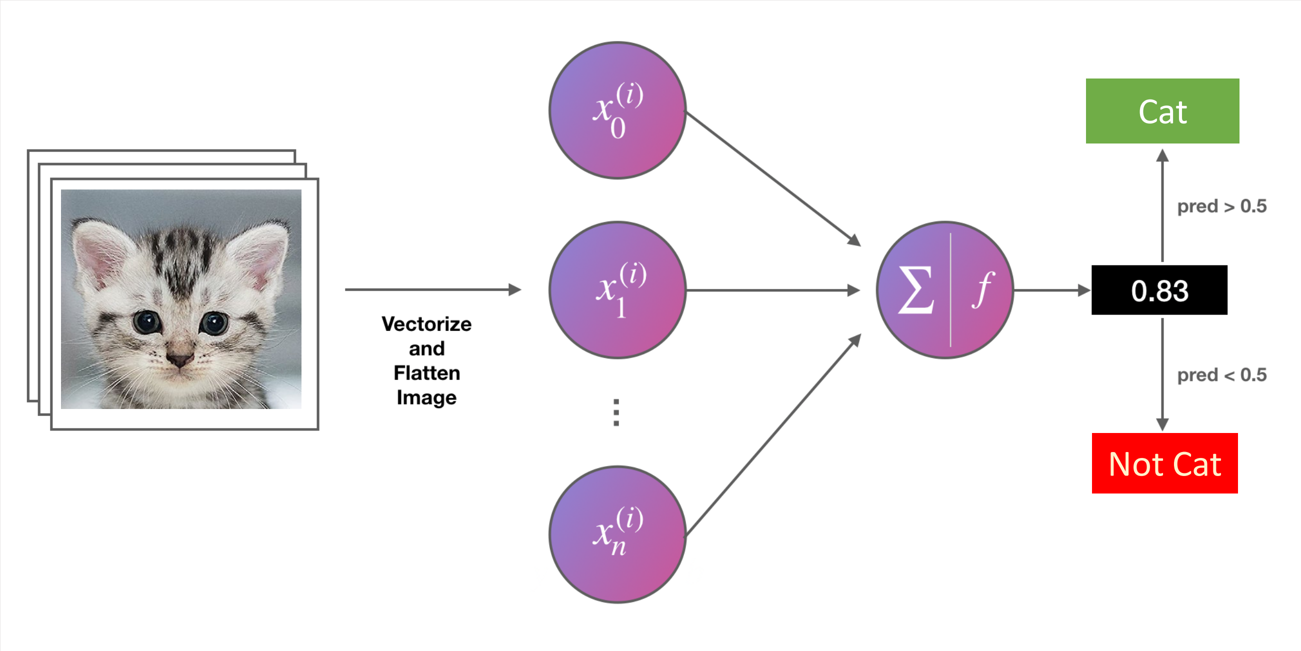
Lecture 6: Logistic Regression & PyTorch for Deep Learning



[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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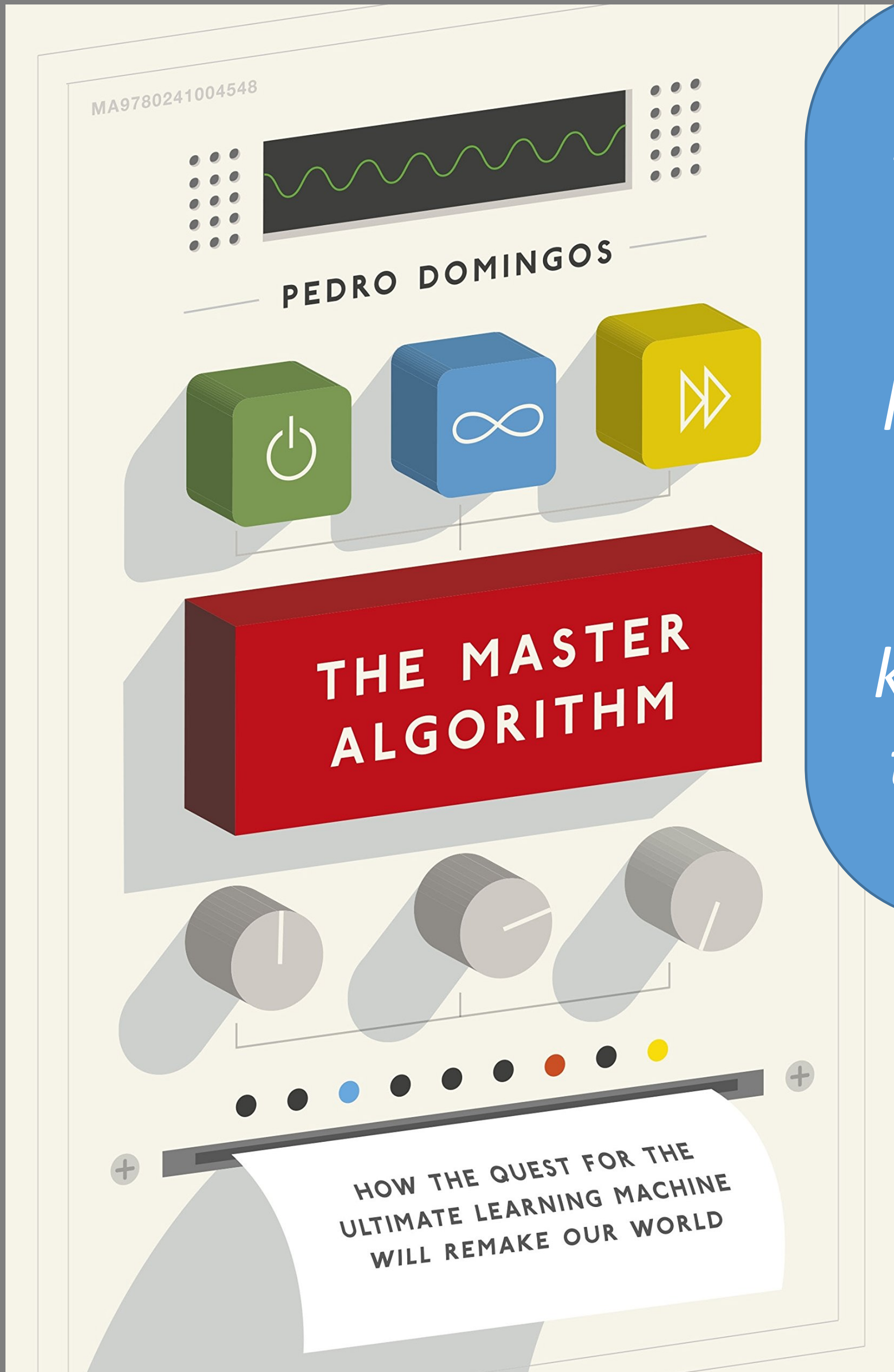
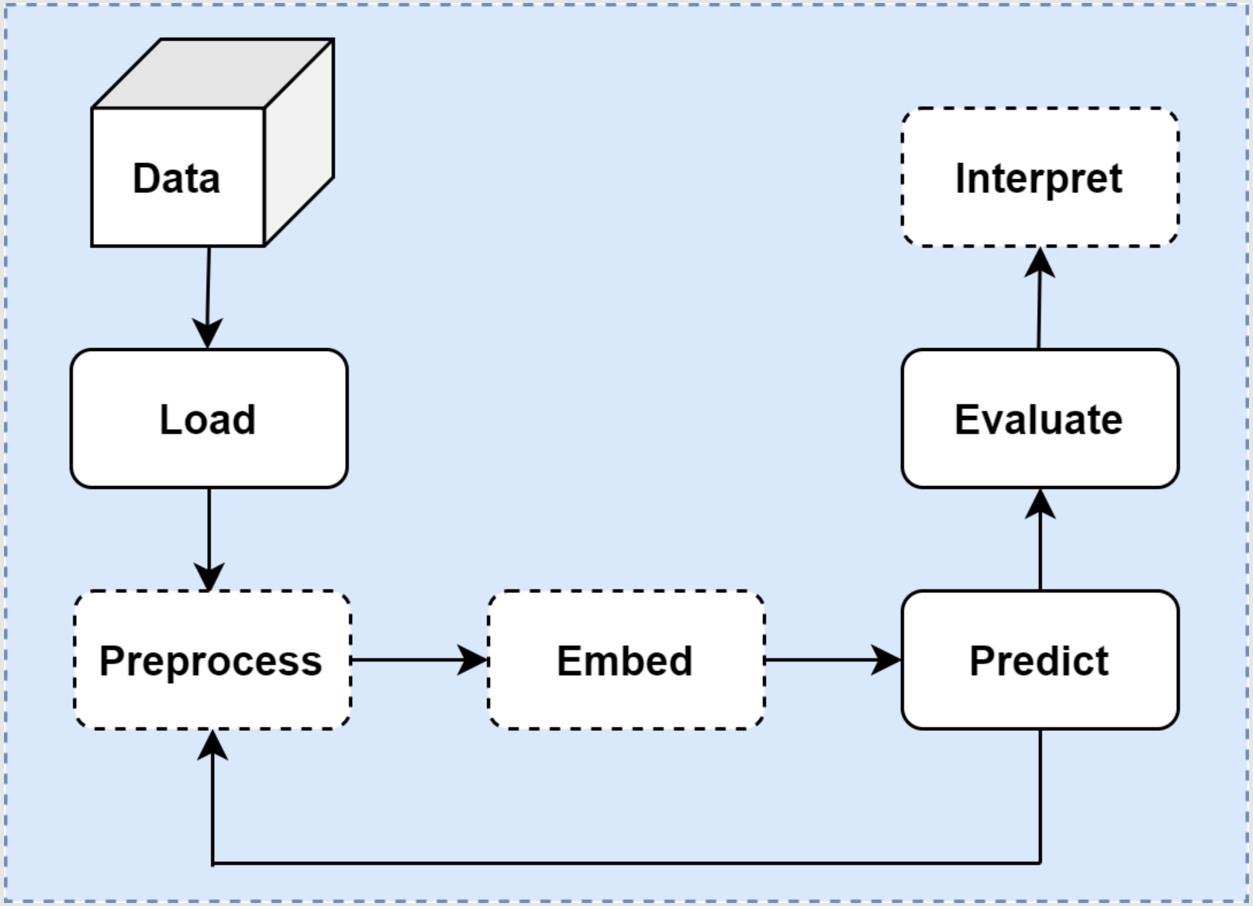


