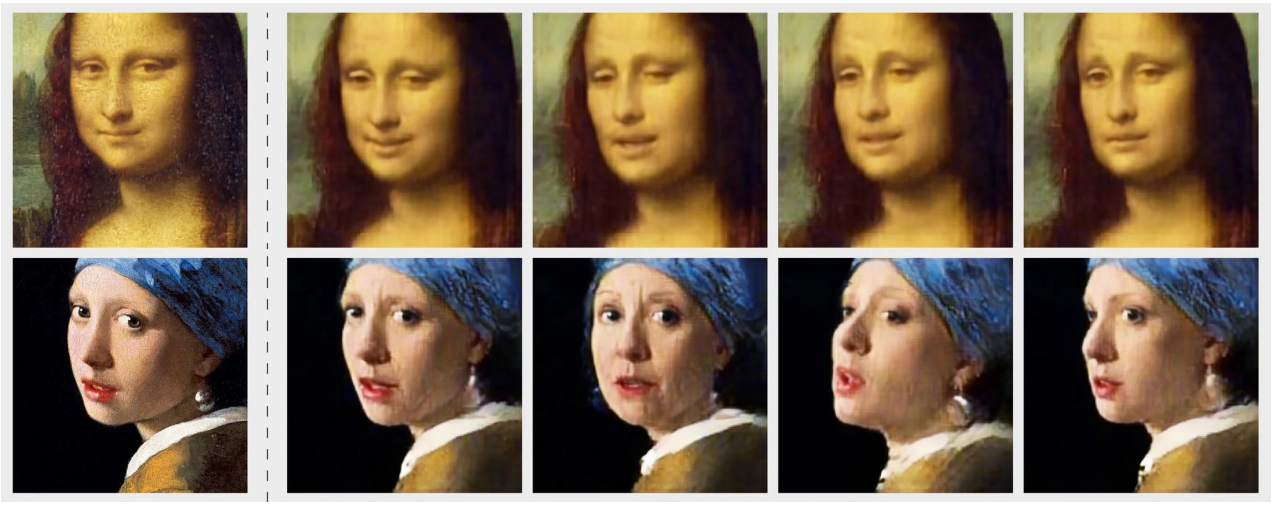
ICME Summer Workshops 2021

Introduction to Deep Learning

Session 1: 8:00—9:30 AM
Instructor: Sherrie Wang

icme-workshops.github.io/deep-learning



Zakharov *et al.* "Few-Shot Adversarial Learning of Realistic Neural Talking Head Models" (2019)

Workshop Schedule

Day 1

Session 1 (Today 8:00—9:30 AM)

- Introduction
- Examples of deep learning
- Math review
- Neural network basics

Session 2 (Today 9:45—11:00 AM)

- Loss functions
- Gradient descent
- Backpropagation
- Walkthrough of an example

Day 2

Session 3 (Tomorrow 8:00—9:30 AM)

- Overfitting and underfitting
- Convolutional neural networks
- Recurrent neural networks

Session 4 (Tomorrow 9:45—11:00 AM)

- Other architectures
- Deep learning libraries
- Walkthrough of an example
- Failures of deep learning

Learning Goals

Day 1

Session 1 (Today 8:00—9:30 AM)

- Introduction
- Examples of deep learning
- Math review
- Neural network basics

- What deep learning is
- Building blocks of neural networks

Session 2 (Today 9:45—11:00 AM)

- Loss functions
- Gradient descent
- Backpropagation
- Walkthrough of an example

- How neural networks learn from data

Learning Goals

- More complex neural networks
- Limitations and pitfalls when training neural networks

Day 2

Session 3 (Tomorrow 8:00—9:30 AM)

- Overfitting and underfitting
- Convolutional neural networks
- Recurrent neural networks

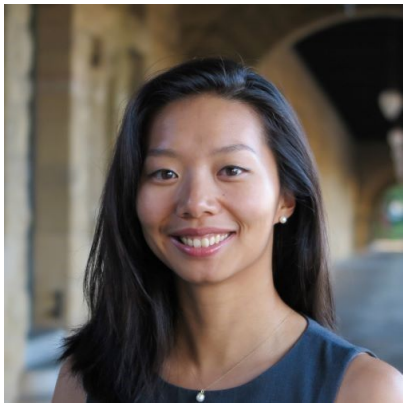
Session 4 (Tomorrow 9:45—11:00 AM)

- Other architectures
- Deep learning libraries
- Walkthrough of an example
- Failures of deep learning

Workshop Logistics

- Workshop website:
  https://icme-workshops.github.io/deep-learning/
- Slides for today's lectures are available online
- We will be using Slido for polls throughout lecture:
  https://tinyurl.com/dlworkshop2021
- Please post all questions during lecture to Piazza:
  https://piazza.com/icme/summer2021/icme
- At the end of each session, I will take questions over Zoom
- New 2-day format! I encourage everyone to ask questions so that on day 2 all previous concepts are clear
- Will be recorded and uploaded online

About me



Hello
my name is

Sherrie Wang

@sherwang

- **PhD graduate** of ICME (2021)
- **Research focus:** Machine learning methods for remote sensing and applications in sustainability
- **Relevant courses:**
  - CS 221 (Artificial Intelligence)
  - CS 229 (Machine Learning)
  - CS 228 (Probabilistic Graphical Models)
  - CS 230 (Deep Learning)
  - CS 231n (Convolutional Neural Networks)
  - CS 236 (Generative Adversarial Networks)
  - CS 330 (Deep Multi-Task and Meta Learning)
- **Relevant teaching:** CME 250 (Introduction to Machine Learning), Summer Workshop 2019-20

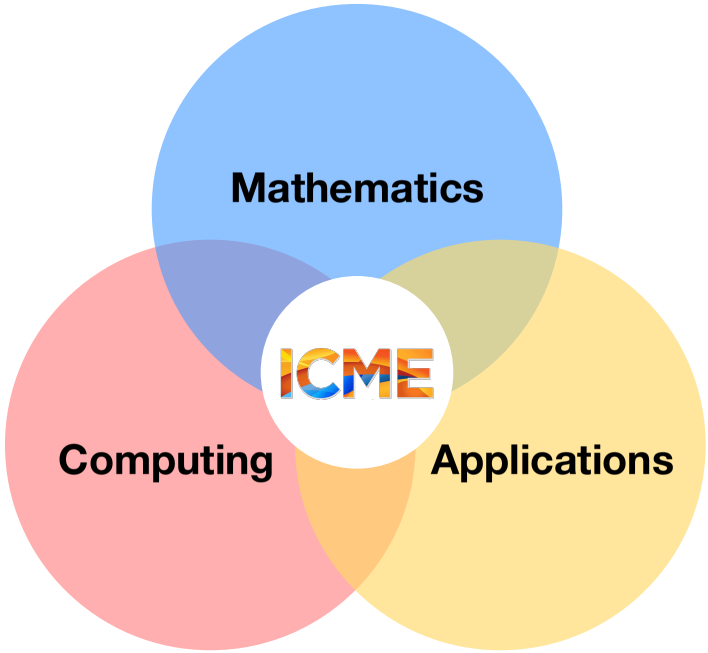
What is ICME?

Stanford Institute for Computational and Mathematical Engineering

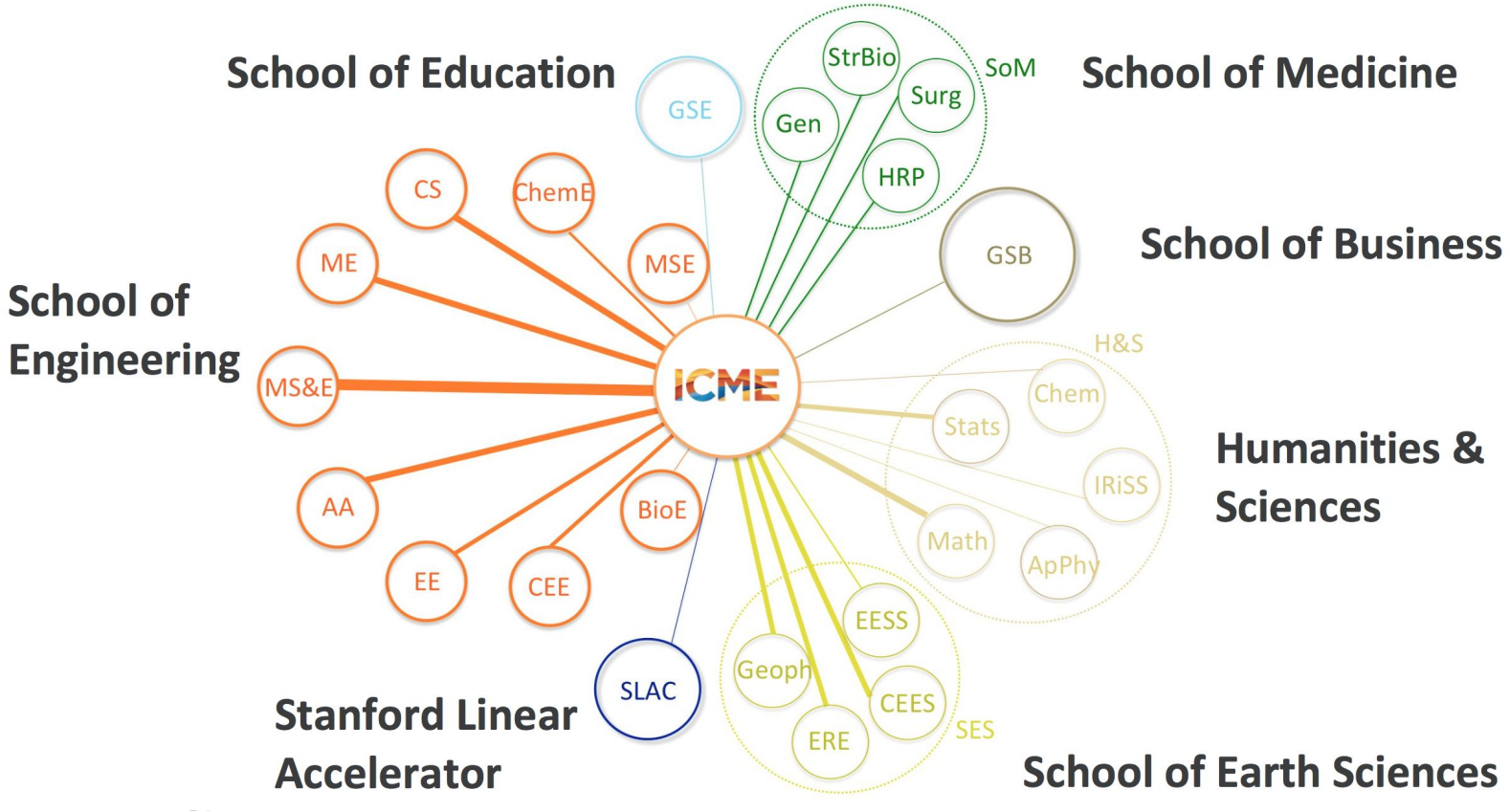
Hub at Stanford

Interdisciplinary field using advanced mathematics and computing to address complex problems

