data in a new space to learn a new representation (feature extraction/selection)
- `predict` predict a desired output
- `evaluate` evaluate the performance using some metrics
- `interpret` interpret the features and outputs via post-prediction analysis mainly via visualisation
- `pipeline` specify a machine learning workflow by combining several other modules

Machine Learning Ingredients

- **Data**: + pre-processing (& visualisation), e.g., $\mathcal{N}(0,1)$
- **Model**
  - Structure ~ Architecture ← expert knowledge
    - Must **specify** before ML, can optimise via cross validation (CV)
  - **Hyper-parameter**, e.g., prior, #degree, layer ← knowledge
    - Must **specify** (choices) and can optimise via CV (***tuning***)
  - Parameters (theta)
    - Compute/learn parameter, e.g., **weights**, bias ← optimisation alg.
- Evaluation metric (what's best): loss/error function
- Optimisation: (how to find the best) learnable parameters

Reproducibility → Trustworthy





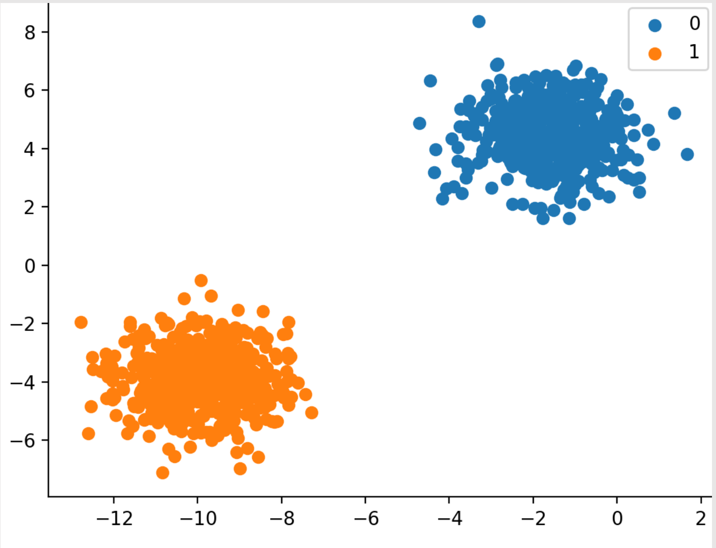
https://www.nature.com/news/1-500-scientists-lift-the-lid-on-reproducibility-1.19970

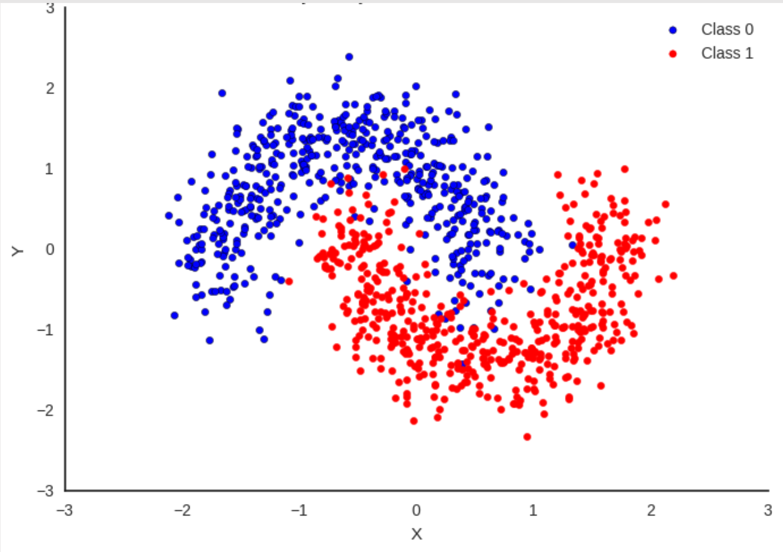
https://www.ucl.ac.uk/pals/research/experimental-psychology/wp-content/uploads/2016/03/reproducibility-small-496x300.jpg

- Reproducible machine learning
  - **Make it modular** to help understanding & tracing
  - **Keep a record** of all assumptions and settings
  - **Set a seed** when there is randomness

Start Simple & Small

- The simplest prediction task: binary classification
  - Input (to predict from): feature vectors
  - Output (to predict): 0 or 1
  - Difficulty determined by the distribution of the input





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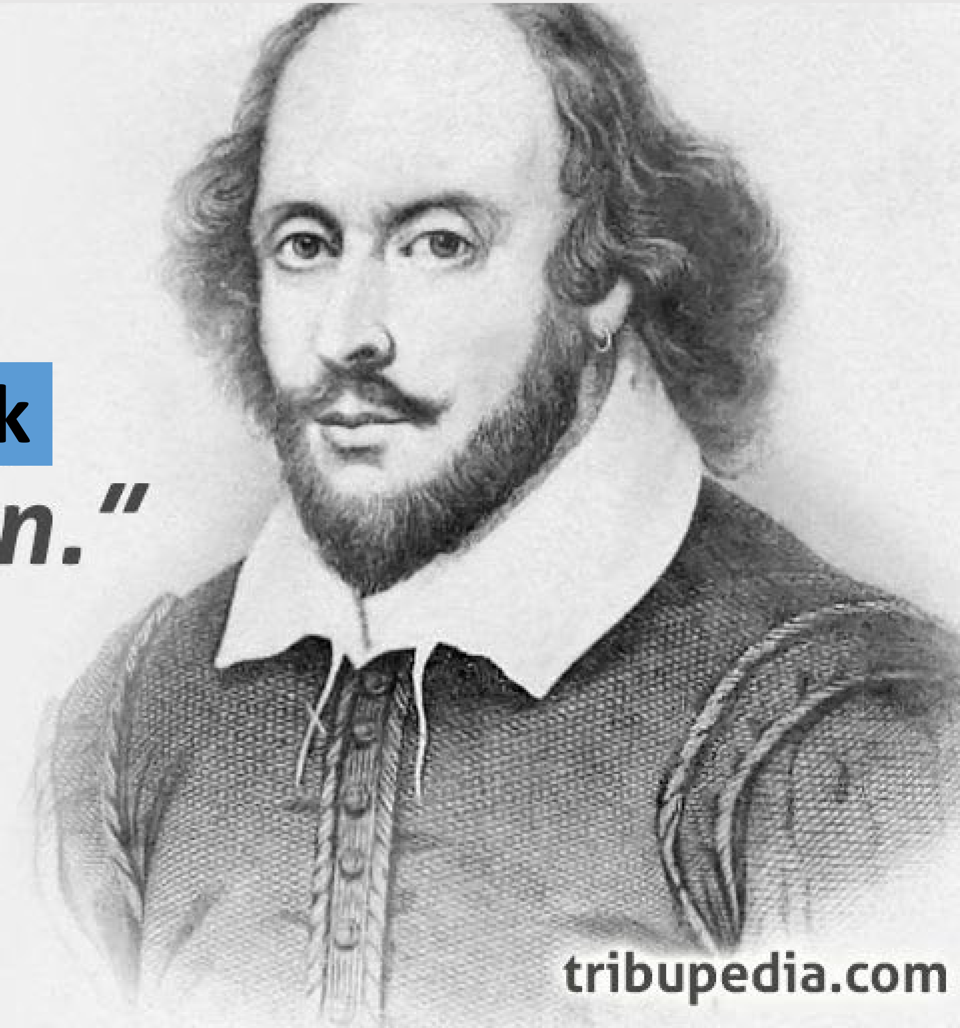
The Question

"To click or not to click that is the question."