Learning algorithms are the seeds, data is the soil, and the learned programs are the grown plants. The machine-learning expert is like a farmer, sowing the seeds, irrigating and fertilizing the soil, and keeping an eye on the health of the crop but otherwise staying out of the way.

Machine Learning Pipeline



- Example: a library defined in this pipeline→PyKale

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

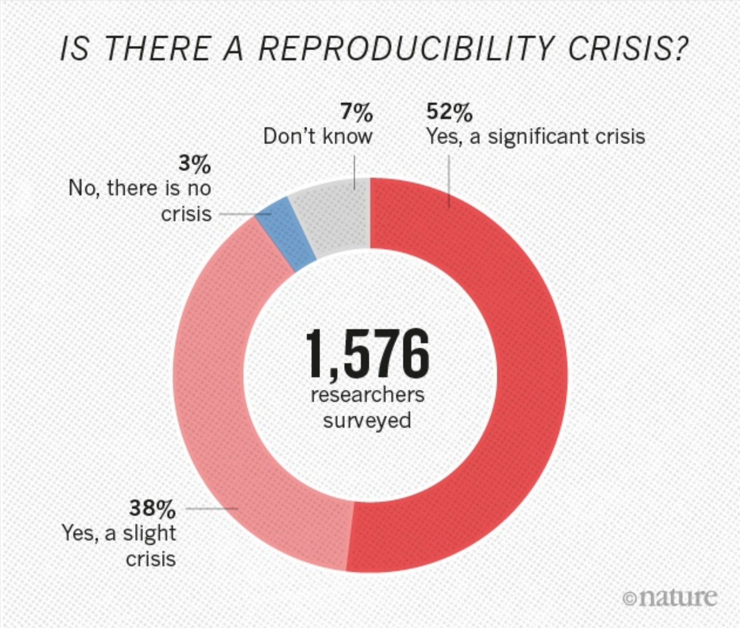
Pipeline-based modules

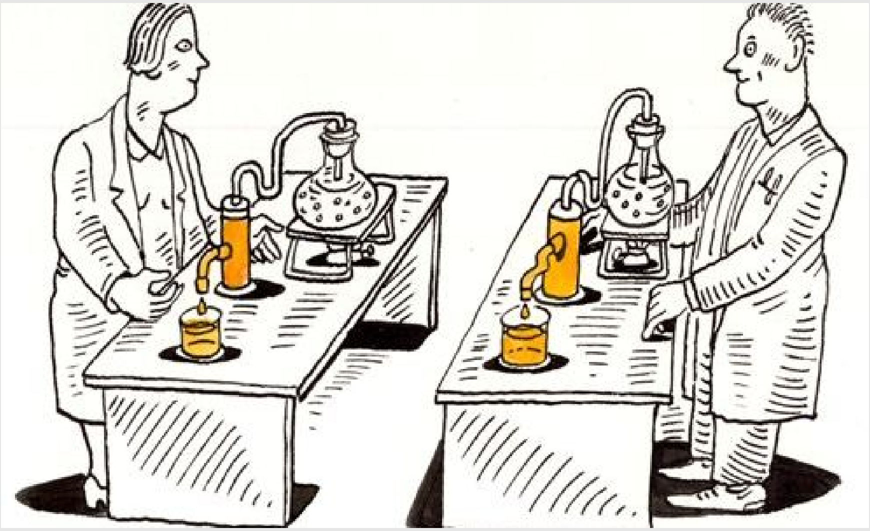
- `loaddata` load data from disk or online resources as in input
- `prepdata` preprocess data to fit machine learning modules below (transforms)
- `embed` embed data in a new space to learn a new representation (feature extraction/selection)
- `predict` predict a desired output
- `evaluate` evaluate 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





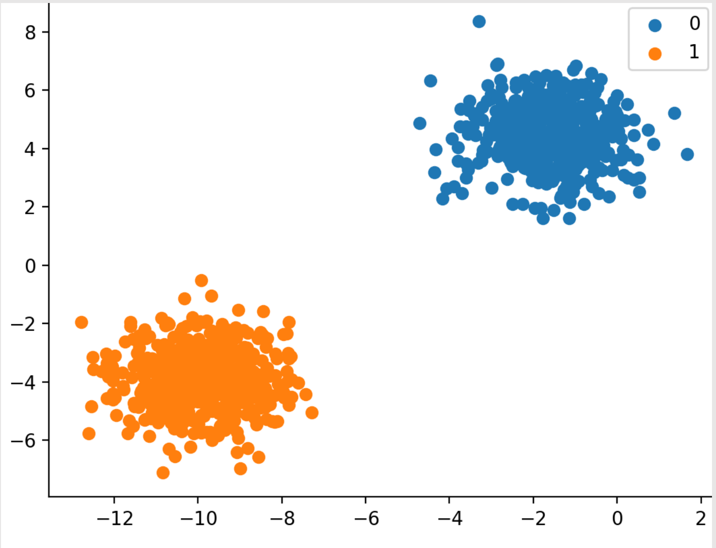
https://www.nature.com/news/1-500-scientists-lift-the-lid-on-reproducibility-1.19970