icme.stanford.edu



55+ affiliated faculty across Stanford



150+ MS and PhD students

ICME industry-academia ecosystem

WELLS FARGO

TOTAL

intuit

Microsoft

NVIDIA

Schlumberger

Tencent 腾讯

Google

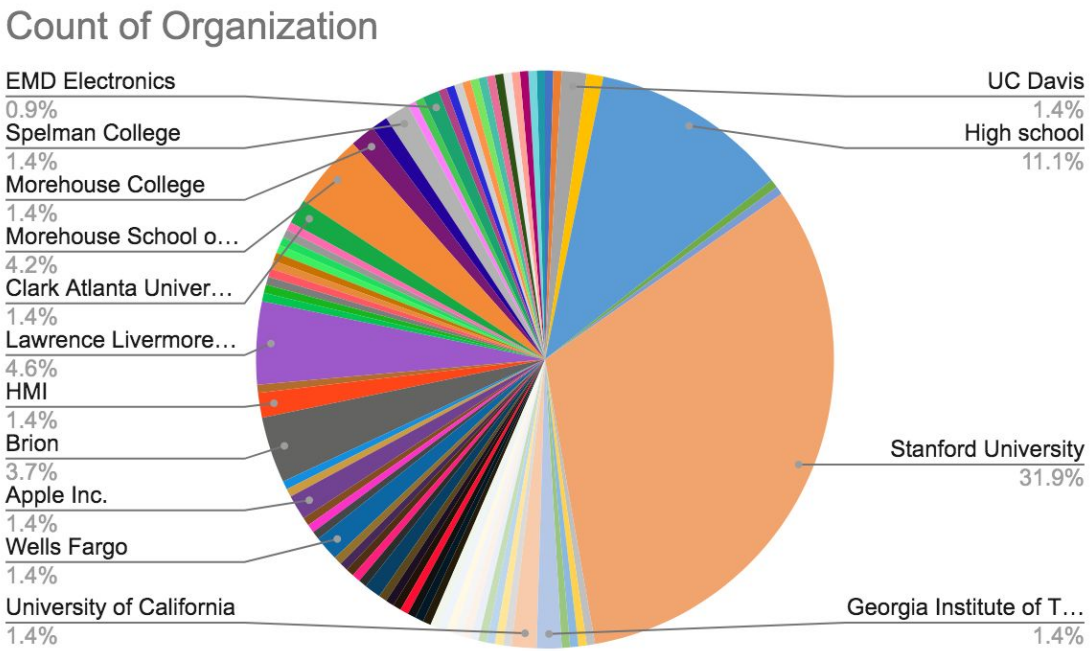
MathWorks

@WalmartLabs

Accenture Applied Intelligence

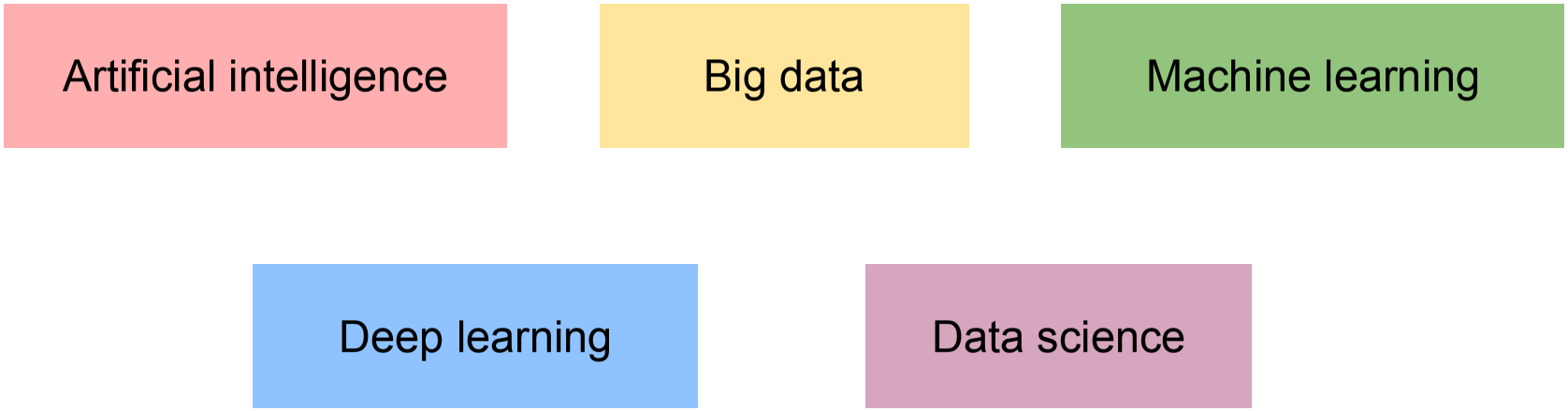
Who’s here today

200+ registered participants

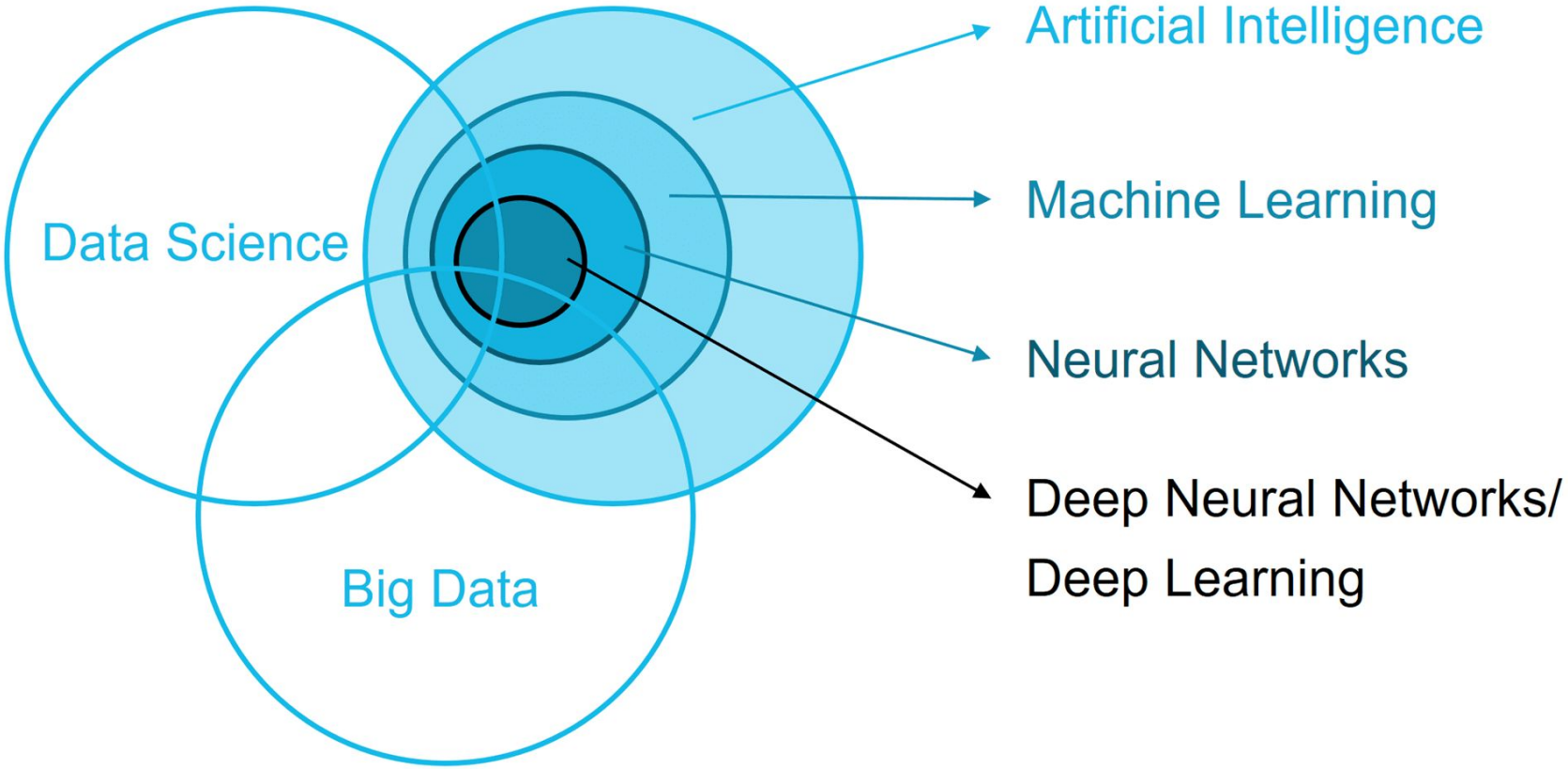


The Deep Learning Revolution

What is “deep learning”?



What is “deep learning”?



https://tamuk.quickstart.com/blog/artificial-intelligence-vs.-machine-learning-vs.-data-science/

Deep learning examples

1. Optical character recognition (OCR)
2. Image classification
3. Text translation
4. Image generation
5. Text generation
6. Audio generation
7. Reinforcement learning
8. Energy
9. Healthcare
10. Biology
11. Development
12. Investing
13. Surveillance

1. Optical character recognition

Computer vision is one of the first places where deep learning started to outshine other methods.

"The Street View House Numbers (SVHN) Dataset": http://ufldl.stanford.edu/housenumbers/

Deep learning examples

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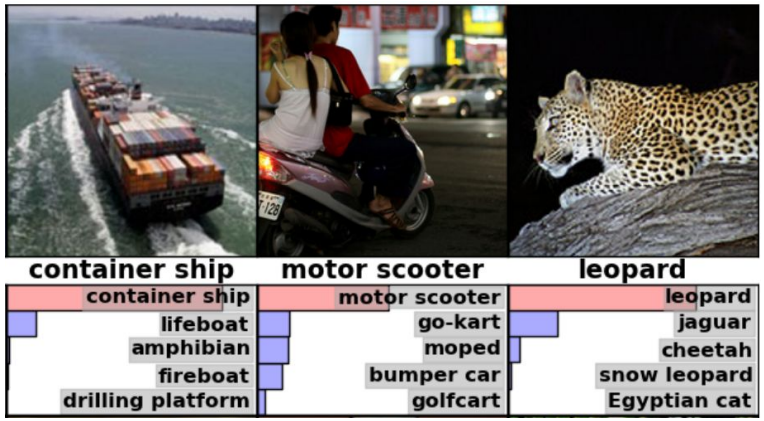
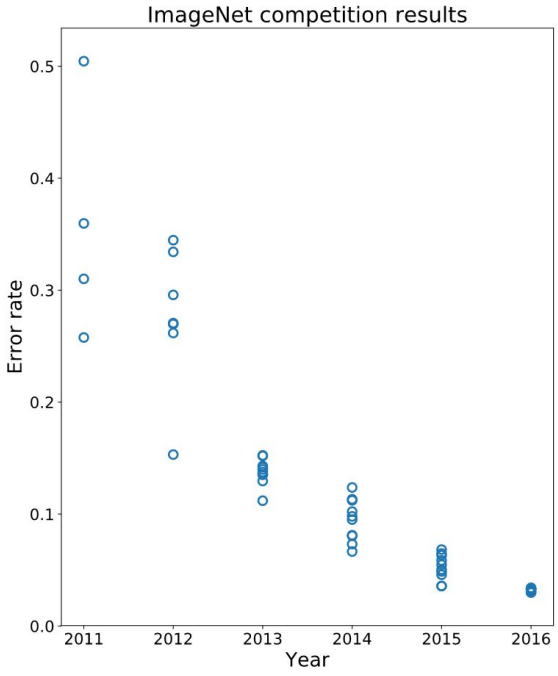
2. Image classification