William Shakespeare



Click-Through Rate (CTR) Prediction

- Estimating click probabilities: What is the probability that user *i* **will click** on ad *j*
  - Not important just for ads:
    - Optimize search results
    - Suggest news articles
    - Recommend products
- Logistic regression is used by many internet companies, making lots of money for them
  - E.g., Facebook ad matching

A Binary Classification Problem

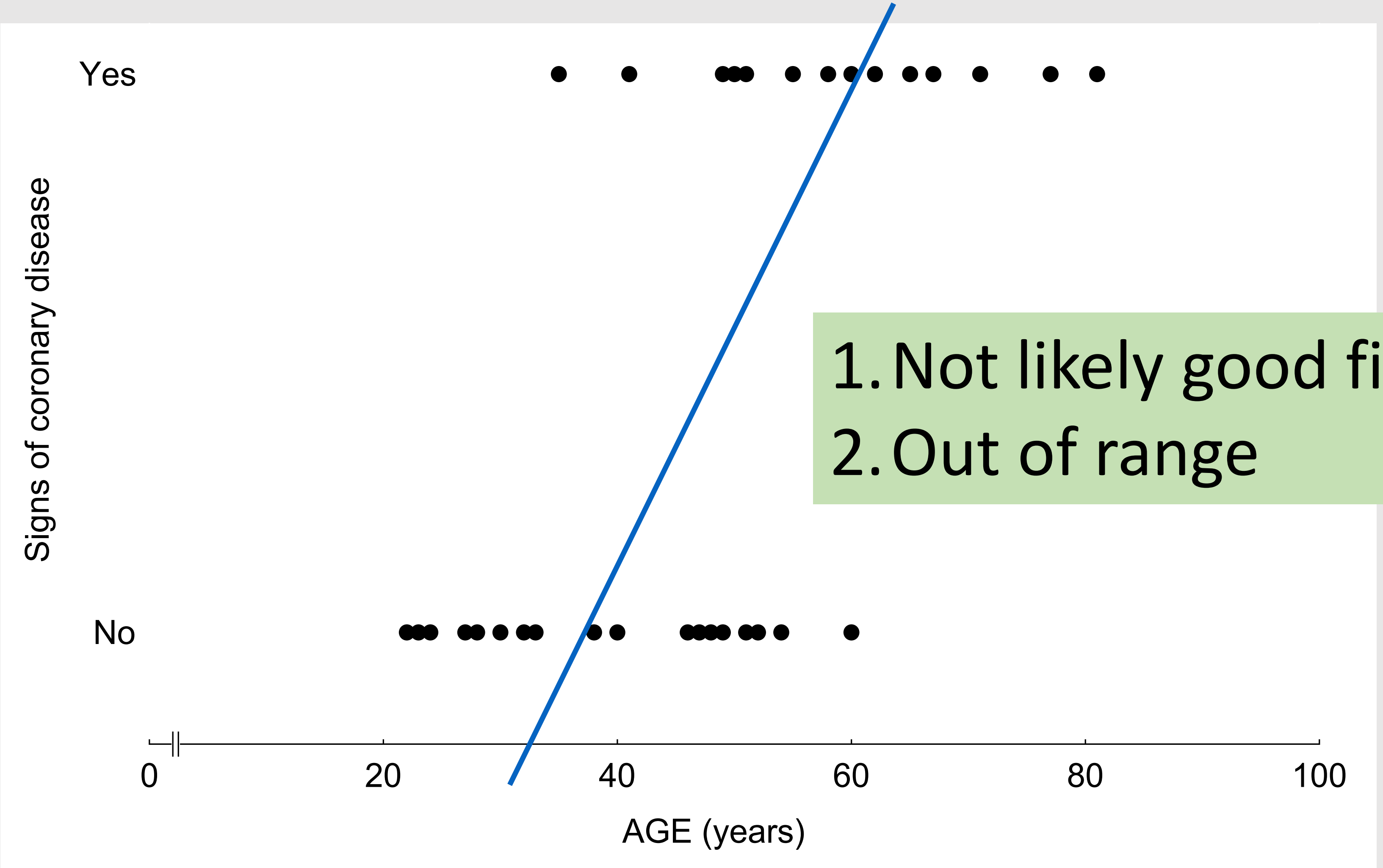
Table 1: Age and signs of coronary heart disease (CD)

Age	CD
22	0
23	0
24	0
27	0
28	0
30	0
30	0
32	0
33	0
35	1
38	0
40	0
41	1
46	0
47	0
48	0
49	1
49	0
50	1
51	0
51	1
52	0
54	0
55	1
58	1
60	1
60	0
62	1
65	1
67	1
71	1
77	1
81	1

Prediction question: a particular age → CD

Linear regression?