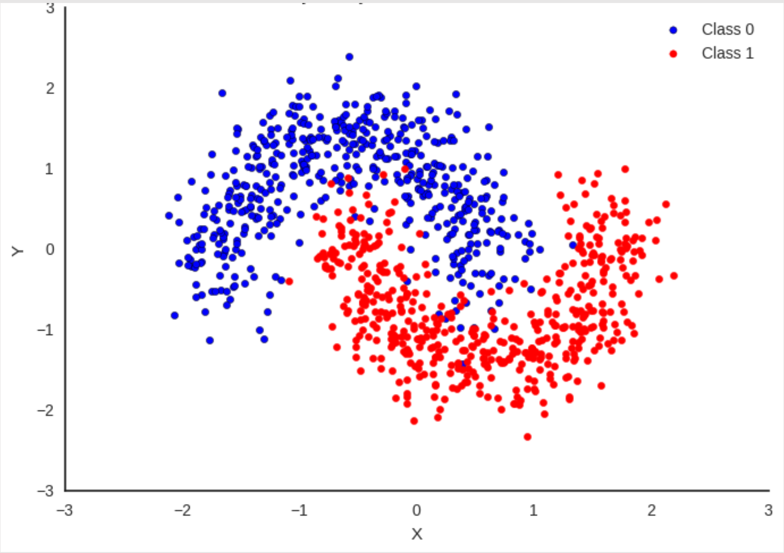
https://www.ucl.ac.uk/pals/research/experimental-psychology/wp-content/uploads/2016/03/reproducibility-small-496x300.jpg

- 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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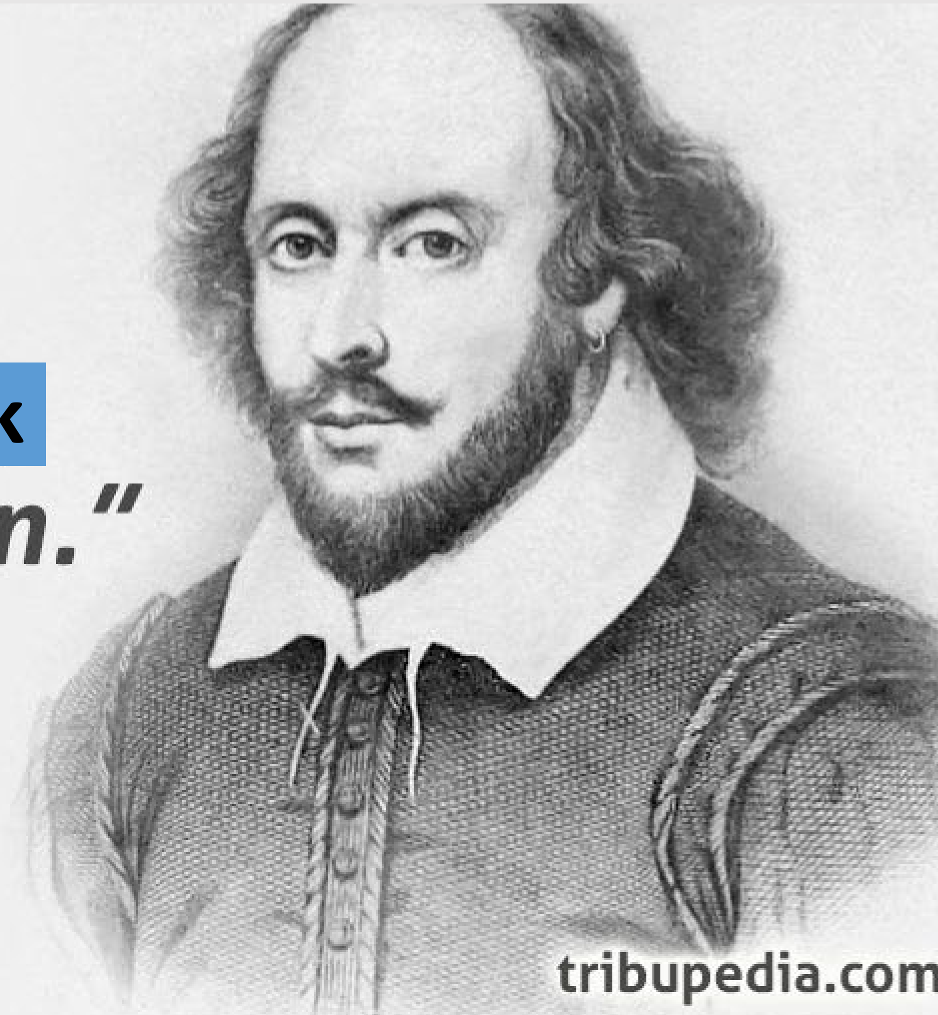
The Question



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

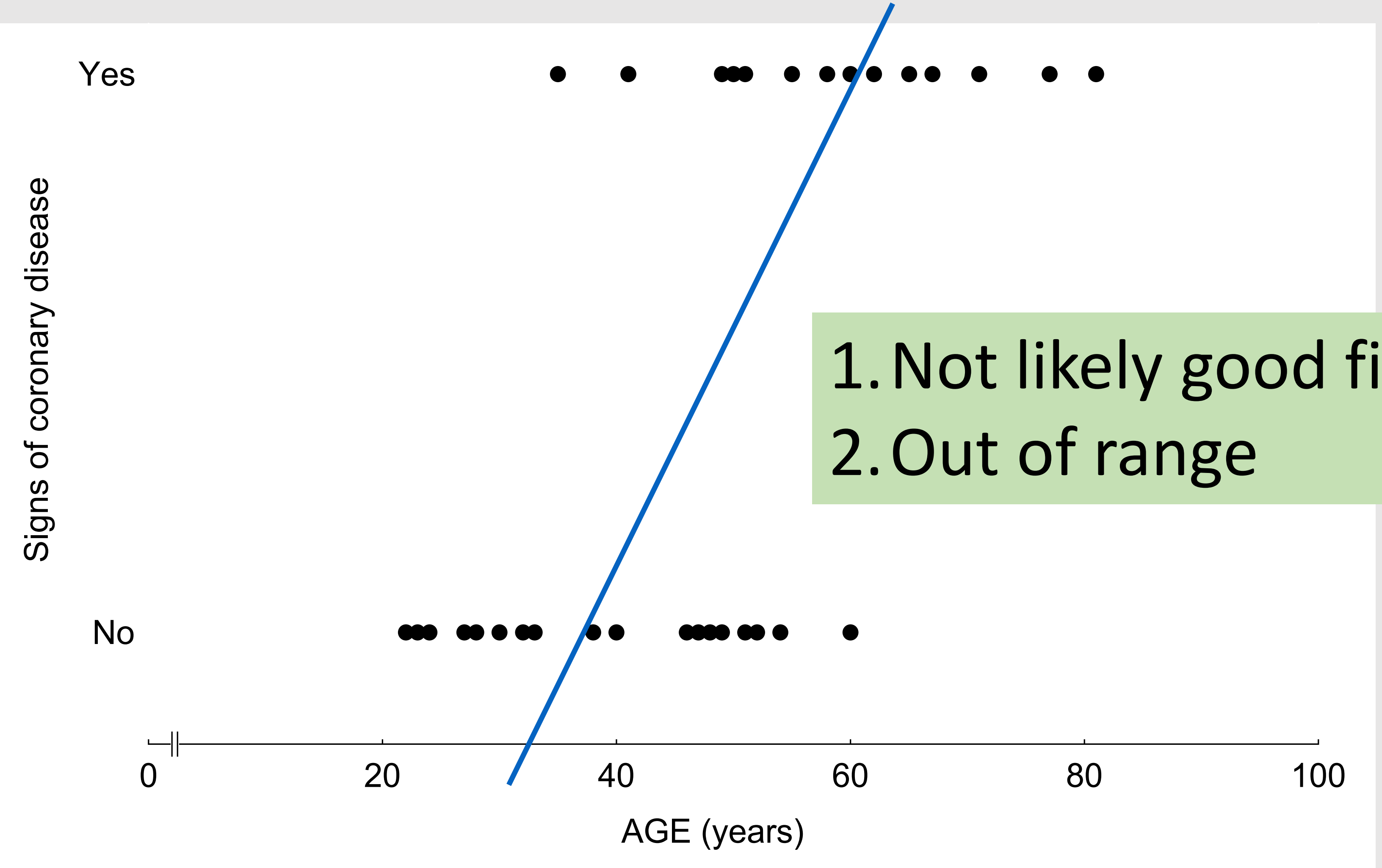
Table 1: Age and signs of coronary heart disease (CD)

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

Prediction question: a particular age → CD

Linear regression?