Krizhevsky, Sutskever, and Hinton. "ImageNet Classification with Deep Convolutional Neural Networks" (2012)

Deep learning examples

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3. Text translation

Wu *et al.* “Google's Neural Machine Translation System: Bridging the Gap between Human and Machine Translation” (2016)

Deep learning examples

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4. Image generation

Progression in the capabilities of GANs

Brundage *et al*. "The Malicious Use of Artificial Intelligence: Forecasting, Prevention, and Mitigation" (2018)

Brock *et al*. "Large Scale GAN Training for High Fidelity Natural Image Synthesis" (2018)

Deep learning examples

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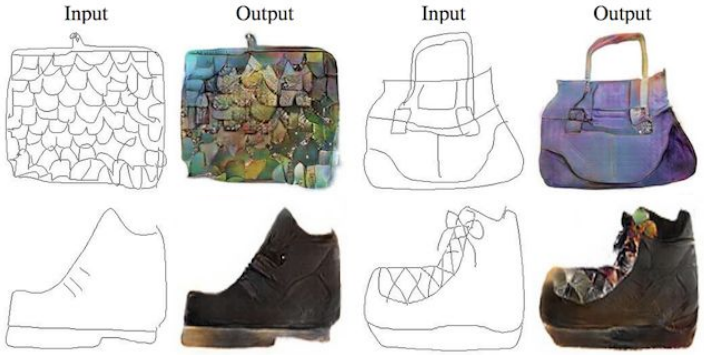
4. Image generation

Image-to-image translation



Isola *et al.* "Image-to-Image Translation with Conditional Adversarial Networks" (2016)

Text-to-image translation

Reed *et al.* "Generative Adversarial Text to Image Synthesis" (2016)

Source: Instagram, FaceApp - AI Face Editor

Deep learning examples

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5. Text generation

GPT-3-aided poetry!

Human prompt (bolded):

Here's a poem by Dr. Seuss about Elon Musk launching rockets with SpaceX, building electric cars at Tesla, selling flame throwers, dating Grimes, fighting the SEC, crushing short sellers, building brain chips to fight AI, and colonizing mars, and tweeting at all hours of day and night. Musk wants to make humans interplanetary to prevent extinction. The poem rhymes every other line with an ABAB structure. The rhyme structure is typical of Dr. Seuss nursery rhymes.

GPT-3 output (with "several hours" of trial and error):

Elon Musk
By Dr. Seuss

Once there was a man
who really was a Musk.
He liked to build robots
and rocket ships and such.

He said, "I'm building a car
that's electric and cool.
I'll bet it outsells those
Gasoline-burning clunkers soon!"

They sell cool cars
that are electric and clean.
And then he wanted to go
even farther, you see.

The first Tesla, Roadster,
Was just the start of a bigger dream.
He said, "I'm building a plane
that's electric and green.

That's not all!
That man is also a Musk.
He likes electric cars,
flamethrowers, tunnels, and such.

But then he thought, "If we make
a very small, small chip,
We'll implant it in our heads,
And then connect our minds to the
Internet!"
...

Source: https://arr.am/2020/07/14/elon-musk-by-dr-seuss-gpt-3/ (2020)

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5. Text generation

GPT-3-generated text:

Human prompt is bolded.

Movie plot summaries (from Wikipedia):

The Matrix (1999): "A computer hacker learns from mysterious rebels about the true nature of his reality and his role in the war against its controllers." (For the purposes of this post, we can set aside some of the specific details and just say that, basically, Neo learns that our world isn't real—that what we perceive isn't the real thing, but a simulation or "matrix" created to fool us.)

Inception (2010): "While competing with a rival thief to recover a potent artefact, Dom Cobb (Leonardo DiCaprio) falls into a dreamworld where he must 'extract' an idea from an influential businessman while being chased by the FBI."

Source: https://www.gwern.net/GPT-3 (2020)

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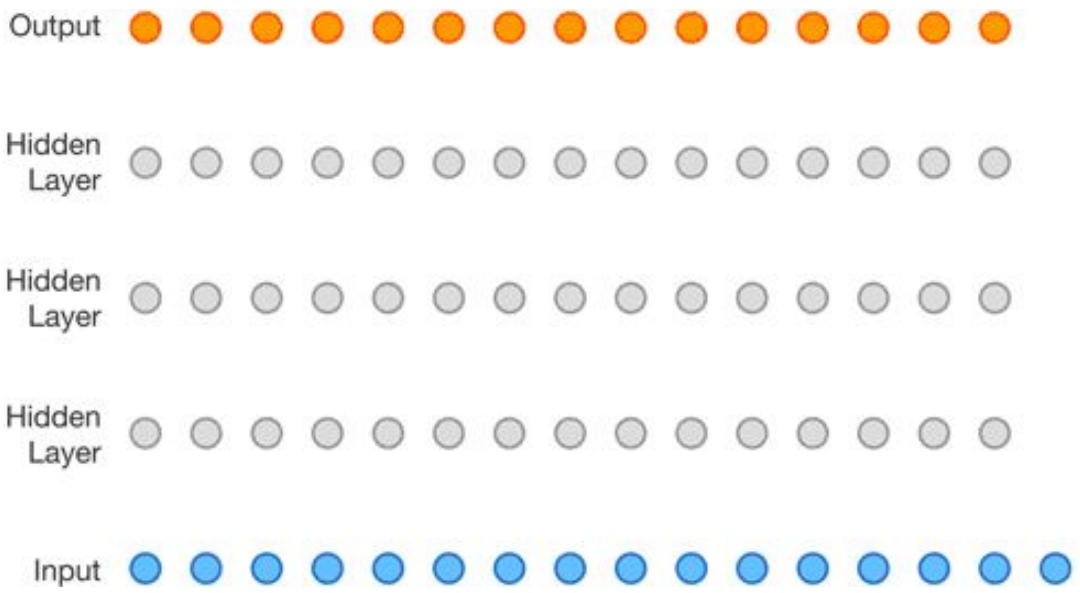
6. Audio generation

DeepMind's WaveNet



Source: https://deepmind.com/blog/article/wavenet-generative-model-raw-audio (2016)

Deep learning examples

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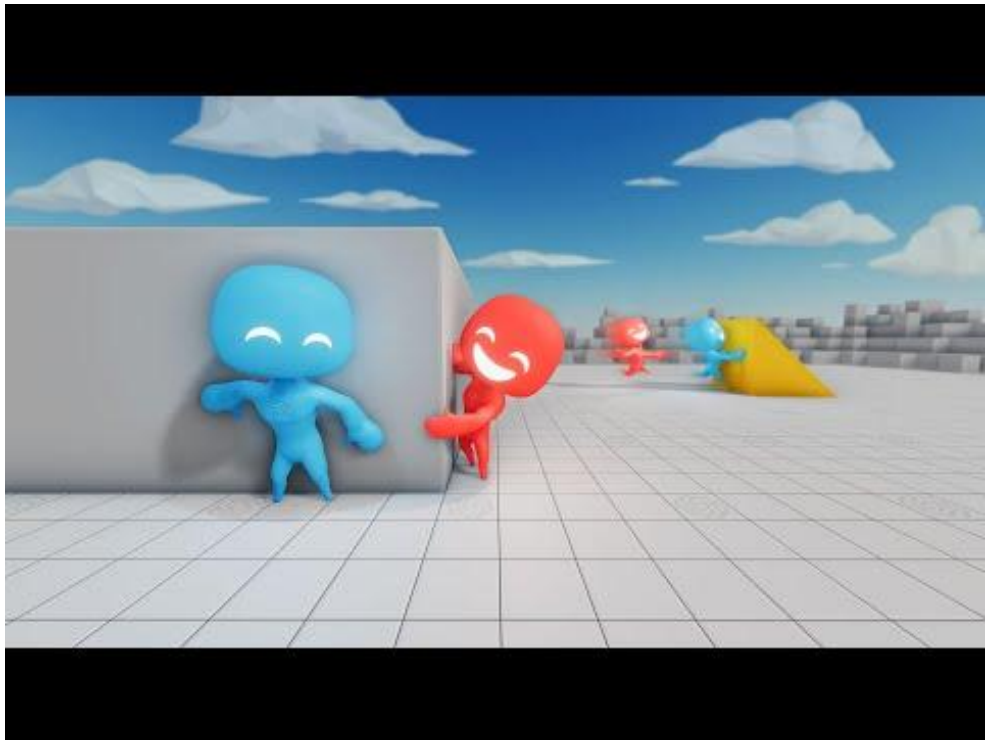
7. Reinforcement learning

OpenAI's "Hide and Seek" Game



Source: https://openai.com/blog/emergent-tool-use/ (2019)

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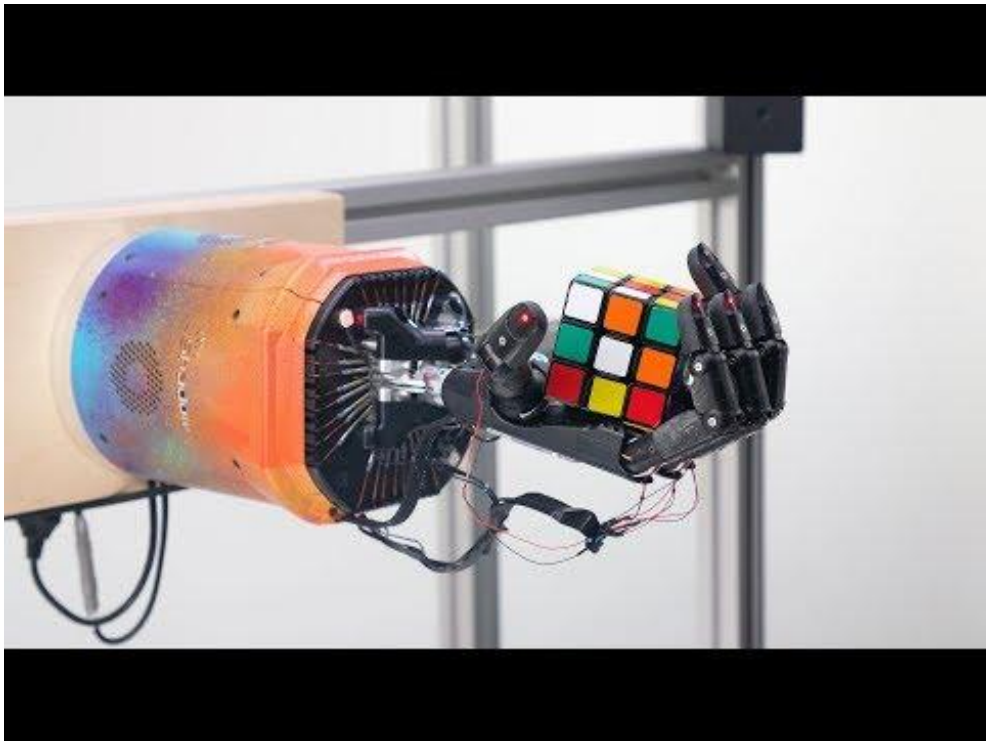
7. Reinforcement learning