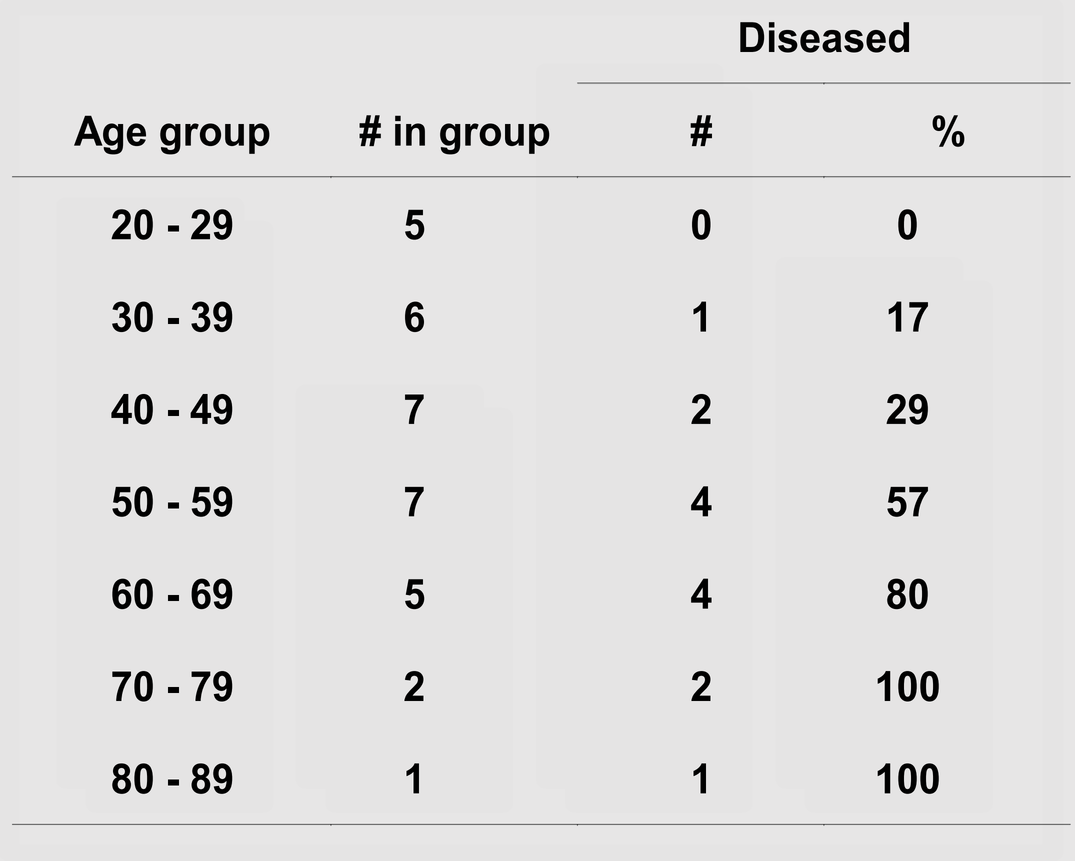
Dot-plot: Data from Table 1



1. Not likely good fit
2. Out of range

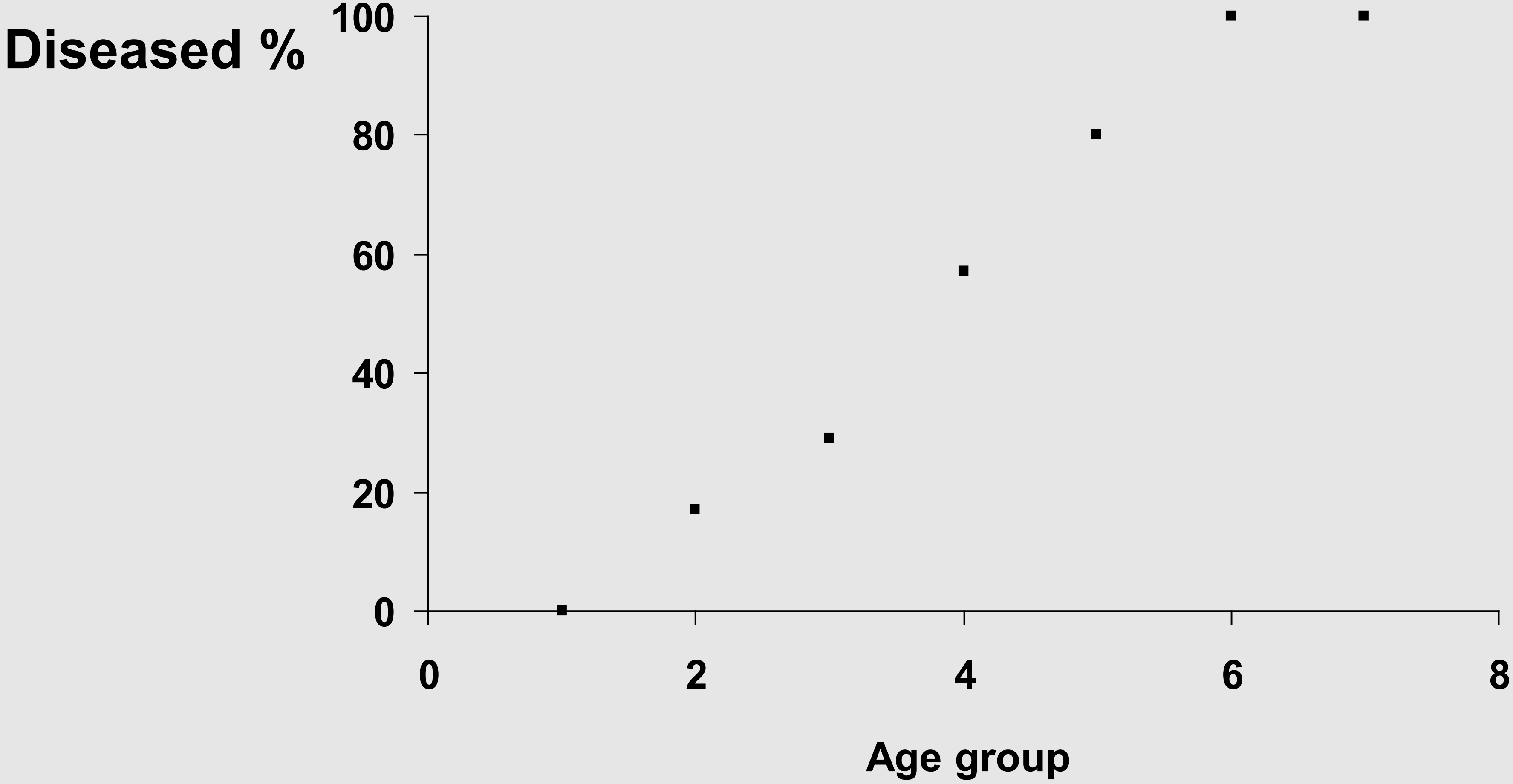
Transform the Data→ Probability

Table 2 Prevalence (%) of signs of CD according to age group

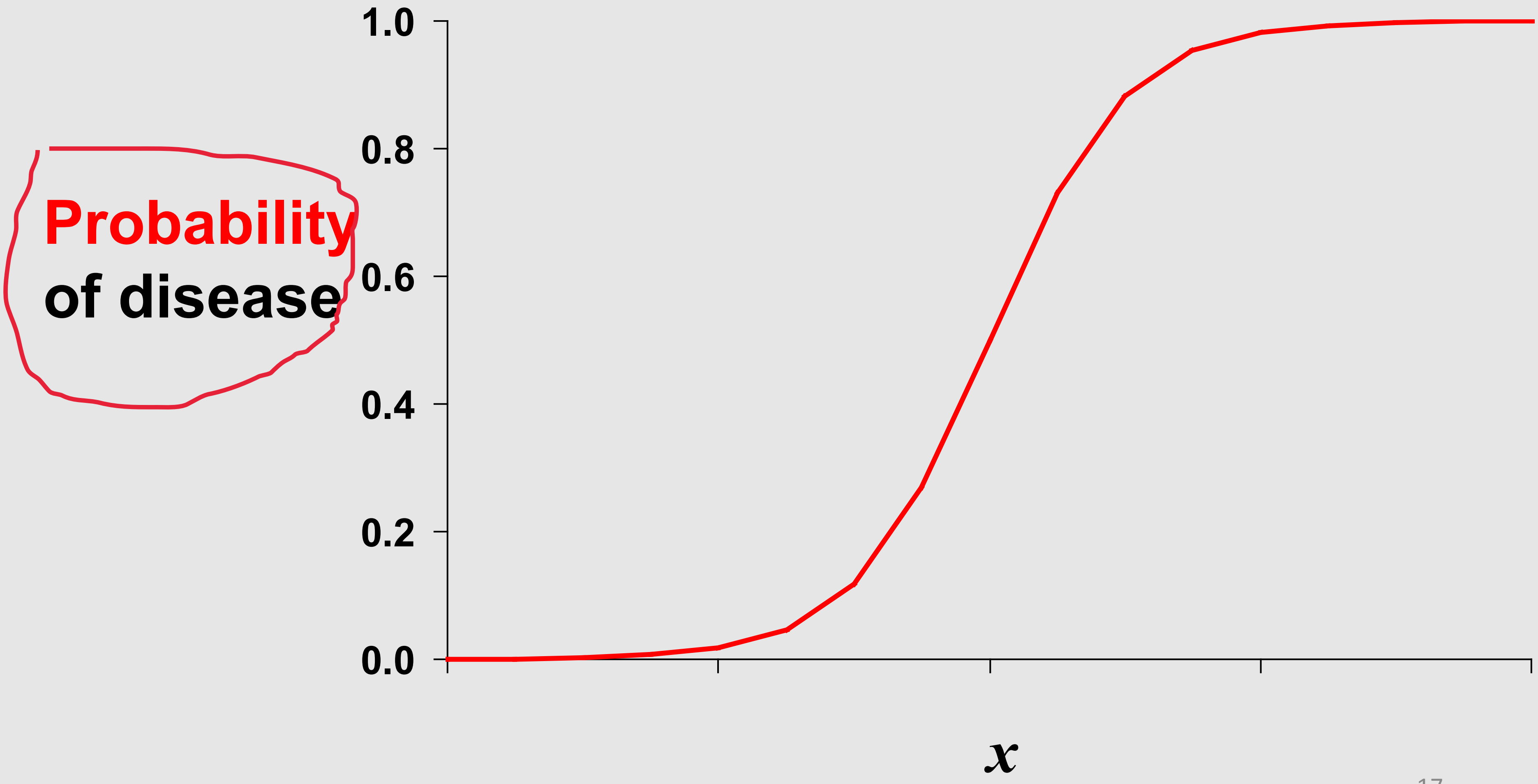


		Diseased	
Age group	# in group	#	%
20 - 29	5	0	0
30 - 39	6	1	17
40 - 49	7	2	29
50 - 59	7	4	57
60 - 69	5	4	80
70 - 79	2	2	100
80 - 89	1	1	100

Dot-plot: Data from Table 2



Logistic Function



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Probabilistic Classification

- Training classifiers: estimating f: X → Y, or P(Y|X)
- **Discriminative** classifiers
  - Assume some functional form for P(Y|X)
  - Estimate parameters of P(Y|X) directly from training data
- **Generative** classifiers
  - Assume some functional form for P(X|Y), P(X)
  - Estimate parameters of P(X|Y), P(X) directly from training data
  - Use Bayes rule to calculate $P(Y|X= x_i)$

Log Odds

- **Odds**: the ratio of π, the probability of a positive outcome *P*(*y=1*|**x**), to *(1- π)*, the probability of a negative outcome *P*(*y=0*|**x**).

$$\frac{\pi}{1-\pi}$$

- Probability: [0, 1]

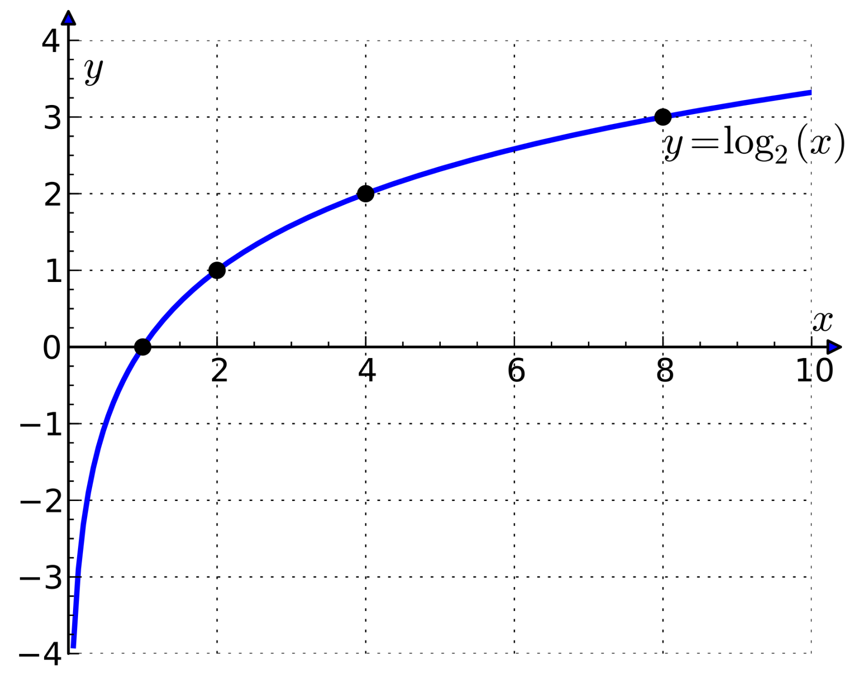
- → Odds: [0, ∞]

x

- → Log odds (**logit**): **[-∞, ∞]**

$$\text{logit}(\pi) = \log \frac{\pi}{1-\pi}$$

y



Logit Function→ Logistic Function

- Linear **regression** on **logit** function = logistic *regression*

$$\mathrm{logit}(\pi) = \log \frac{\pi}{1-\pi} = \mathbf{w}^\top \mathbf{x} = w_0 + w_1 x_1 + \cdots$$