Dot-plot: Data from Table 1



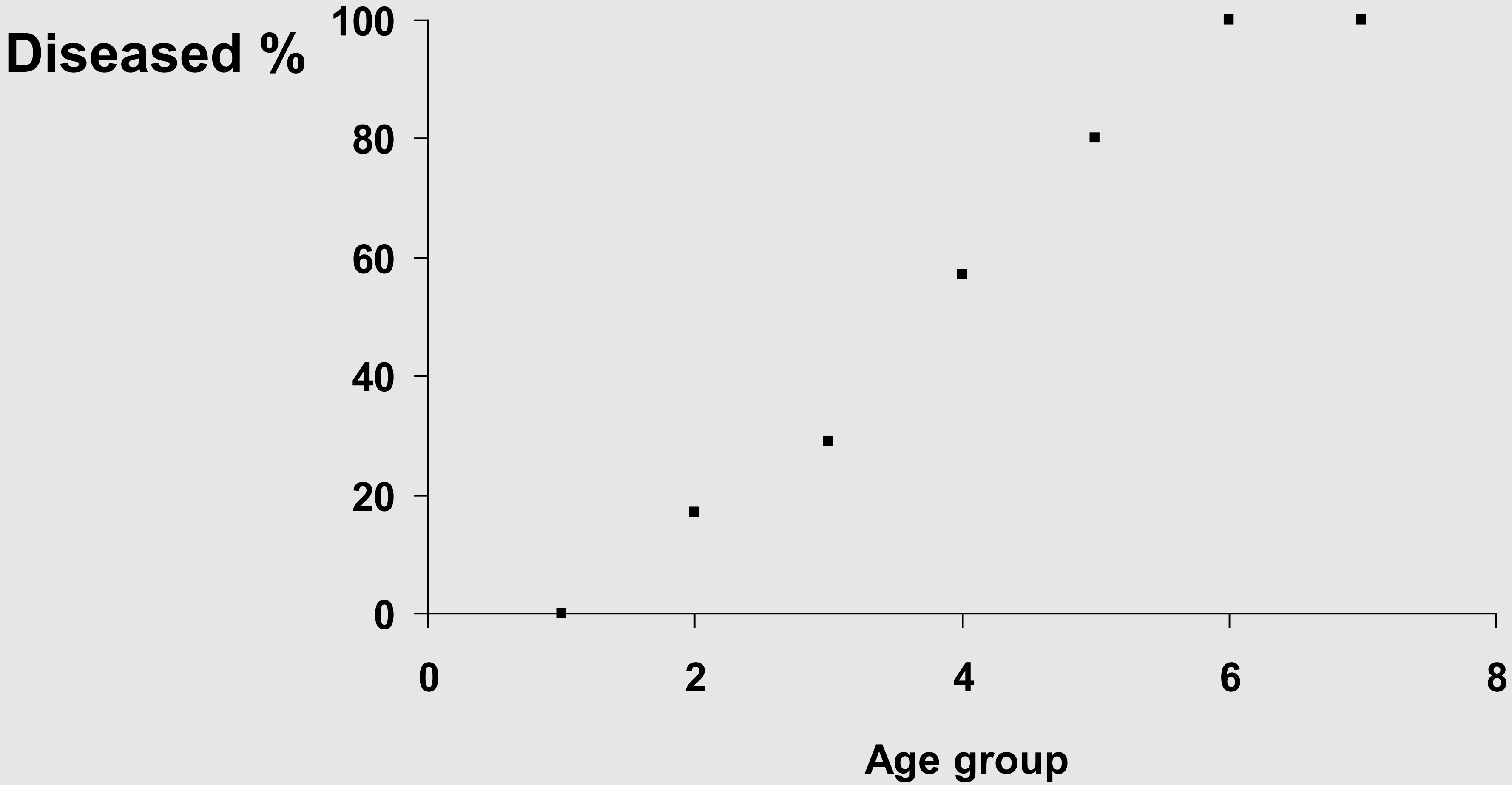
1. Not likely good fit
2. Out of range

Transform the Data→ Probability

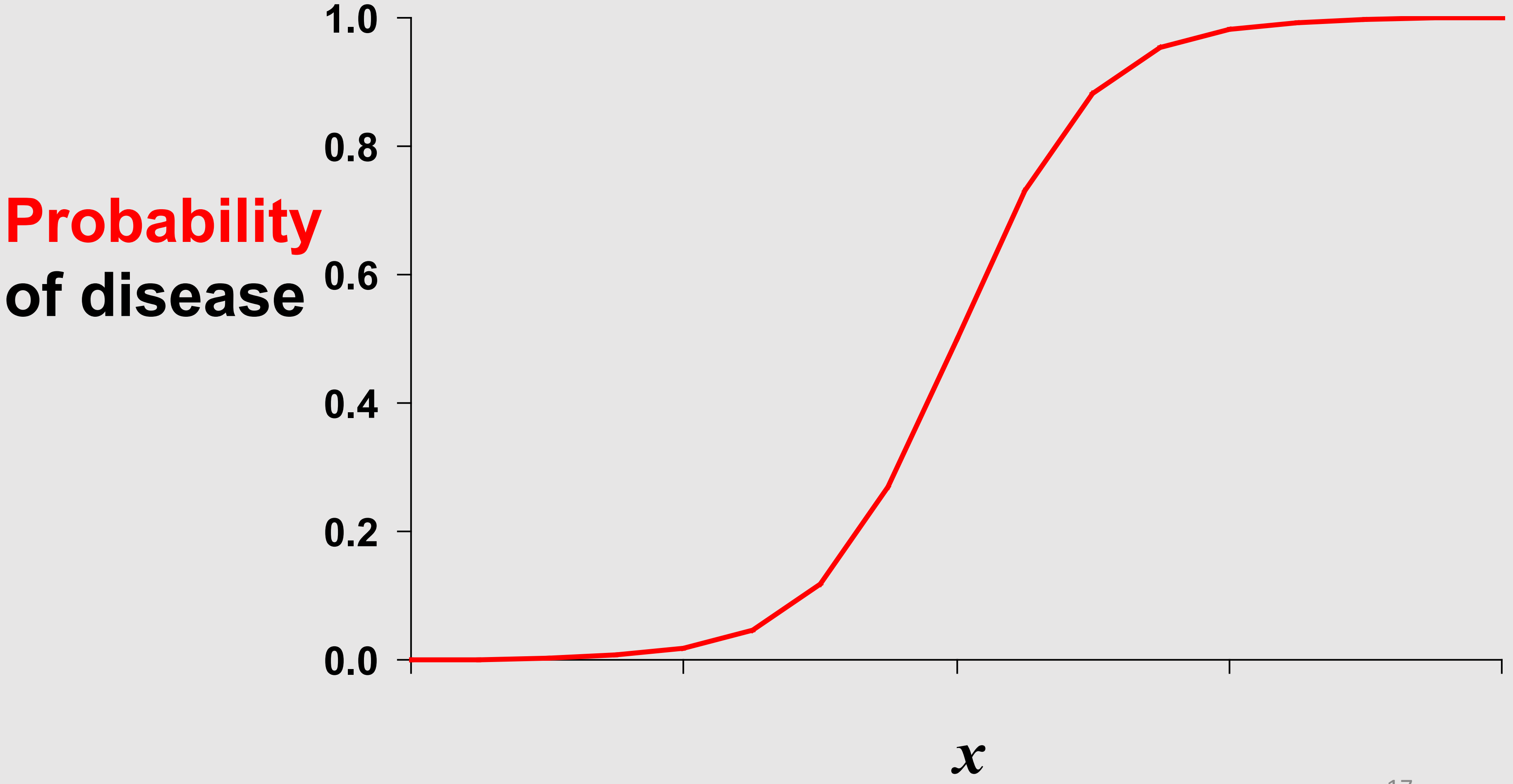
Table 2 Prevalence (%) of signs of CD according to age group

		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)