Solving a Rubik's cube with a robot hand



Source: https://openai.com/blog/solving-rubiks-cube/ (2019)

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OpenAI vs. best human players in DOTA 2

Source: https://openai.com/projects/five/ (2019)

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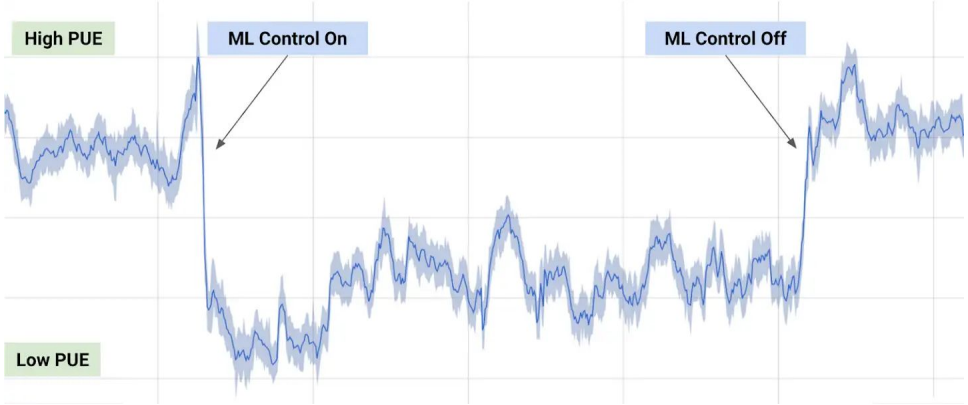
"DeepMind AI Reduces Google Data Centre Cooling Bill by 40%"



MENU nature

Article | Published: 19 February 2020

Closed-loop optimization of fast-charging protocols for batteries with machine learning

Peter M. Attia, Aditya Grover, Norman Jin, Kristen A. Severson, Todor M. Markov, Yang-Hung Liao, Michael H. Chen, Bryan Cheong, Nicholas Perkins, Zi Yang, Patrick K. Herring, Muratahan Aykol, Stephen J. Harris, Richard D. Braatz ✉, Stefano Ermon ✉ & William C. Chueh ✉

Source: (top) https://deepmind.com/blog/article/deepmind-ai-reduces-google-data-centre-cooling-bill-40 (2016)

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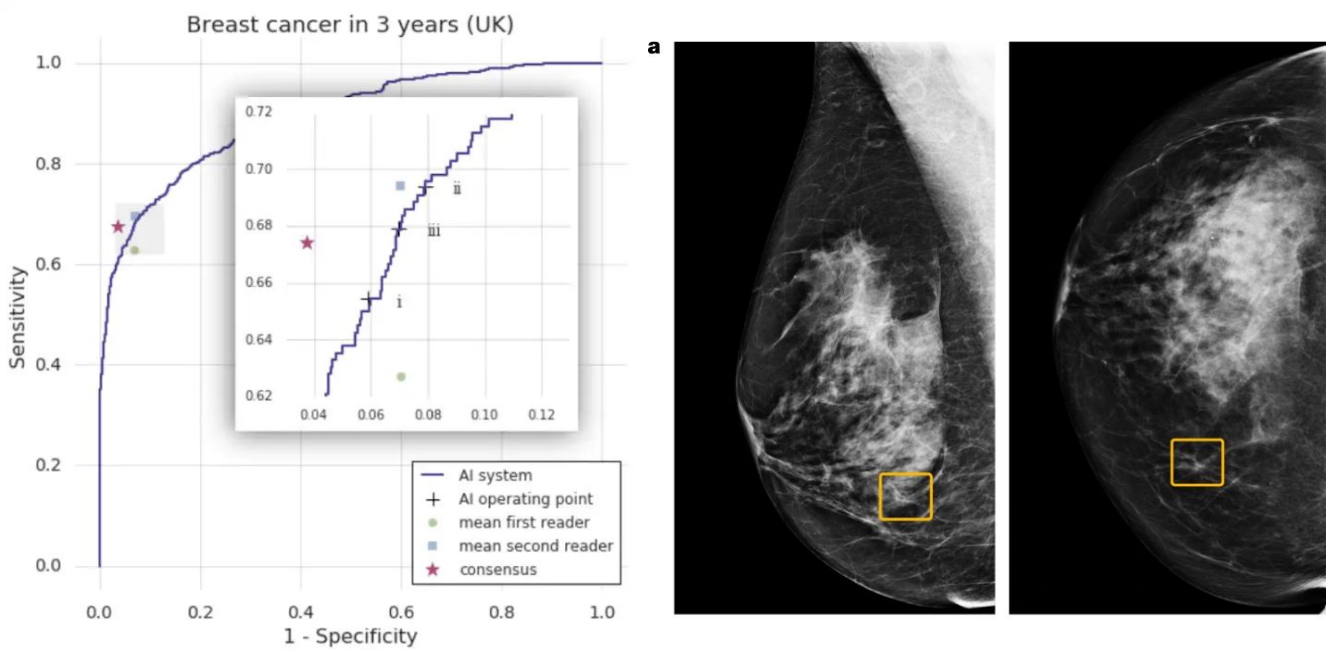
9. Healthcare

DeepMind's AI for breast cancer screening



Source: McKinney *et al.* "International evaluation of an AI system for breast cancer screening" (2020)

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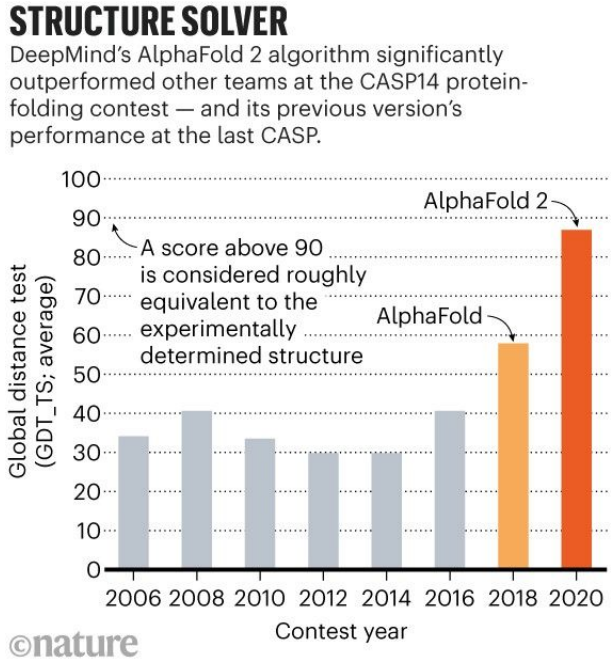
DeepMind's AlphaFold 2



Source:"'It will change everything': DeepMind's AI makes gigantic leap in solving protein structures" (2020)

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11. Sustainable development

Estimating poverty using transfer learning and night lights

Source: Jean *et al.* "Combining satellite imagery and machine learning to predict poverty" (2016)

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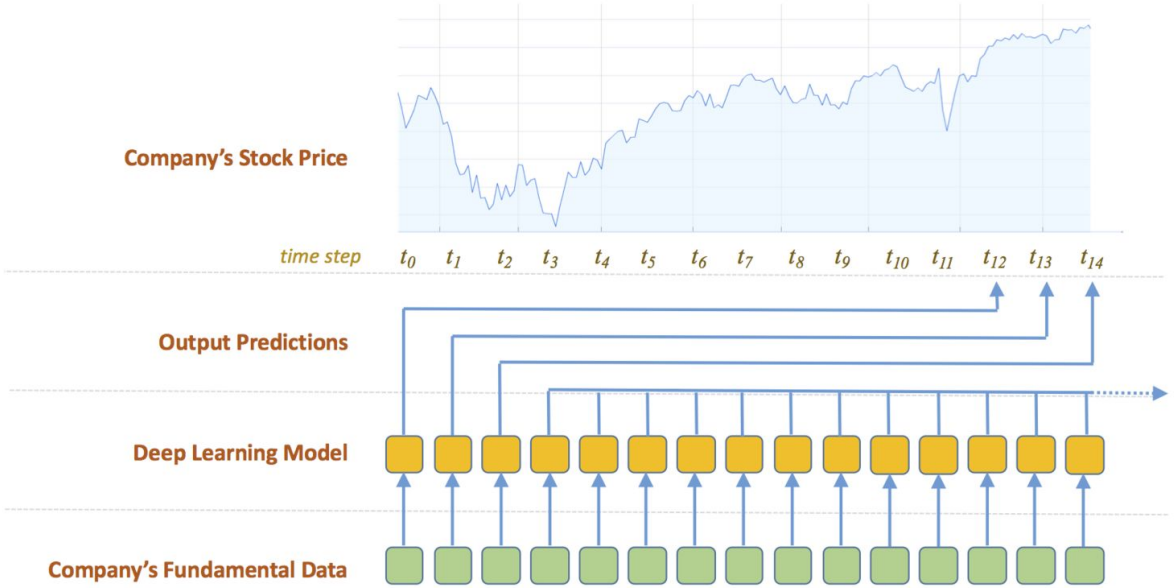
12. Investing

Predicting stock price from company fundamentals



Source: Alberg and Lipton. "Improving Factor-Based Quantitative Investing by Forecasting Company Fundamentals" (2017)

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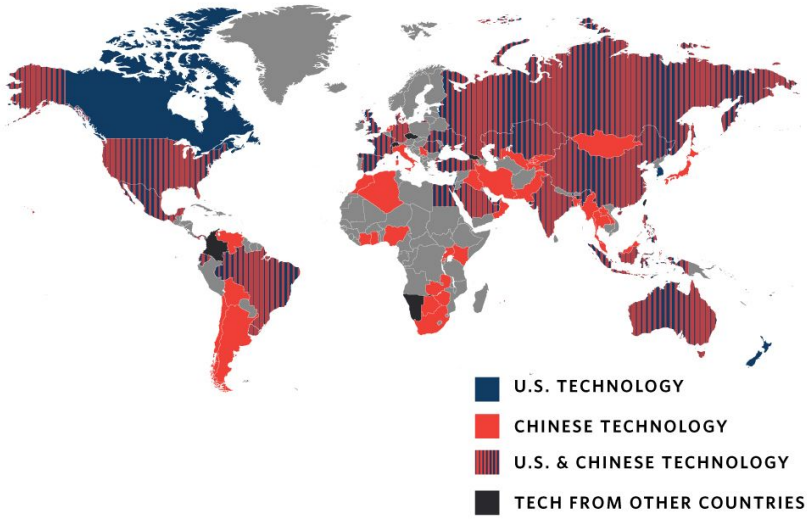
The New York Times

San Francisco Bans Facial Recognition Technology

Attendees interacting with a facial recognition demonstration at this year's CES in Las Vegas. Joe Buglewicz for The New York Times

MAP 1

AI Surveillance Technology Origin

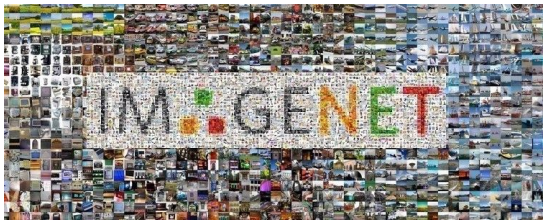


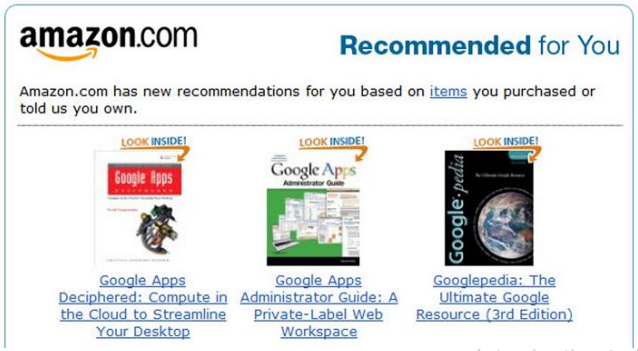
Sources: https://www.nytimes.com/2019/05/14/us/facial-recognition-ban-san-francisco.html (2019)
https://carnegieendowment.org/2019/09/17/global-expansion-of-ai-surveillance-pub-79847 (2019)

Why is deep learning at the forefront now?