- More generally, we can use **basis function** as

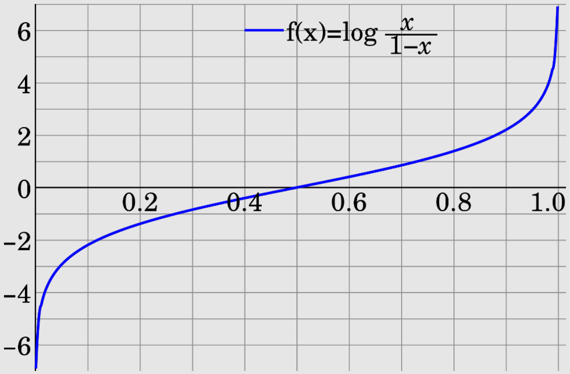
$$\mathrm{logit}(\pi) = \log \frac{\pi}{1-\pi} = \mathbf{w}^\top \phi(\mathbf{x}) = w_0 + w_1 \phi(x_1) + \cdots$$

  In the following, we use the simpler first form above

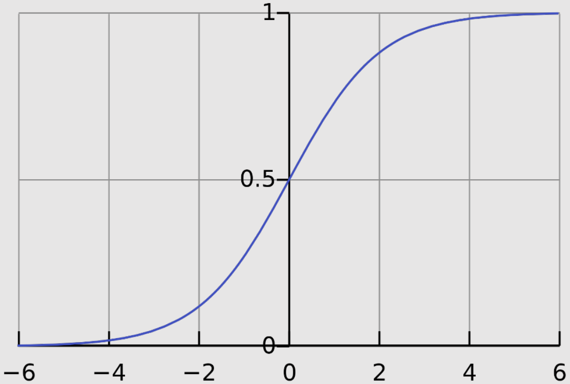
- Logistic function (**sigmoid**)= inverse of logit

$$P(y=1|\mathbf{x}) = \mathrm{logit}^{-1}(\mathbf{w}^\top \mathbf{x}) = \mathrm{logistic}(\mathbf{w}^\top \mathbf{x}) = \frac{1}{1+e^{-\mathbf{w}^\top \mathbf{x}}}$$

- **Exercise**: verify the odds using the above equation



→



How to Estimate **w**? (Learning algo)

- Assumption: Conditional independence of data
- →Likelihood:

$$P(\mathbf{y}|\mathbf{X}) = \prod_{i=1}^{n} P(y_i|\mathbf{x}_i)$$

- **Bernoulli distribution** for binary classification
  - *P(y=1) = π ; P(y=0) =1 – π* (coin flipping)
  - Write the above as a single equation: using *y* as a switch

$$P(y) = \pi^y (1-\pi)^{(1-y)} \qquad \pi_i = P(y_i = 1|\mathbf{x}_i)$$

- Log likelihood (negative log likelihood → *cross entropy*)

$$\log P(\mathbf{y}|\mathbf{X}) = \sum_{i=1}^{n} \log P(y_i|\mathbf{x}_i) = \sum_{i=1}^{n} y_i \log \pi_i + \sum_{i=1}^{n} (1-y_i) \log(1-\pi_i)$$

- MLE: no closed form solution

→ SGD on negative log likelihood (minimisation)

Machine Learning Ingredients

- **Data**: + pre-processing (& visualisation), e.g., $\mathcal{N}(0,1)$
- **Model**
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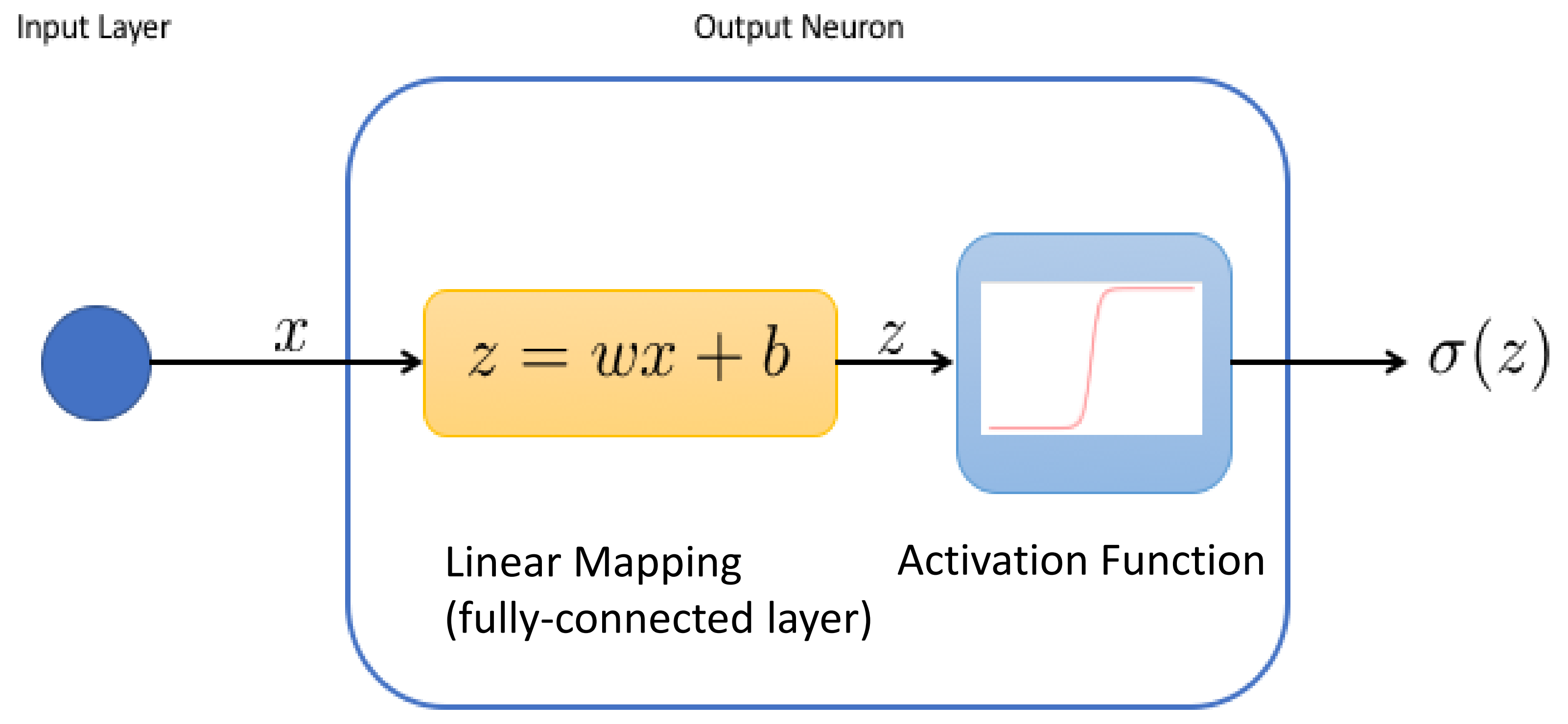
    - Parameters (theta)
        - Compute/learn parameter, e.g., **weights**, bias ← optimisation alg.
- Evaluation metric (what's best): loss/error function
- Optimisation: (how to find the best) learnable parameters