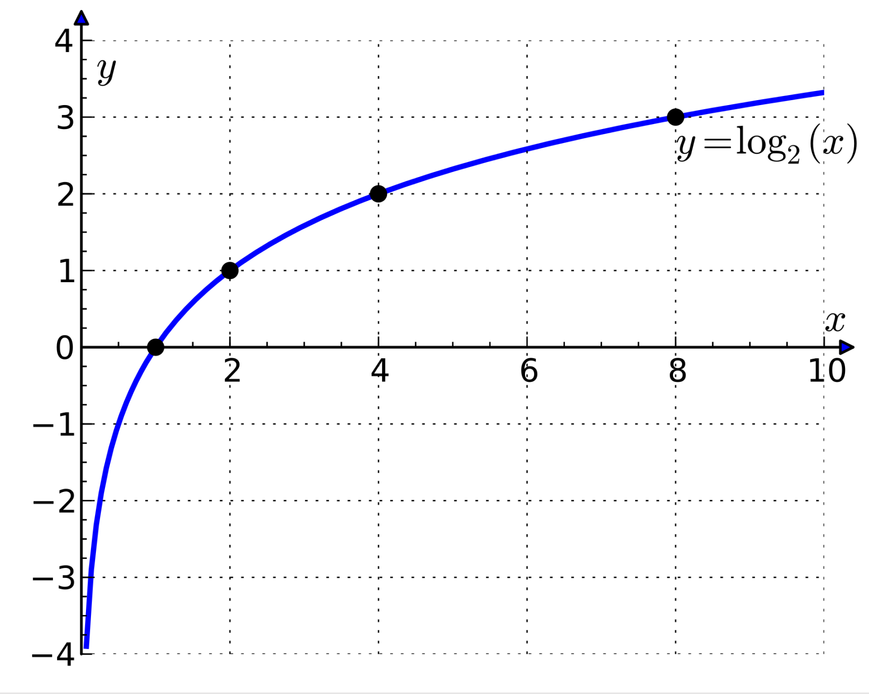
Log Odds

- **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, ∞]
- → Log odds (**logit**): **[-∞, ∞]**

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



Logit Function → Logistic Function

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

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

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

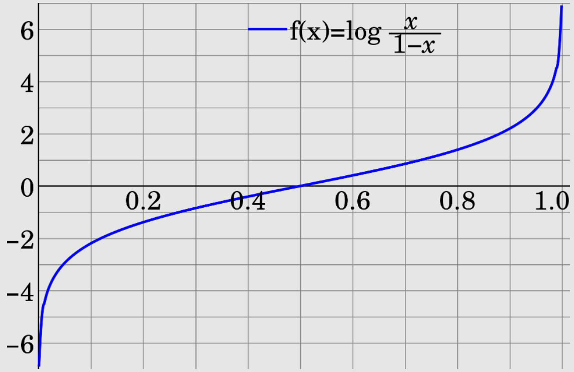
$$\text{logit}(\pi) = \log \frac{\pi}{1-\pi} = \mathbf{w}^\top \phi(\mathbf{x}) = w_0 + w_1 \phi(x_1) + \cdots$$

  In the following, we use the simpler first form above

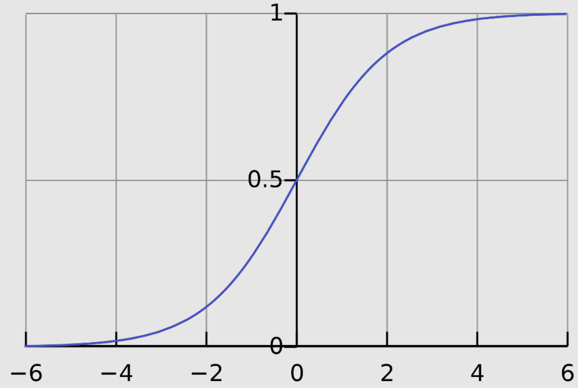
- Logistic function (**sigmoid**)= inverse of logit

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

- **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

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- Evaluation metric (what's best): loss/error function
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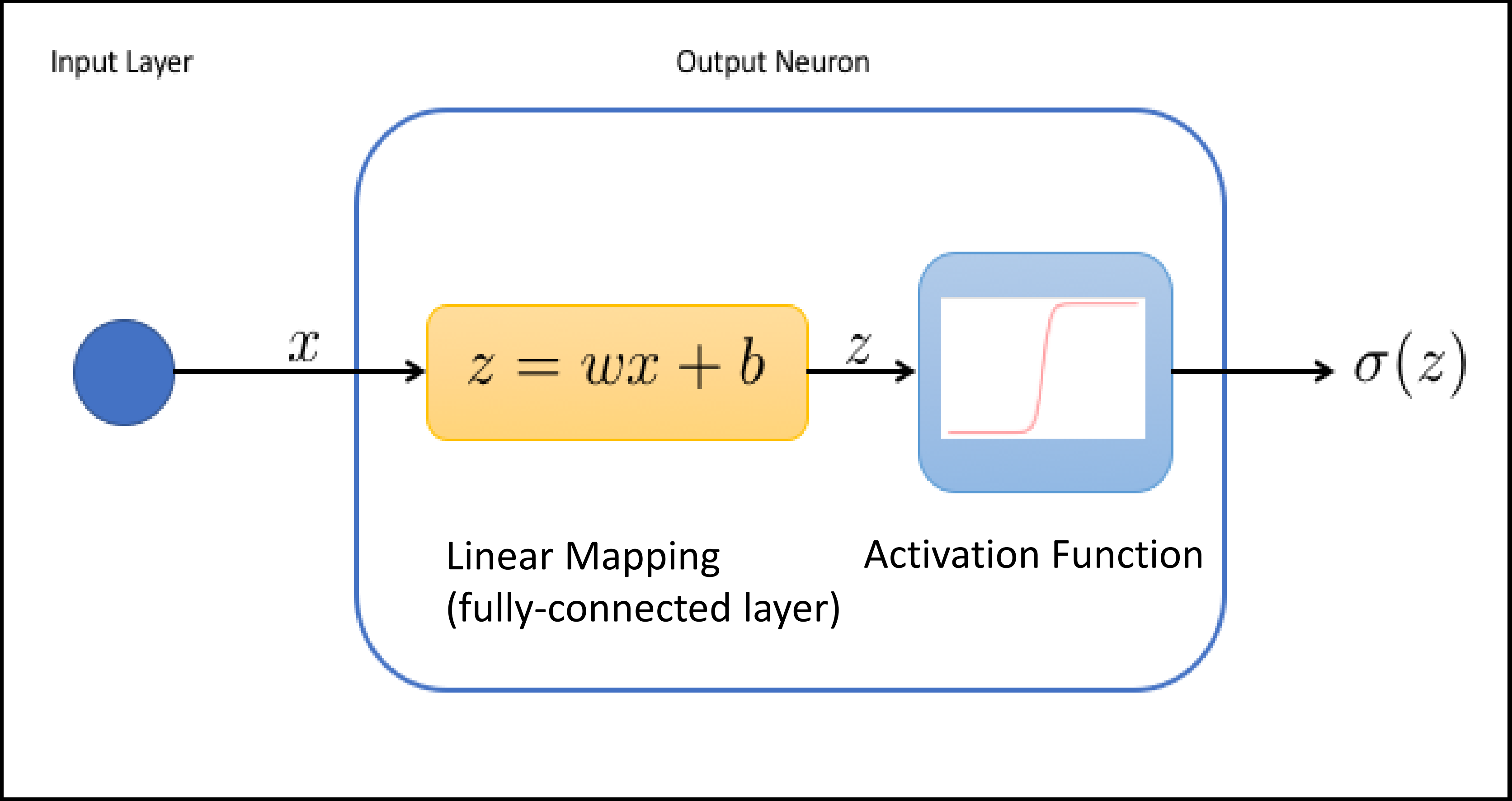
Logistic Regression Ingredients