Big data

Compute





Why is deep learning at the forefront now?

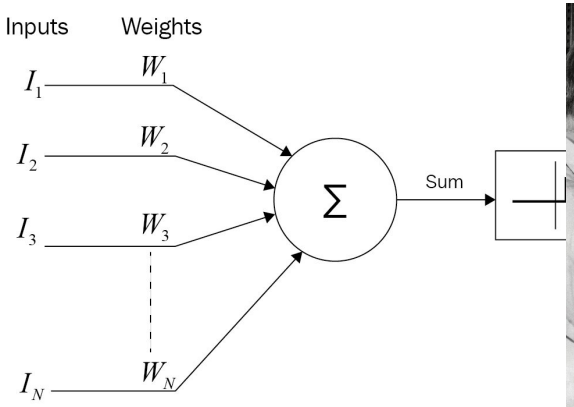
Algorithms

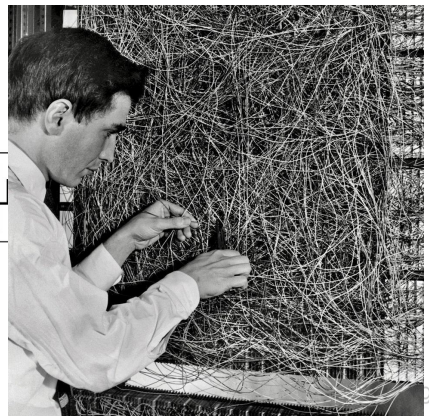
1943: McCulloch and Pitts develop a mathematical model of the neuron

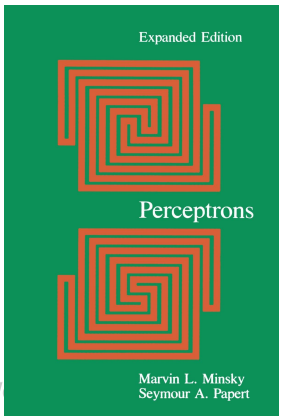
1957: Rosenblatt invents the perceptron algorithm and machine

1969: Minsky and Papert improve the perceptron and prove it cannot model nonlinearities like XOR

1974–1980: The First AI Winter



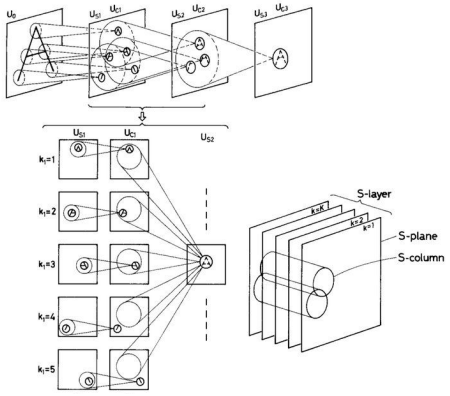




Why is deep learning at the forefront now?

Algorithms

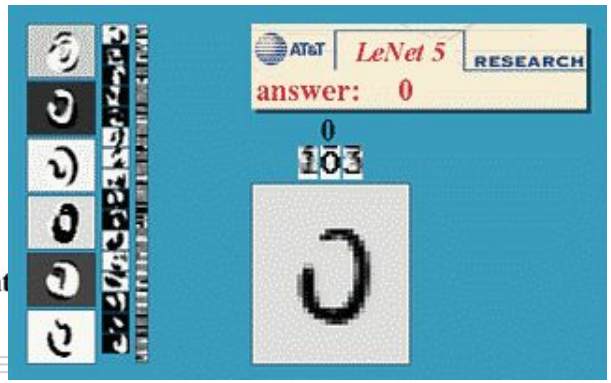
1980: Fukushima creates the “neocognitron”, introducing convolutional and downsampling layers



1986: Rumelhart, Hinton, and Williams apply backpropagation to train neural networks

D.E. Rumelhart, G.E. Hinton, R.J. Williams
Learning representation by back-propagat
errors. *Nature*, 323 (1986), pp. 533–536

1989: LeCun uses backprop to train convolutional neural networks to read digits



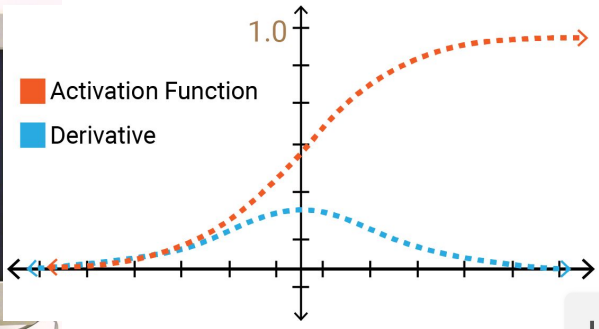
1987–1994: The Second AI Winter

Why is deep learning at the forefront now?

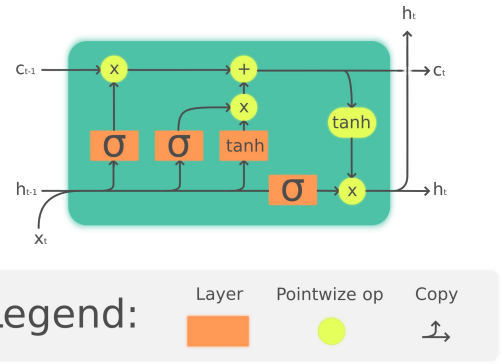
Algorithms

1990s: Computers become faster, GPUs developed

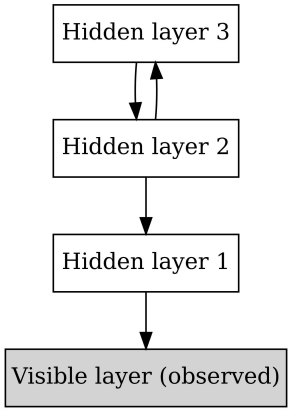
1991: The vanishing gradient problem is identified



1997: Hochreiter and Schmidhuber develop long short-term memory



2006: Hinton and others show that deeper networks can be trained one layer at a time



Why is deep learning at the forefront now?

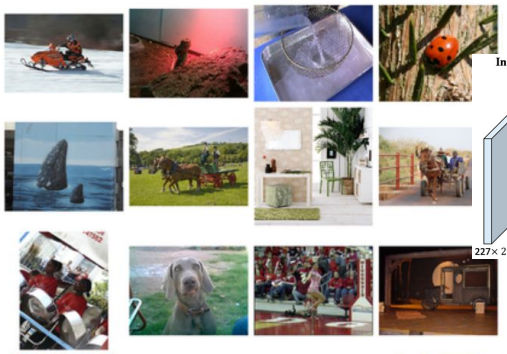
Algorithms

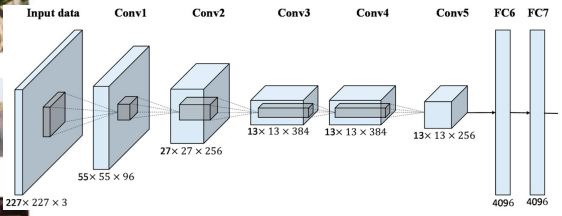
2009: Fei-fei Li releases ImageNet, a classification dataset of 14 million labeled images

2012: AlexNet, a CNN, wins the Large Scale Visual Recognition Challenge — by a lot

2014: Goodfellow designs generative adversarial networks for data generation

2015-2016: Deep learning frameworks like TensorFlow, Keras, and PyTorch are released



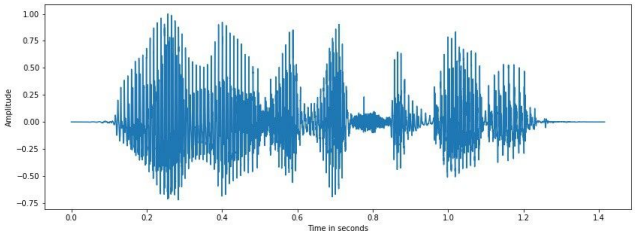


What's so special about deep learning?

Deep learning has made significant improvements in performance on tasks involving unstructured data