Logistic Regression Ingredients

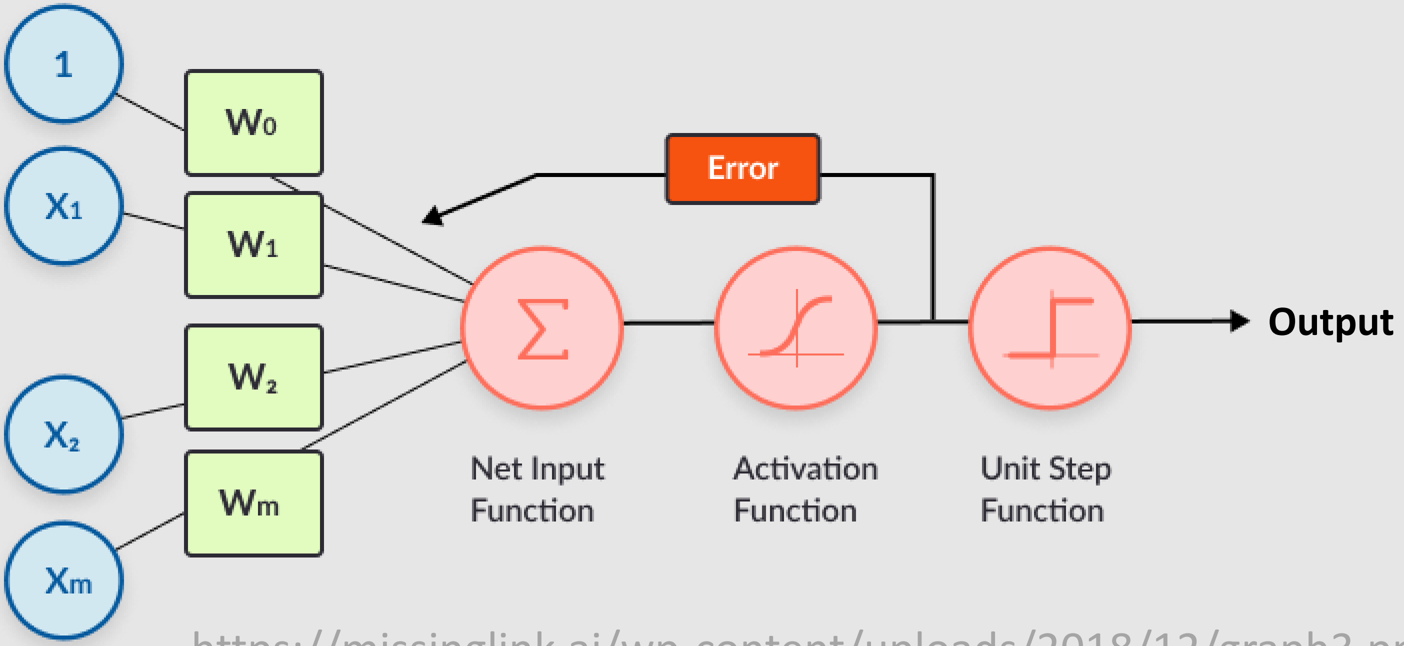
- **Data**: + pre-processing, e.g., $\mathcal{N}(0,1)$
- **Model**
  - Structure/Architecture: linear relationship

$$P(y=1|\mathbf{x}) = \frac{1}{1+e^{-\mathbf{w}^\top \mathbf{x}}}$$

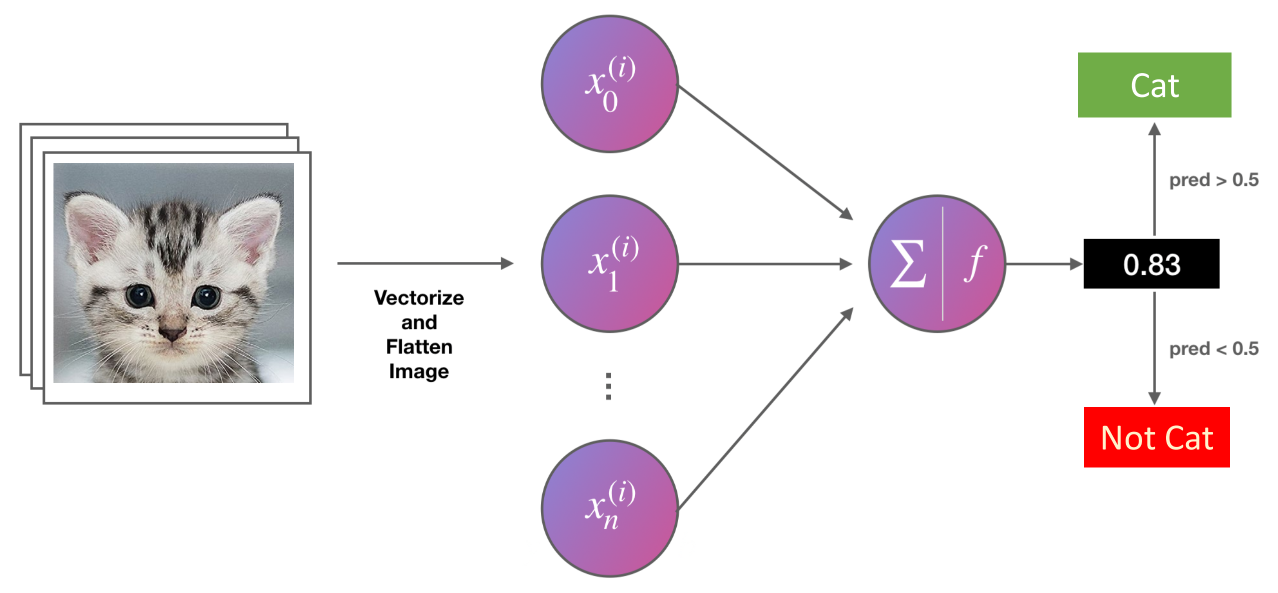
  - **Hyper-parameter**: no (unless + regularisation)
  - Parameters (theta): weights and bias
- Evaluation metric: max likelihood (min NLL)
- Optimisation: SGD or the like



Logistic Regression – The Simplest Neural Network



https://missinglink.ai/wp-content/uploads/2018/12/graph3.png



https://miro.medium.com/max/4112/1*5NV4NEtgR4rDpSVZkWh3oA.png

Multiclass Classification

- A simple way: one-vs-rest logistic regression
  - Run binary classification for all possible classes
  - Pick the one with the highest value
- More mathematical: multinomial logistic regression, also known as **softmax**
  - Generalise logistic regression to multiple classes
    - Binomial → multinomial distribution
    - Sigmoid function → softmax function
  - A linear classifier for multiple classes

Summary on Logistic Regression (LR)

- **Discriminative** classifiers directly model the likelihood *P(Y|X)*
- A simple **linear** classifier that retains a **probabilistic** semantics (see lab)
- Parameters in LR are learned by **iterative** optimization (e.g. SGD), no closed-form solution
- The simplest neural network

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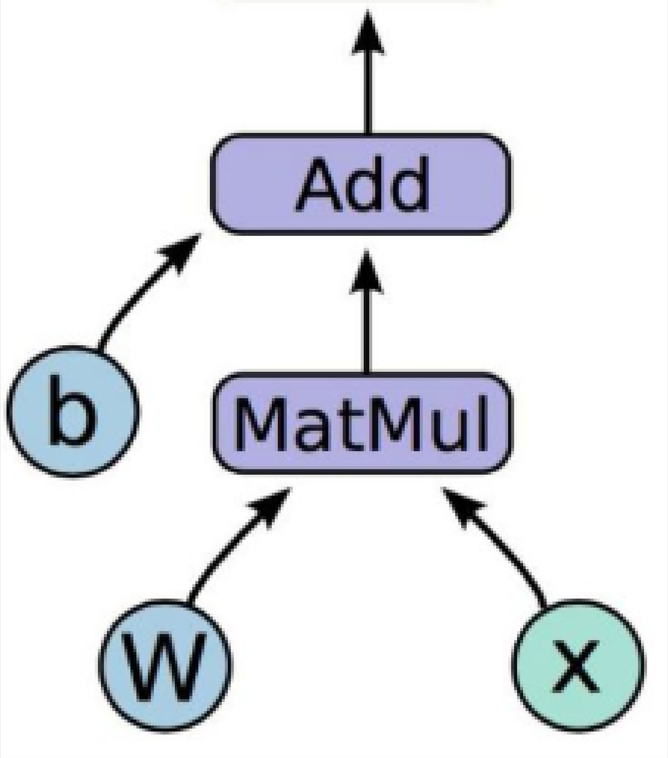
Computational Graph