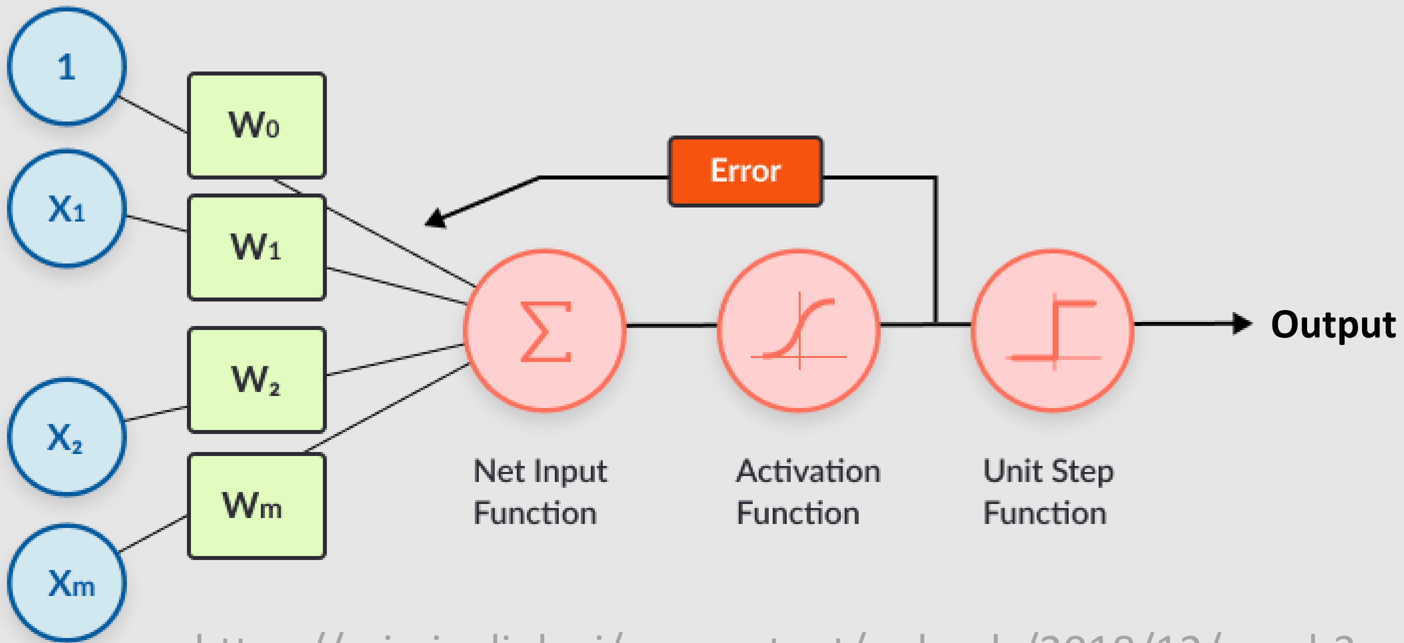
- **Data**: + pre-processing, e.g., $\mathcal{N}(0,1)$
- **Model**
  - Structure/Architecture: linear relationship

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

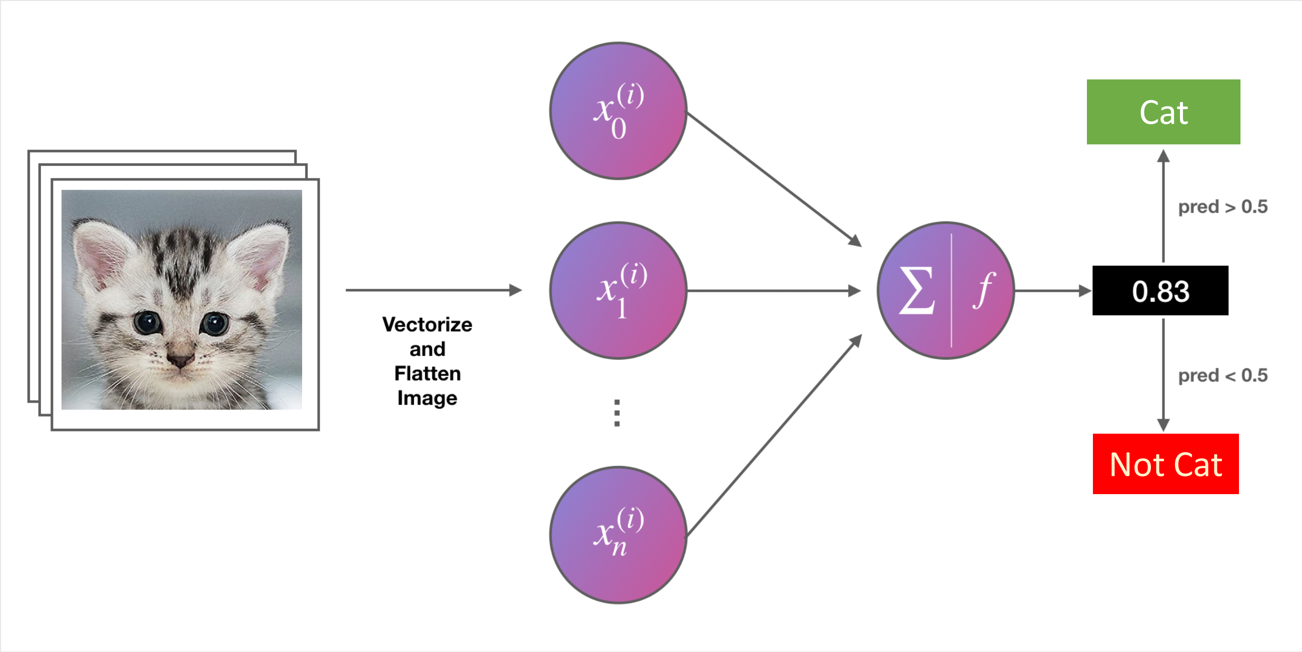
  - **Hyper-parameter**: no (unless + regularisation)
  - Parameters (theta): **w**
- Evaluation metric: max likelihood (min NLL)
- Optimisation: SGD or the like



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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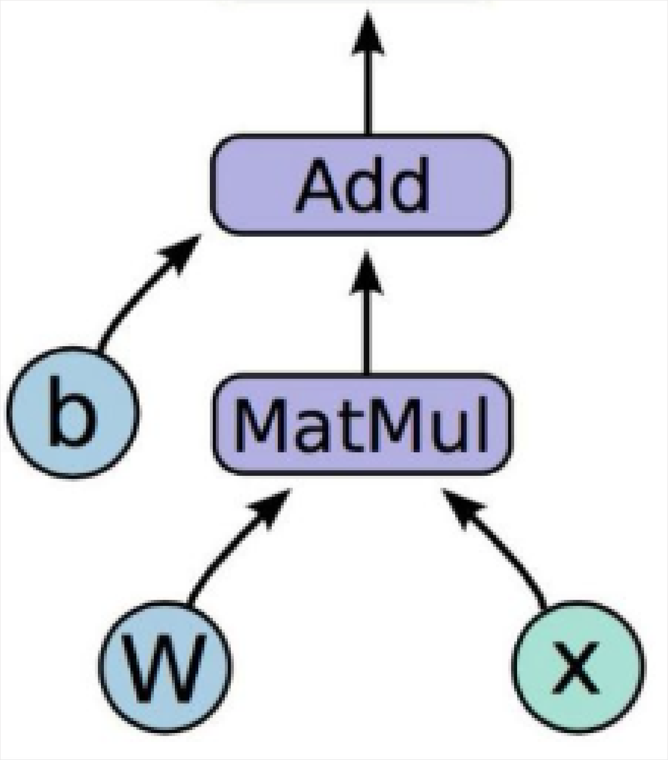
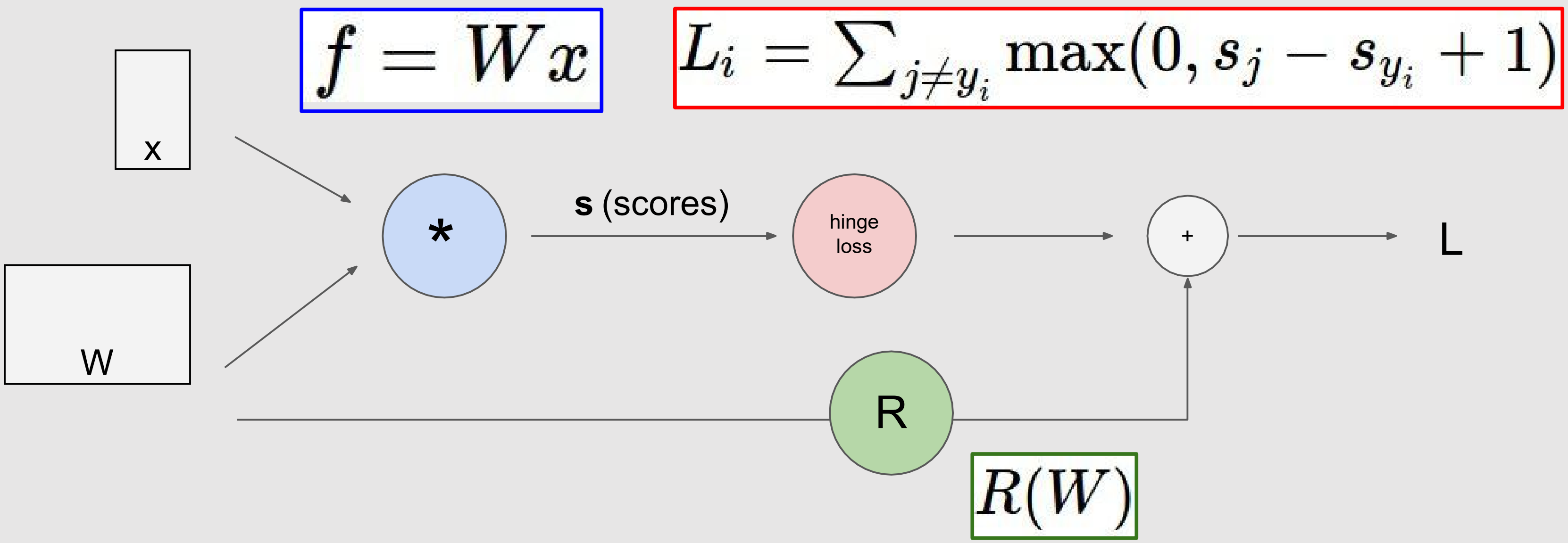
Computational Graph