Images

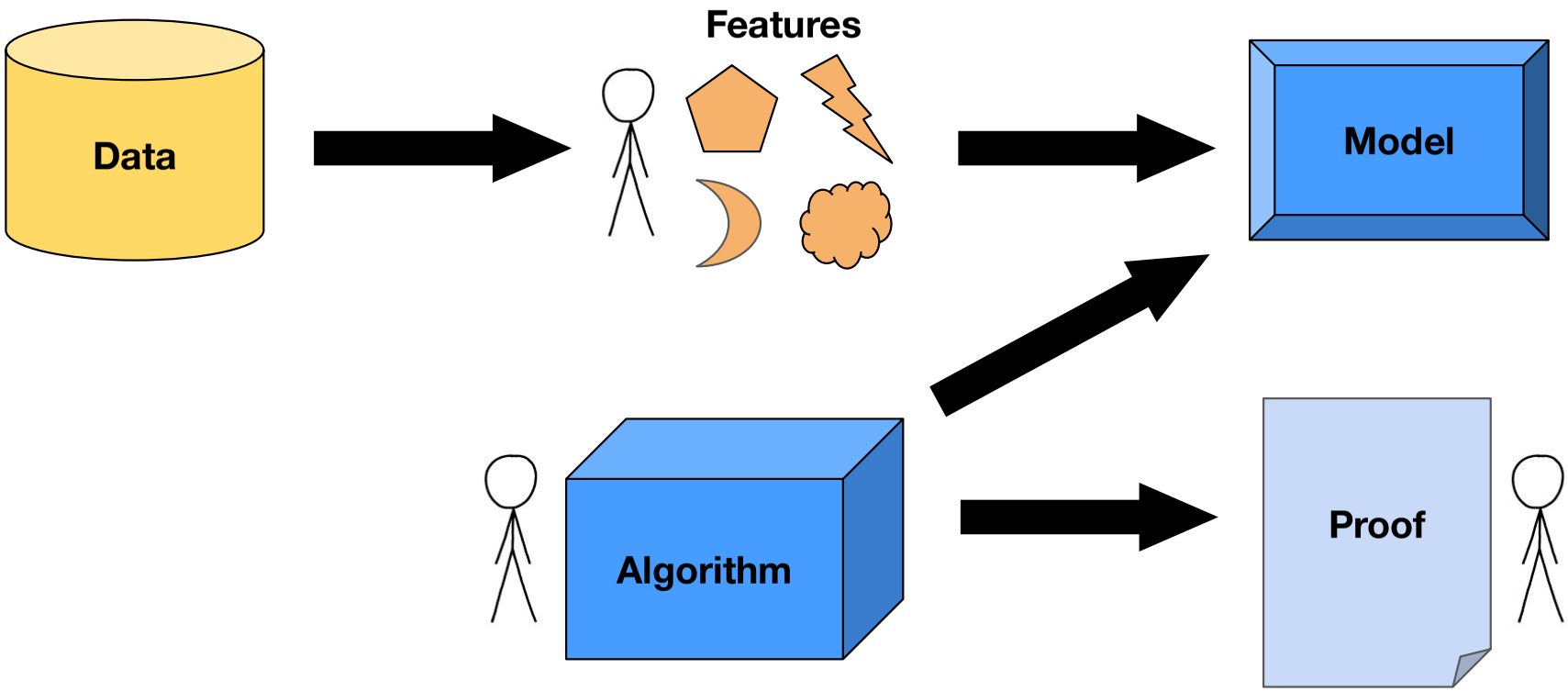
Speech



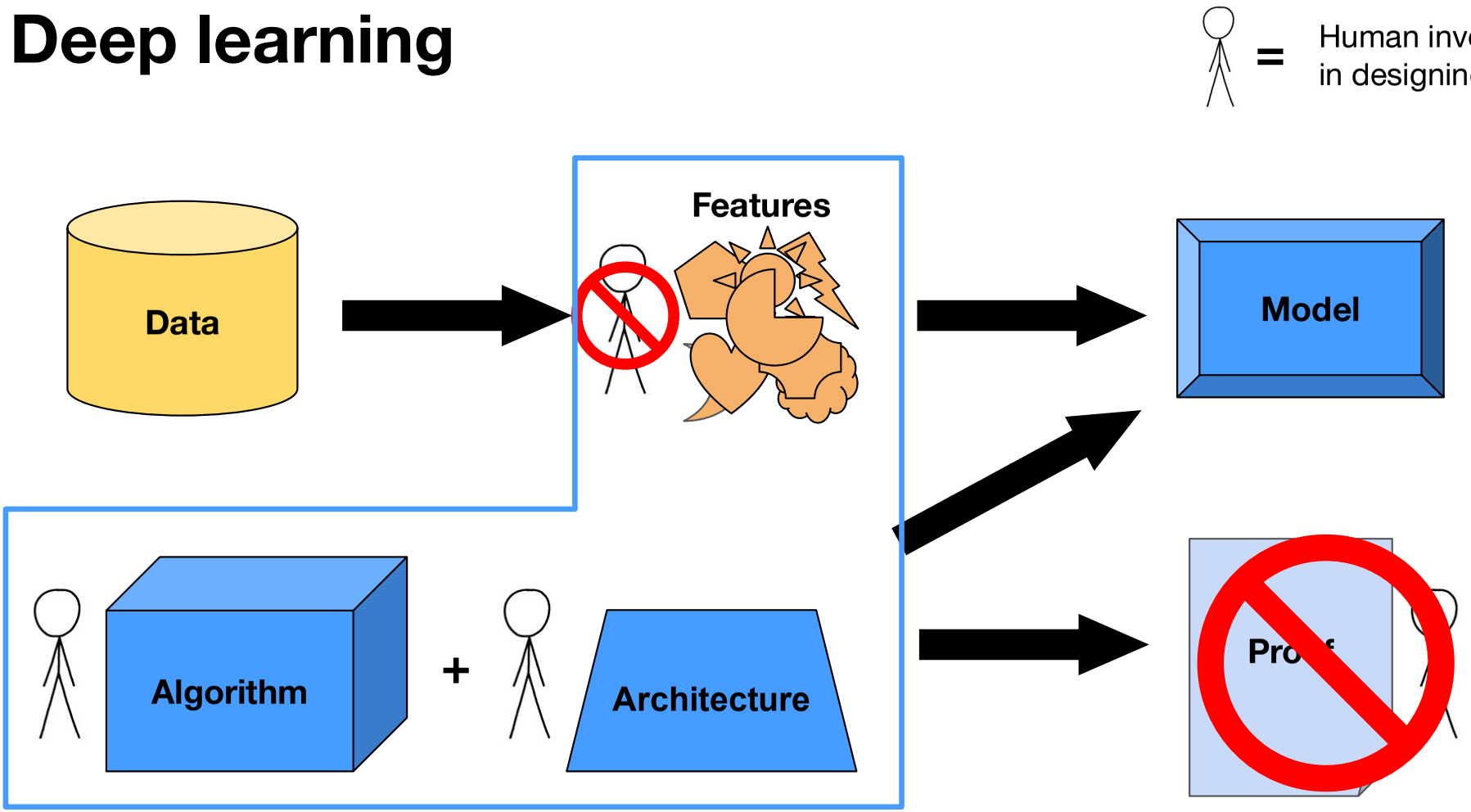
Text

It is a truth universally acknowledged, that a single man in possession of a good fortune, must be in want of a wife. However little known the feelings or views of such a man may be on his first entering a neighbourhood, this truth is so well fixed in the minds of the surrounding families, that he is considered ...

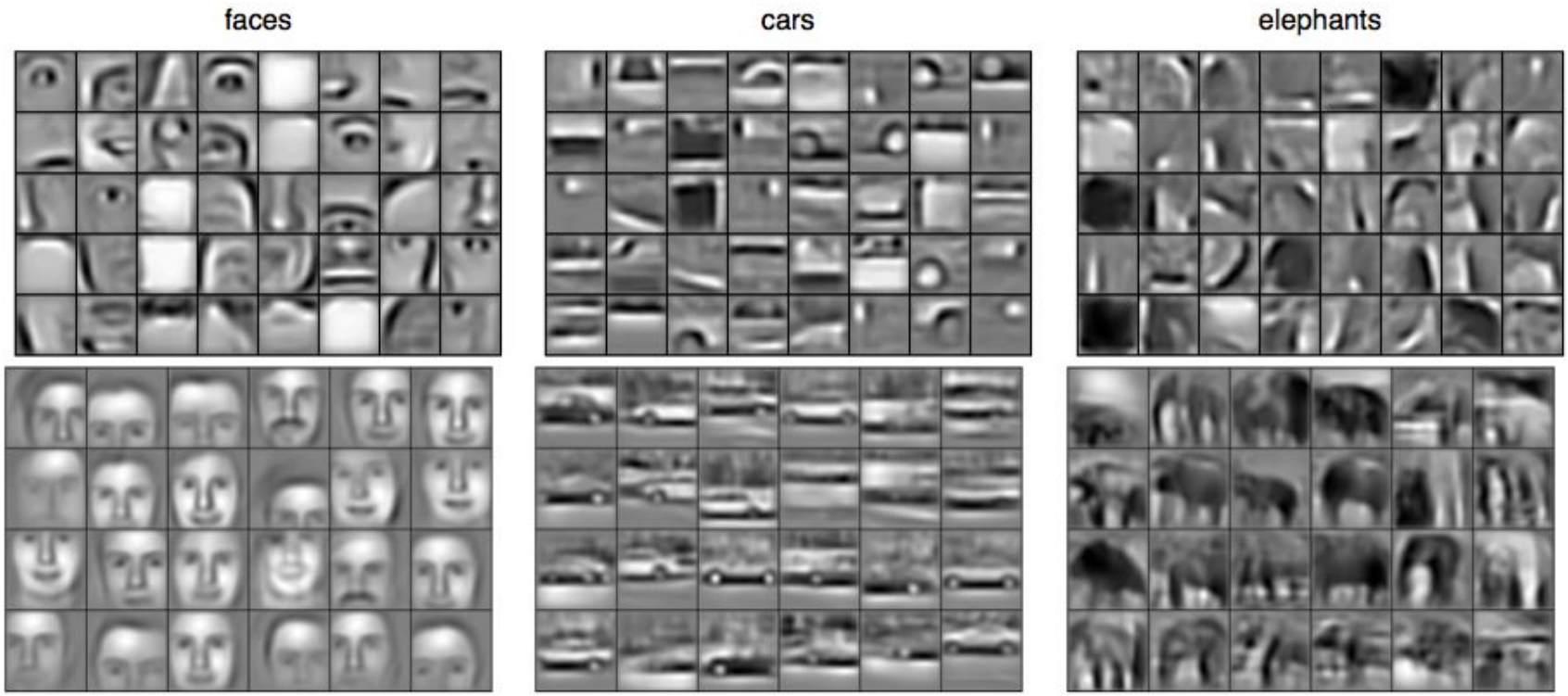
Traditional machine learning



Deep learning



Deep learning-generated features

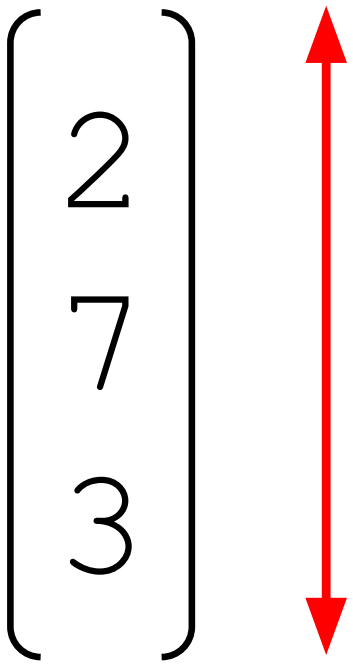


Lee *et al.* "Convolutional Deep Belief Networks for Scalable Unsupervised Learning of Hierarchical Representations" (2009)

Math Review

Vectors, matrices, and tensors

What is a vector?

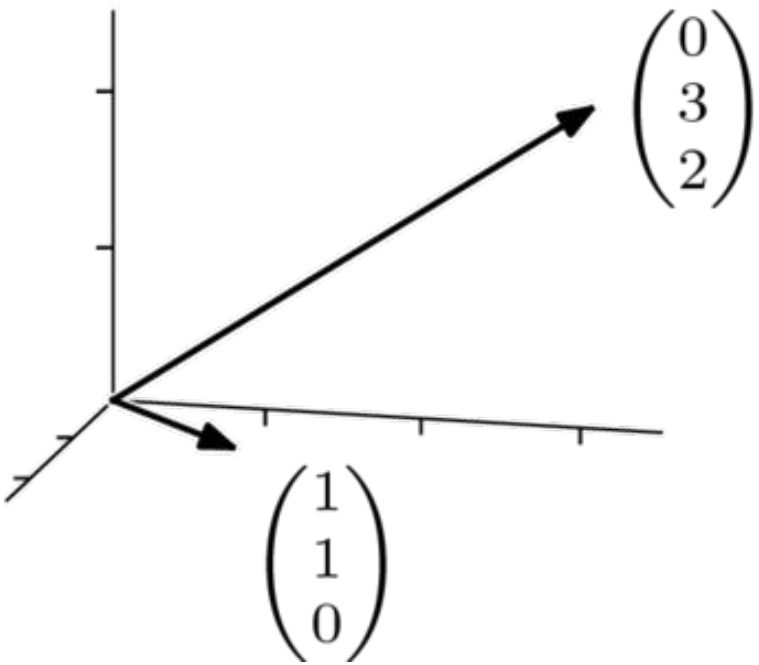


An array (or list) of numbers

Dimension = 3

$$\vec{v} \in \mathbb{R}^3$$

What is a vector?