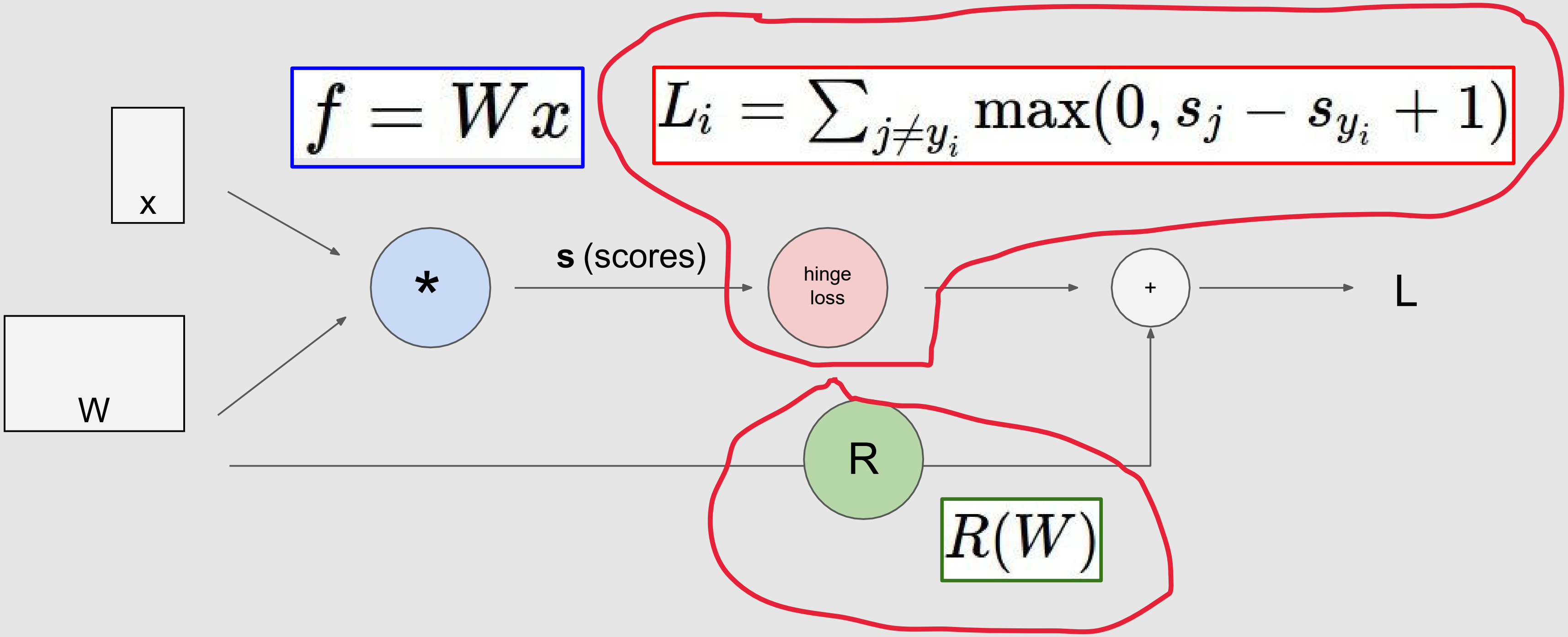
- Linear regression **y = Wx + b**



Source: Nelson Liu: https://colab.research.google.com/drive/11iLtGFDpnIuHj5B0rQDGG5lqq6BQ8FRh

Computational Graph: w/t Reg.

SVM

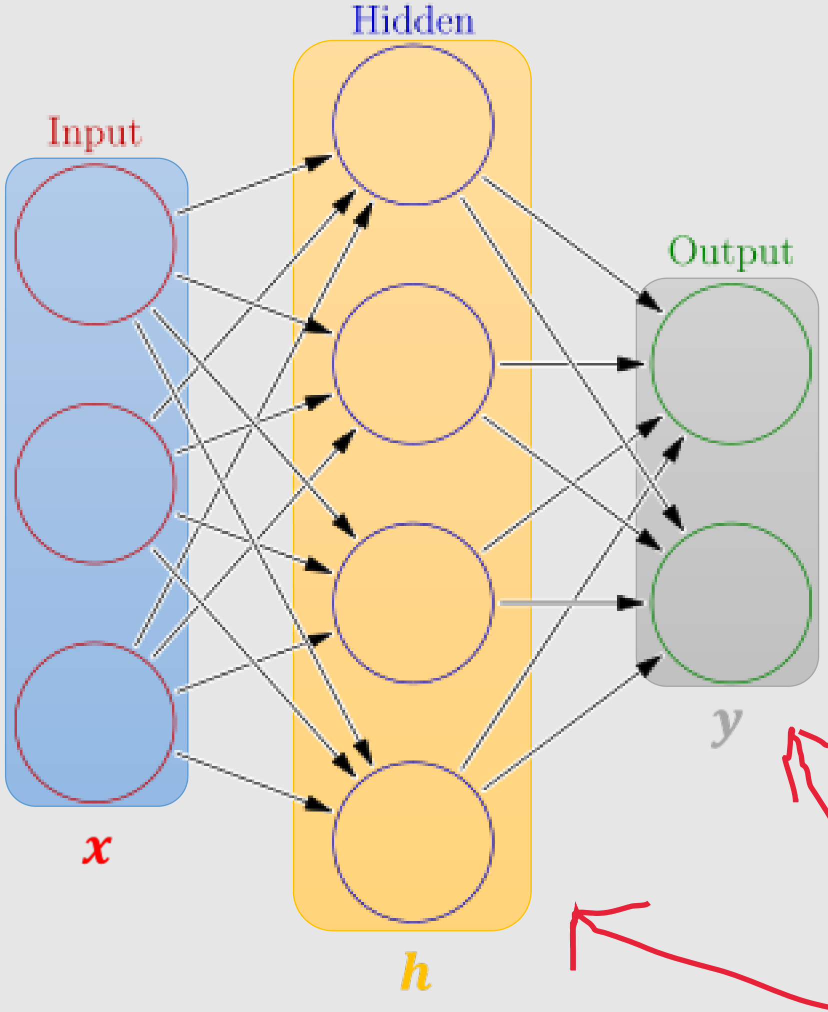


$$f = Wx$$

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

$$R(W)$$

Multilayer Perceptron (NN) vs LR



Weights

$$h = \sigma(W_1 x + b_1)$$

$$y = \sigma(W_2 h + b_2)$$

Activation functions

Question:
How many model parameters?