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

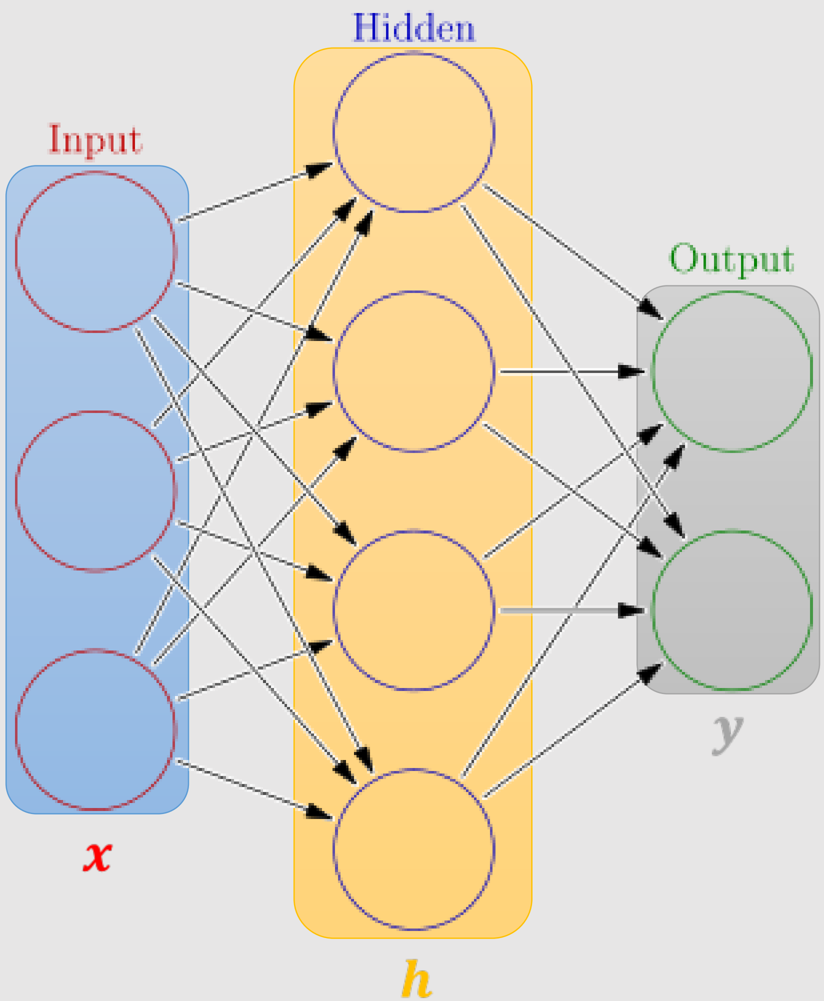


Source: Nelson Liu: https://colab.research.google.com/drive/11iLtGFDpnIuHj5B0rQDGG5lqq6BQ8FRh

Computational Graph: w/t Reg.



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?

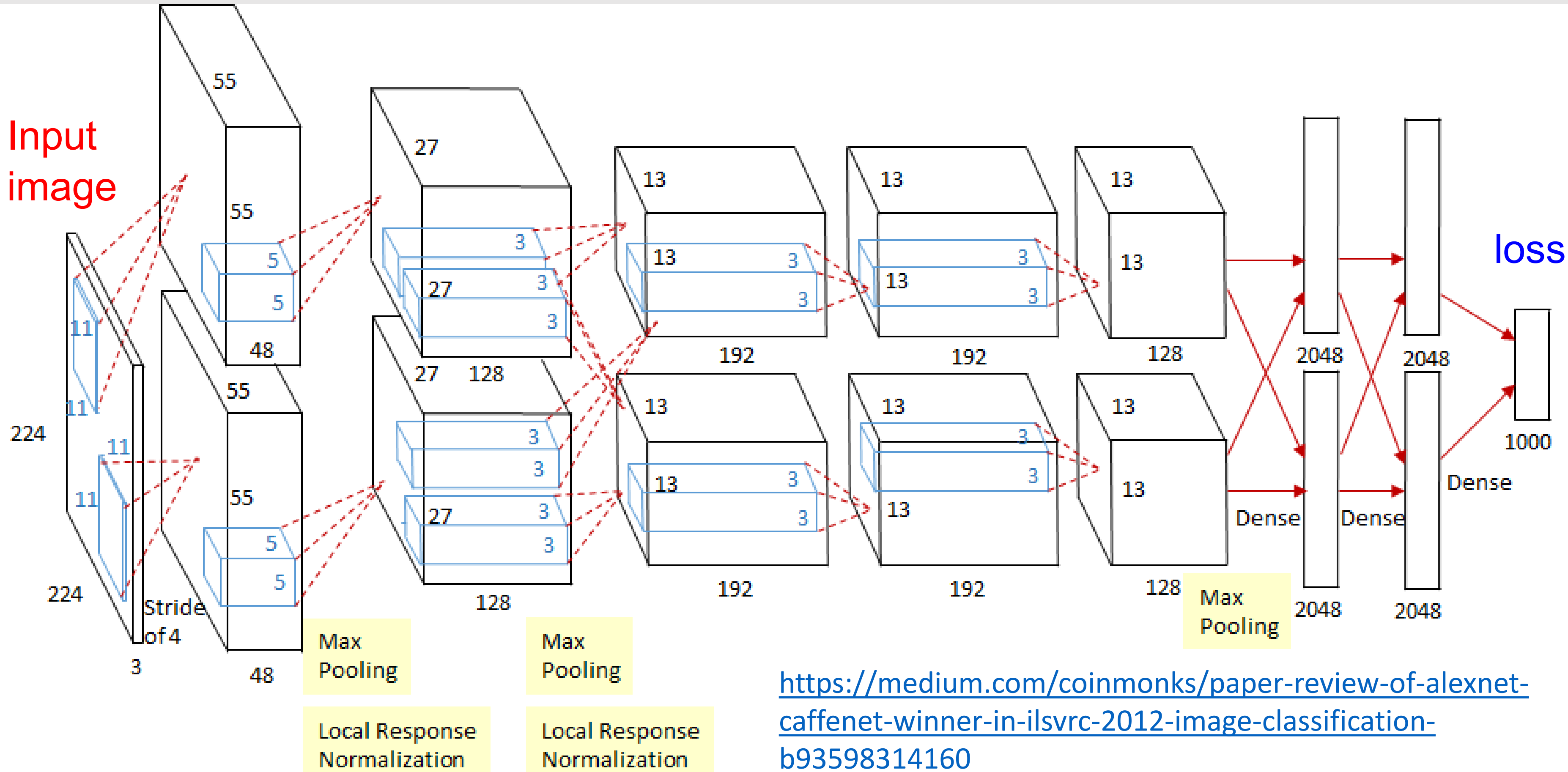
[3 x 4] + [4 x 2] = 20 weights
4 + 2 = 6 biases
26 learnable **parameters**

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 C[...]