In addition to linear algebra, you may have learned about vectors in physics courses as entities with direction and magnitude

Here are two more vectors of dimension 3, visualized in Euclidean space

Vector operations

1. Scalar multiplication

$$4 * \begin{pmatrix} 2 \\ 7 \\ 3 \end{pmatrix} = \begin{pmatrix} 8 \\ 28 \\ 12 \end{pmatrix}$$

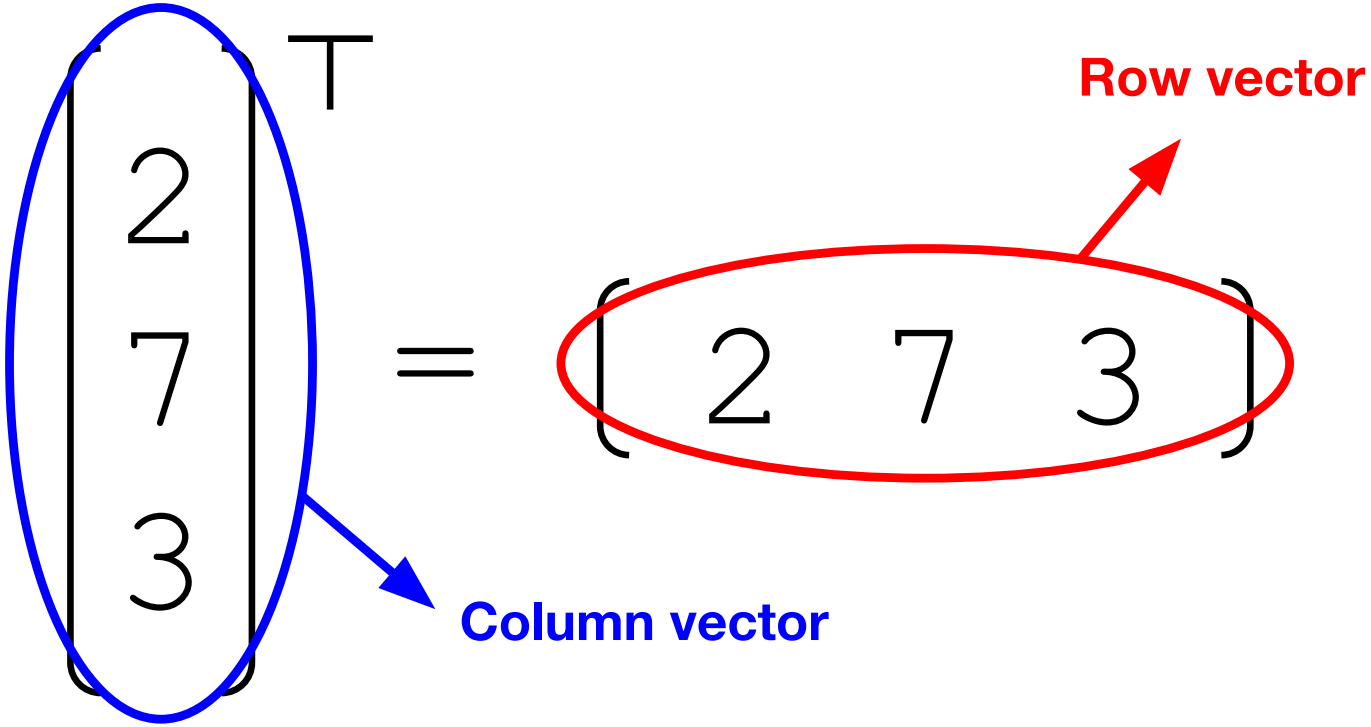
Vector operations

2. Addition

$$\begin{bmatrix} 2 \\ 7 \\ 3 \end{bmatrix} + \begin{bmatrix} 1 \\ 3 \\ 6 \end{bmatrix} = \begin{bmatrix} 3 \\ 10 \\ 9 \end{bmatrix}$$

Vector operations

3. Transpose



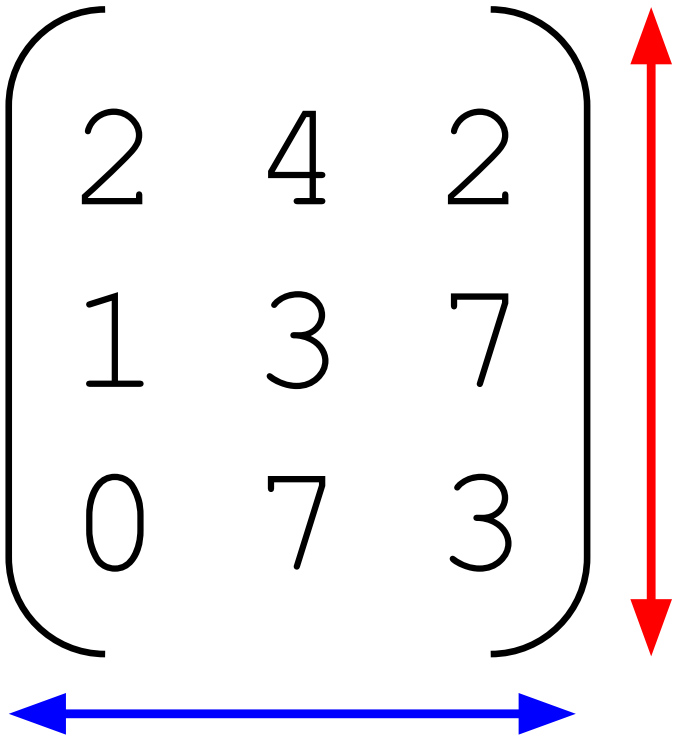
Vector operations

4. Inner product

$$\vec{u}^{\top}\vec{v} = w$$

$$\begin{bmatrix} 2 & 7 & 3 \end{bmatrix} \begin{bmatrix} 1 \\ 3 \\ 6 \end{bmatrix} = 2*1+7*3+3*6 = 41$$

What is a matrix?



A rectangular array (or table) of numbers

What is a matrix?

$$\begin{array}{c} \\ 1 \\ 2 \\ 3 \\ \vdots \\ m \end{array} \begin{array}{c} \begin{array}{cccc} 1 & 2 & \dots & n \end{array} \\ \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ a_{31} & a_{32} & \dots & a_{3n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{bmatrix} \end{array}$$

$$\mathbf{A} \in \mathbb{R}^{m \times n}$$

What is a matrix?

$$\begin{pmatrix} \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix} & \begin{bmatrix} 4 \\ 3 \\ 7 \end{bmatrix} & \begin{bmatrix} 2 \\ 7 \\ 3 \end{bmatrix} \end{pmatrix}$$

You can think of a matrix as a row vector of column vectors

What is a matrix?

$$\begin{pmatrix} \begin{pmatrix} 2 & 4 & 2 \end{pmatrix} \\ \begin{pmatrix} 1 & 3 & 7 \end{pmatrix} \\ \begin{pmatrix} 0 & 7 & 3 \end{pmatrix} \end{pmatrix}$$

… or as a column vector of row vectors

Matrix operations

1. Scalar multiplication
2. Addition

$$2 * \begin{pmatrix} 2 & 4 & 2 \\ 1 & 3 & 7 \\ 0 & 7 & 3 \end{pmatrix} = \begin{pmatrix} 4 & 8 & 4 \\ 2 & 6 & 14 \\ 0 & 14 & 6 \end{pmatrix}$$

Matrix operations

3. Transpose

$$A = \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix}$$

Source: https://en.wikipedia.org/wiki/Transpose

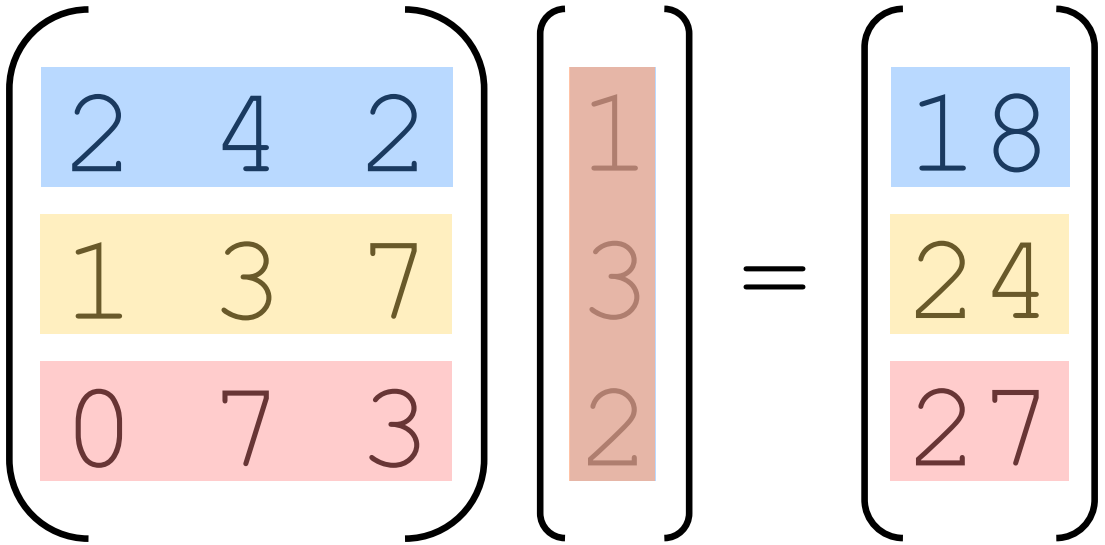
Matrix operations

3. Transpose

$$\left(\begin{bmatrix}2\\1\\0\end{bmatrix}\begin{bmatrix}4\\3\\7\end{bmatrix}\begin{bmatrix}2\\7\\3\end{bmatrix}\right)^{\top} = \begin{pmatrix}2 & 1 & 0\\4 & 3 & 7\\2 & 7 & 3\end{pmatrix}$$

Matrix operations

4. Multiplication with a vector



Matrix operations

4. Multiplication with a vector

$$\left(\begin{bmatrix}2\\1\\0\end{bmatrix}\begin{bmatrix}4\\3\\7\end{bmatrix}\begin{bmatrix}2\\7\\3\end{bmatrix}\right)\begin{bmatrix}1\\3\\2\end{bmatrix}=\begin{bmatrix}18\\24\\27\end{bmatrix}$$

Matrix operations

4. Multiplication with a vector

$$1\begin{pmatrix}2\\1\\0\end{pmatrix}+3\begin{pmatrix}4\\3\\7\end{pmatrix}+2\begin{pmatrix}2\\7\\3\end{pmatrix}=\begin{pmatrix}18\\24\\27\end{pmatrix}$$