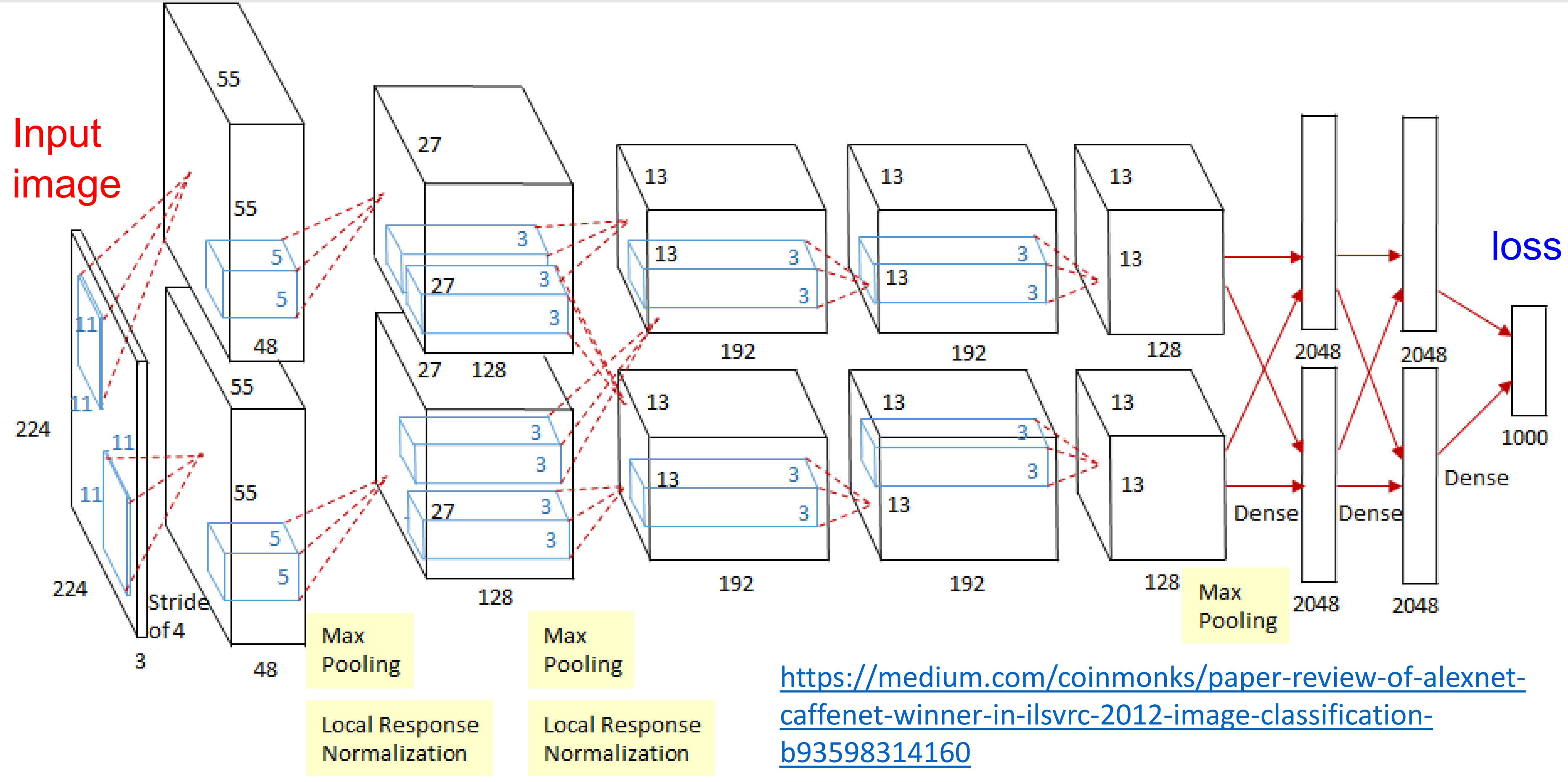
[3 x 4] + [4 x 2] = 20 weights
4 + 2 = 6 biases
26 learnable **parameters**

4 + 2 = 6 neurons (not counting inputs)

Source: https://miro.medium.com/max/570/0*y8AuUHSoTGRqX40h.jpeg

Computational Graph: DL

Weights (60 million parameters)



https://medium.com/coinmonks/paper-review-of-alexnet-caffenet-winner-in-ilsvrc-2012-image-classification-b93598314160

ImageNet I 010 (

Dataset: 1.2 million **1000 cla**
CNN for Image Clas evsky, S
Hinton, 2011) → 17.5% error

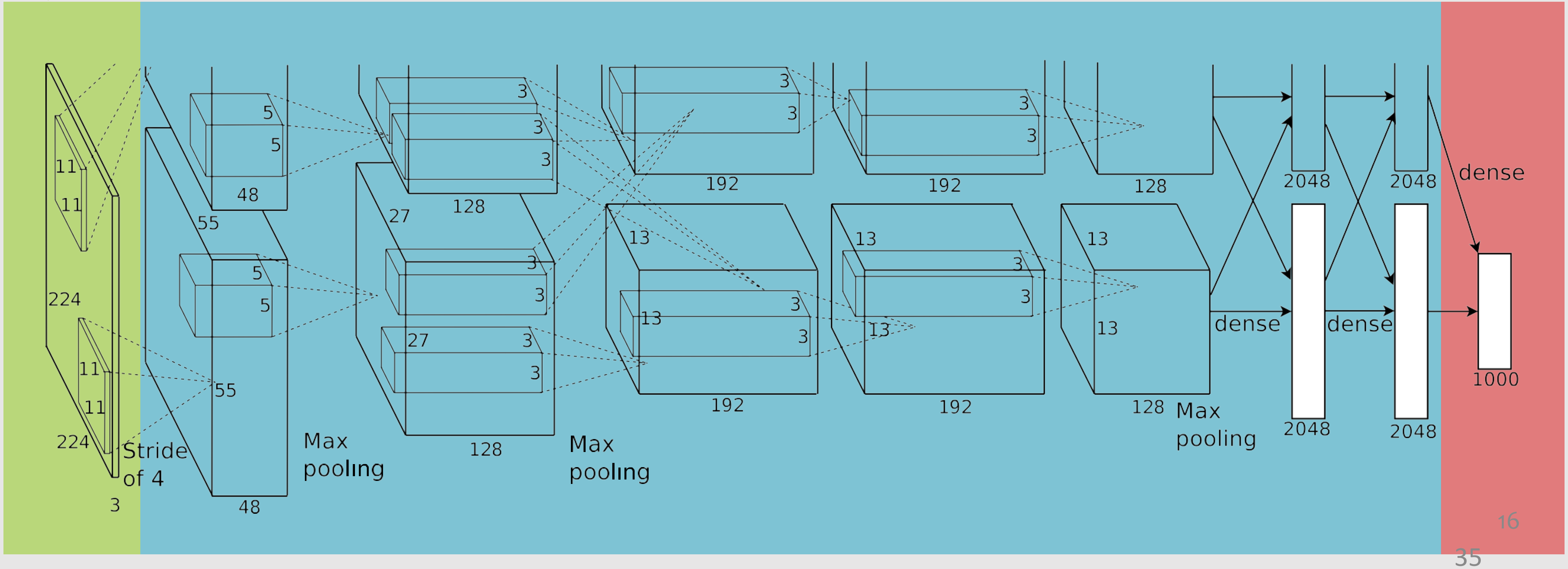
Fancy feature extraction **/representation learning**

Logistic Regression!
Softmax: sigmoid for multiclass

Input image (pixels)

- Five convolutional layers (w/max-pooling)
- Three fully connected layers

1000-way softmax



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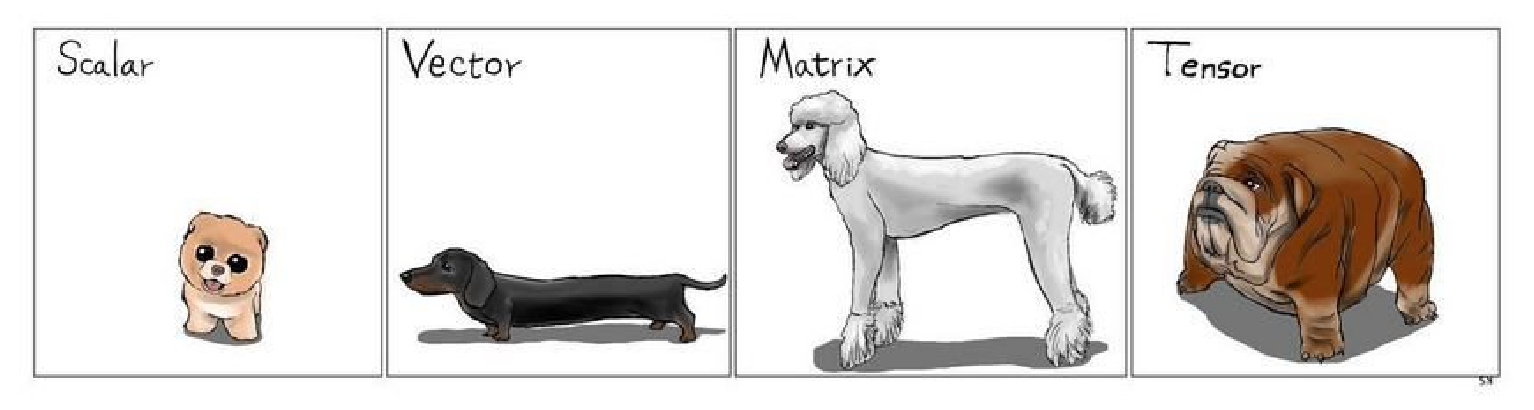
PyTorch

- An open source deep learning library by Facebook
  - **Tensor** computing with GPU acceleration
  - Deep neural networks built on autodiff
- **torch.Tensor**
  - multidimensional data structures/arrays for programming
  - Scalar: 0-D tensor; Vector: 1-D tensor; Matrix: 2-D tensor