Fancy feature extraction /representation learning

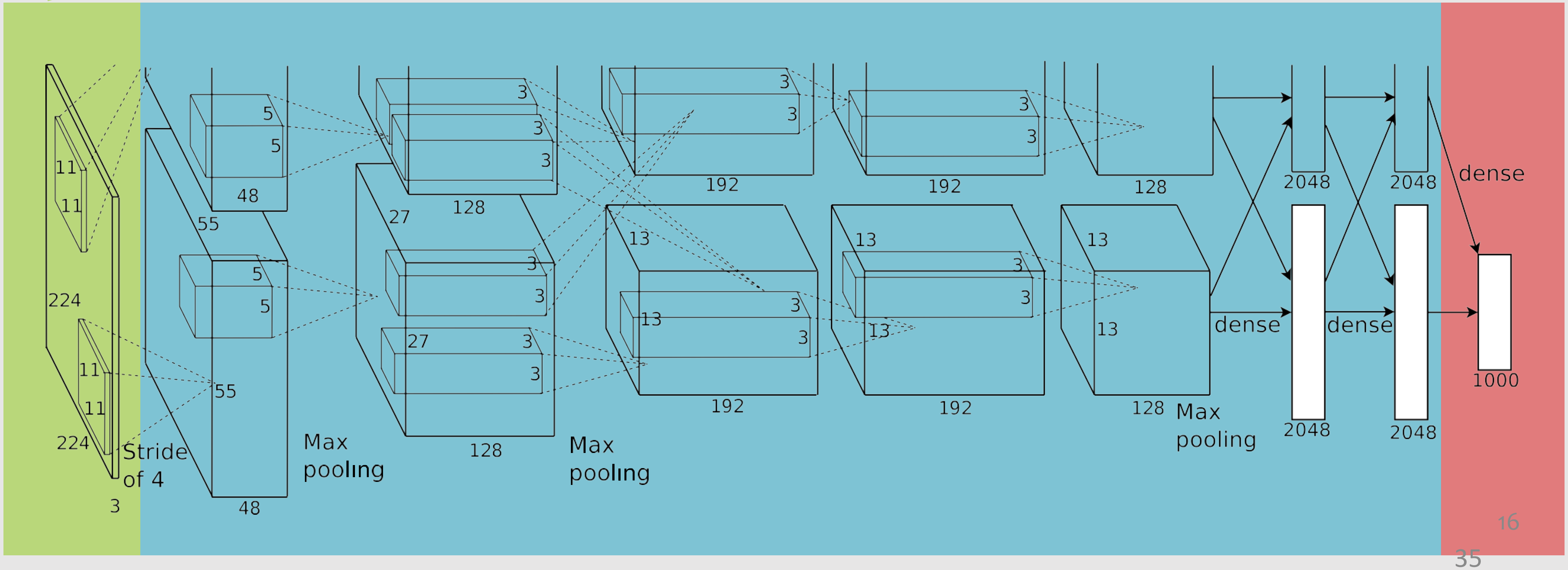
Logistic Regression!
Softmax: sigmoid for multiclass

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

Input image (pixels)

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

1000-way softmax



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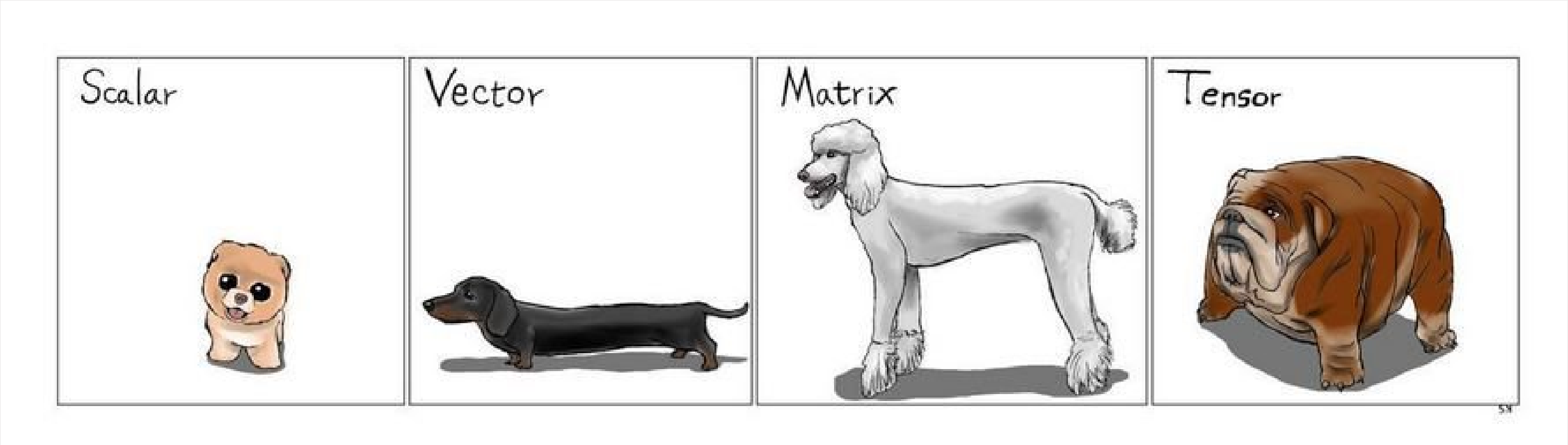
PyTorch

- 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



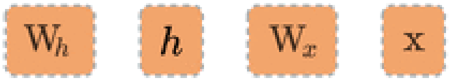
https://pbs.twimg.com/media/D2xTDMJWwAADHQt.jpg

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

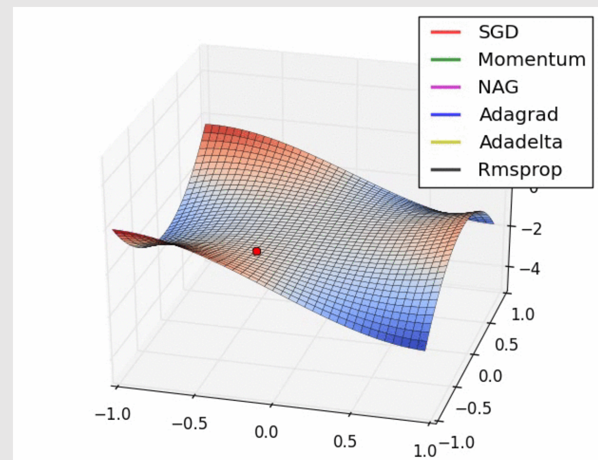
A graph is created on the fly



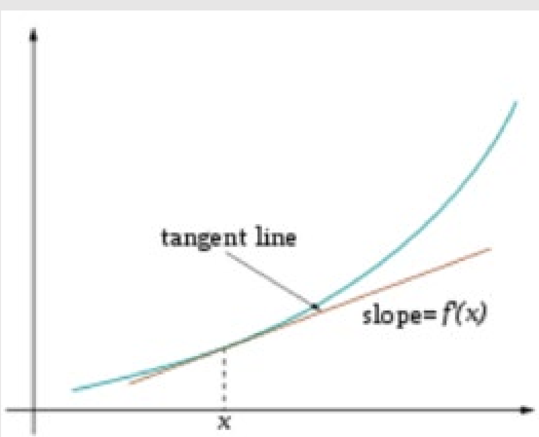

```
W_h = torch.randn(20, 20, requires_grad=True)
W_x = torch.randn(20, 10, requires_grad=True)
x = torch.randn(1, 10)
prev_h = torch.randn(1, 20)
```

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