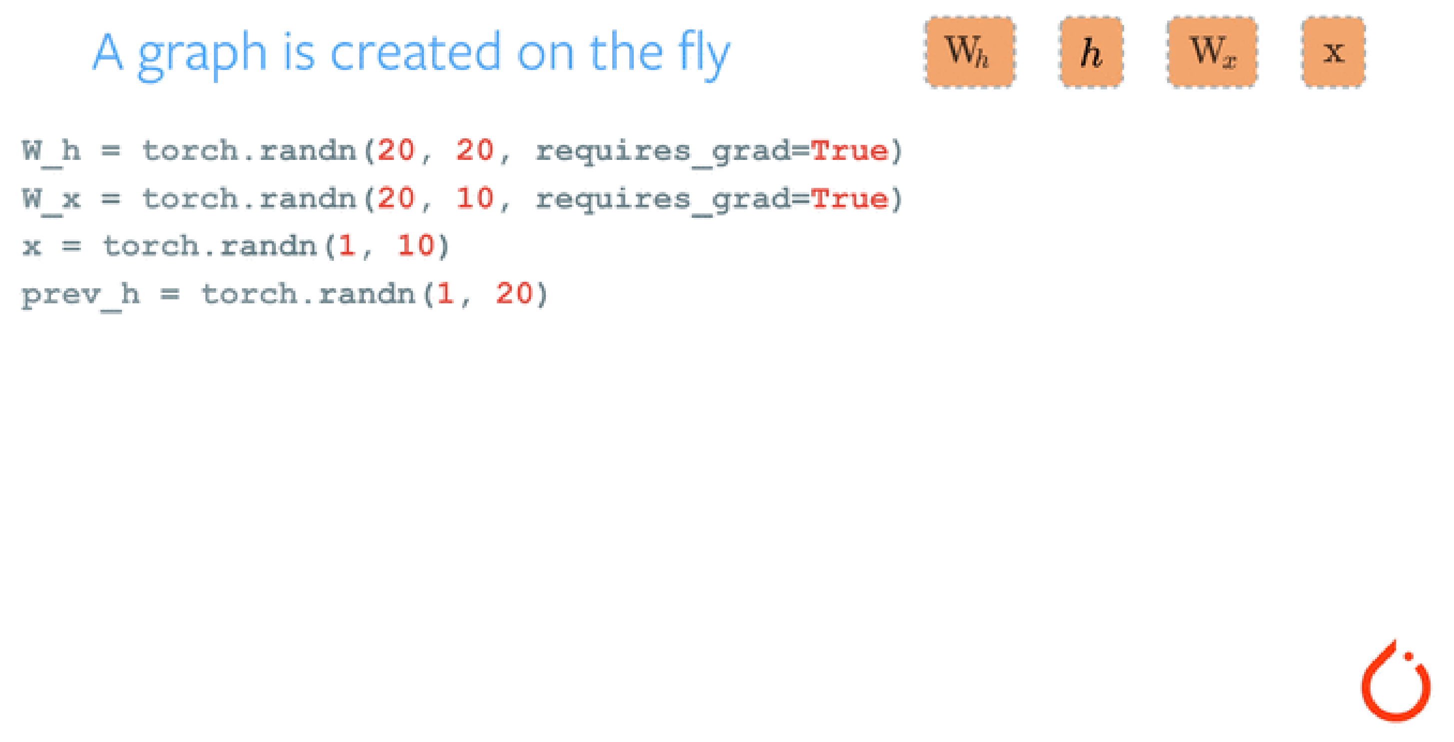


https://pbs.twimg.com/media/D2xTDMJWwAADHQt.jpg

Key Modules in PyTorch

- **torch.autograd**
  - Automatic differentiation. A recorder records what operations have performed, and then it replays it backward to compute the gradients.
- **torch.optim**
  - Implementation of various optimization algorithms used for building neural networks (and other ML algorithms).
- **torch.nn**
  - High-level definition of the **computational graphs (architecture)** of complex neural networks (and other ML algorithms)

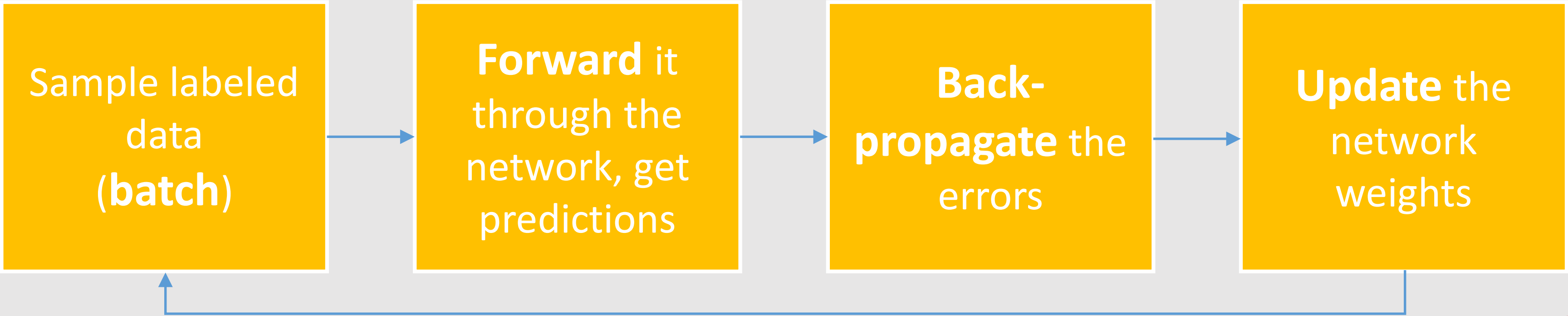
Dynamic Computational Graph



A graph is created on the fly

```
W_h = torch.randn(20, 20, requires_grad=True)
W_x = torch.randn(20, 10, requires_grad=True)
x = torch.randn(1, 10)
prev_h = torch.randn(1, 20)
```

Training



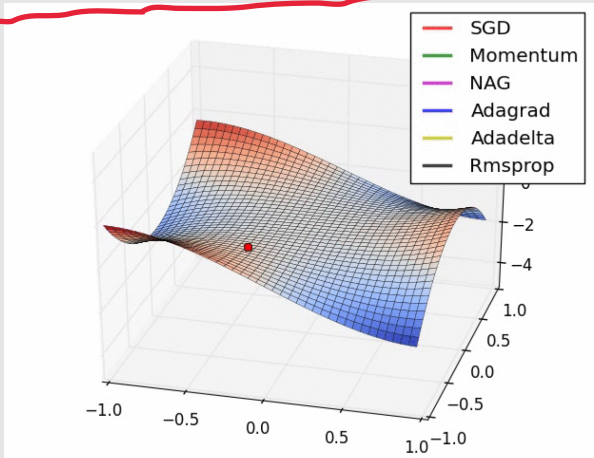
Sample labeled data (**batch**)

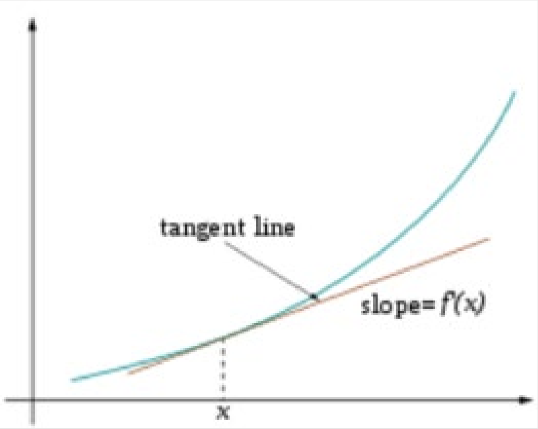
Forward it through the network, get predictions

Back-propagate the errors

Update the network weights

Optimize (min. or max.) **objective/cost function $J(\theta)$**
Generate **error signal** that measures difference between predictions and target values





Use error signal to change the **weights** and get more accurate predictions
Subtracting a fraction of the **gradient** moves you towards the **(local) minimum of the cost function**

https://medium.com/@ramrajchandradevan/the-evolution-of-gradient-descend-optimization-algorithm-4106a6702d39

Acknowledgement

- The slides used materials from: *Colin Bernet, Ismini Lourentzou, Fei-Fei Li & Justin Johnson & Serena Yeung, Rui Zhang, Nelson Liu, Matt Gormley, Rachid Salmi, Jean-Claude Desenclos, Thomas Grein, Alain Moren, Christophe Giraud-Carrier, Bart Selman, Sham Kakade, Raymond J. Mooney, Neil Lawrence, and Andrew Ng*

Recommended Reading

- Notes Logistic Regression by Andrew Ng
- Wikipedia entries on topics, e.g. multiclass classification, softmax, multinomial logistic regression,
- PyTorch documentations
- The lab notebook and references

Next

Lab notebooks

Feedback (if any)

@end of the week