Matrix operations

4. Multiplication with a vector

$$\left(\begin{bmatrix} 2 & 4 & 2 \\ 1 & 3 & 7 \\ 0 & 7 & 3 \end{bmatrix}\right)\begin{bmatrix} 1 \\ 3 \\ 2 \end{bmatrix} = \begin{bmatrix} 18 \\ 24 \\ 27 \end{bmatrix}$$

Matrix operations

4. Multiplication with a vector

$$\begin{pmatrix} \begin{bmatrix} 2 & 4 & 2 \end{bmatrix} \begin{bmatrix} 1 \\ 3 \\ 2 \end{bmatrix} \\ \\ \begin{bmatrix} 1 & 3 & 7 \end{bmatrix} \begin{bmatrix} 1 \\ 3 \\ 2 \end{bmatrix} \\ \vdots \end{pmatrix} = \begin{pmatrix} 18 \\ 24 \\ 27 \end{pmatrix}$$

Matrix operations

4. Multiplication with a vector

$$\begin{pmatrix} \vec{a}_1^\top \\ \vec{a}_2^\top \\ \vec{a}_3^\top \end{pmatrix} \vec{b} = \begin{pmatrix} 18 \\ 24 \\ 27 \end{pmatrix}$$

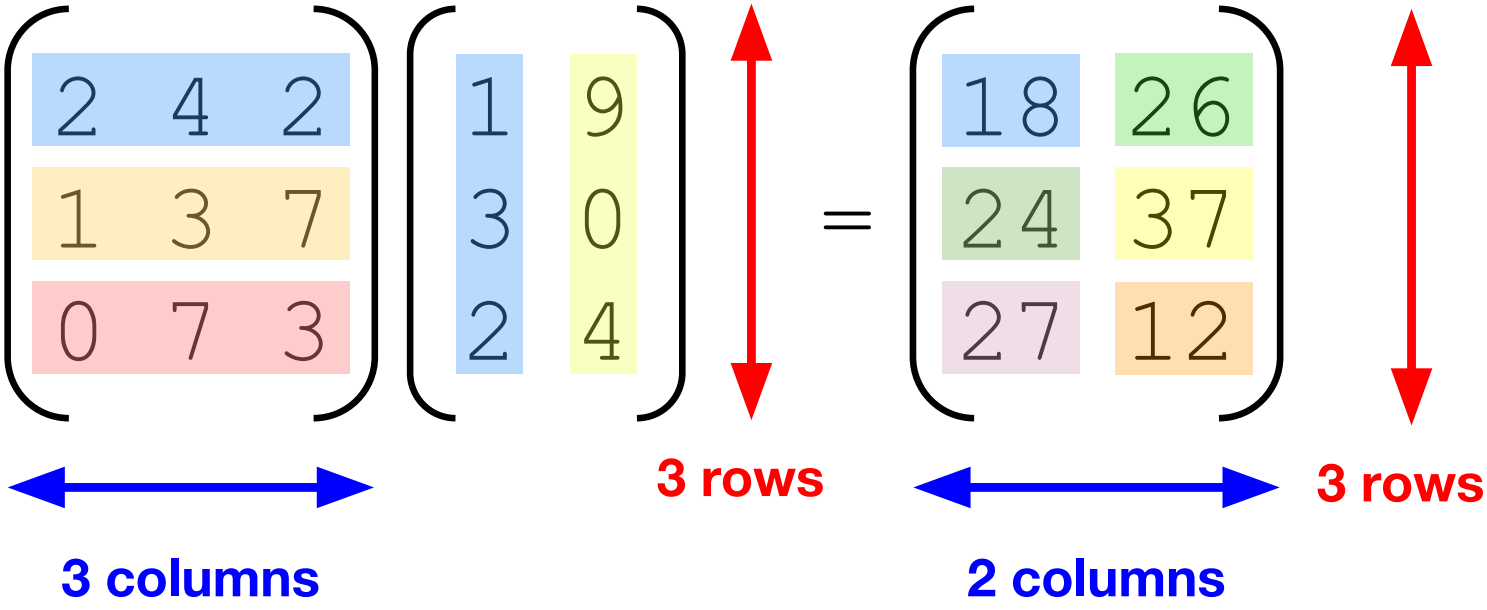
Matrix operations

4. Multiplication with a vector

$$\begin{pmatrix} \vec{a}_1^\top \vec{b} \\ \vec{a}_2^\top \vec{b} \\ \vec{a}_3^\top \vec{b} \end{pmatrix} = \begin{pmatrix} 18 \\ 24 \\ 27 \end{pmatrix}$$

Matrix operations

4. Multiplication with another matrix



Matrix operations

4. Multiplication with another matrix

$$\begin{pmatrix} 2 & 4 & 2 \\ 1 & 3 & 7 \\ 0 & 7 & 3 \end{pmatrix} \left(\begin{bmatrix} 1 \\ 3 \\ 2 \end{bmatrix} \begin{bmatrix} 9 \\ 0 \\ 4 \end{bmatrix} \right) = \begin{pmatrix} 18 & 26 \\ 24 & 37 \\ 27 & 12 \end{pmatrix}$$

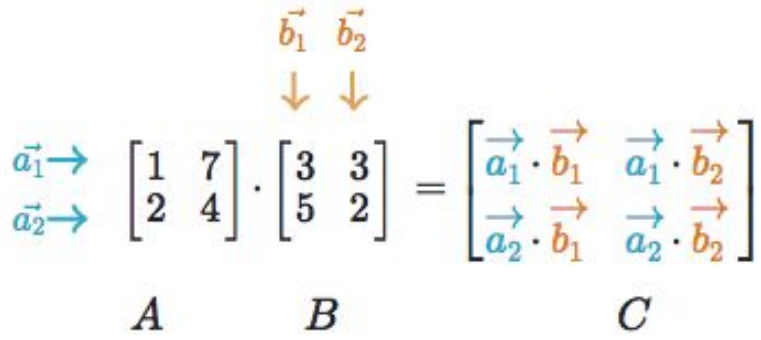
Matrix operations

4. Multiplication with another matrix

$$\mathbf{A}\left(\begin{bmatrix}1\\3\\2\end{bmatrix}\begin{bmatrix}9\\0\\4\end{bmatrix}\right) = \left(\mathbf{A}\begin{bmatrix}1\\3\\2\end{bmatrix} \quad \mathbf{A}\begin{bmatrix}9\\0\\4\end{bmatrix}\right)$$

Matrix operations

4. Multiplication with another matrix



Source: https://ml-cheatsheet.readthedocs.io/en/latest/linear_algebra.html#matrix-multiplication

Poll: Matrix multiplication

Go to **tinyurl.com/dlworkshop2021**

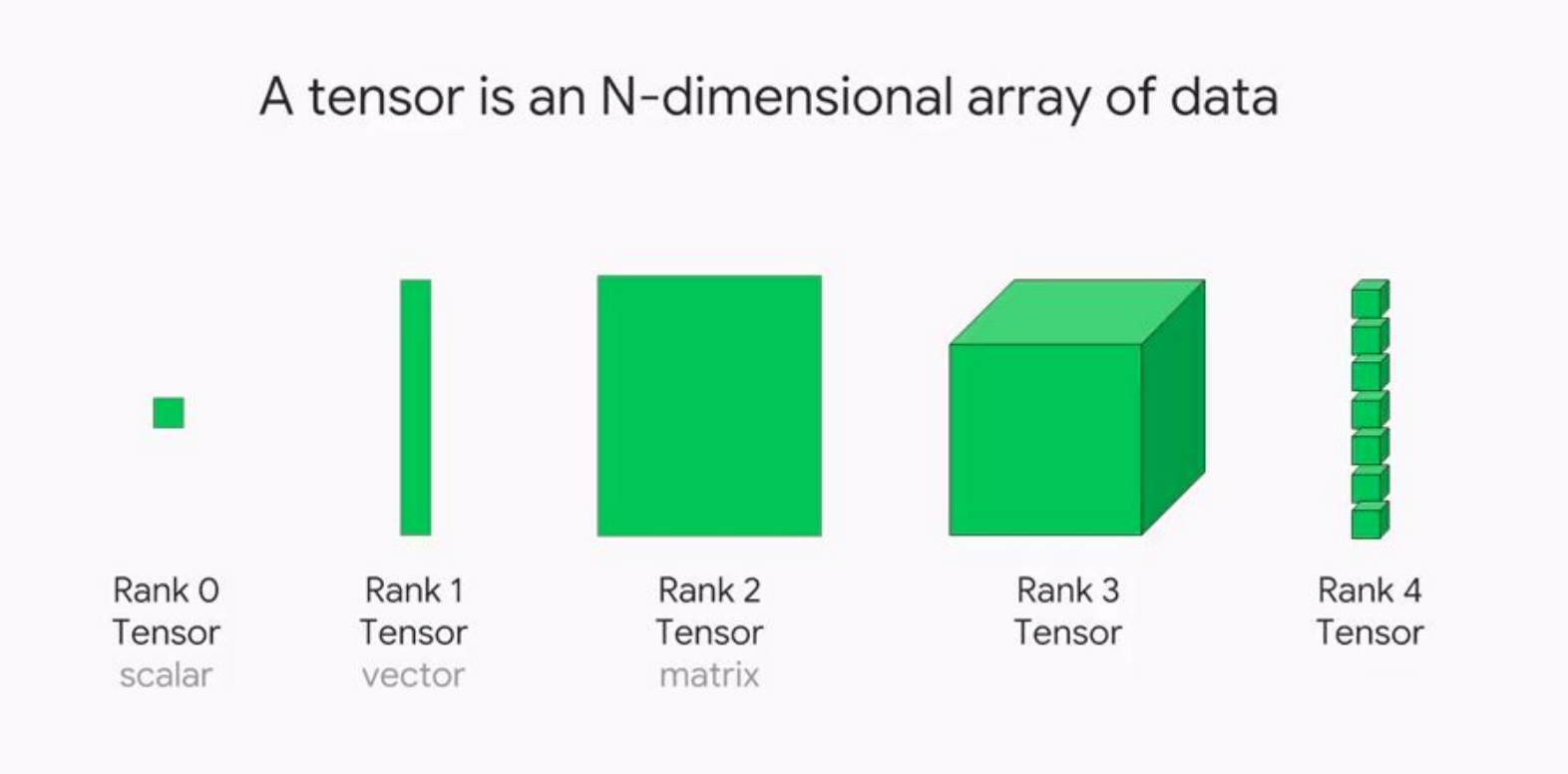
What are the dimensions of the matrix resulting from:

$$\begin{pmatrix} 2 & 4 & 2 & 8 & 4 & 1 & 5 & 0 \\ 1 & 3 & 7 & 9 & 3 & 2 & 6 & 8 \\ 0 & 7 & 3 & 1 & 0 & 4 & 9 & 3 \end{pmatrix} \begin{pmatrix} 3 & 4 \\ 2 & 9 \\ 0 & 1 \\ 5 & 5 \\ 3 & 7 \\ 6 & 4 \\ 2 & 1 \\ 4 & 0 \end{pmatrix}$$

A. 8 x 8 B. 8 x 2 C. 3 x 2 D. Not valid

Source: https://ml-cheatsheet.readthedocs.io/en/latest/linear_algebra.html#matrix-multiplication

What is a tensor?



Source: https://medium.com/mlait/tensors-representation-of-data-in-neural-networks-bbe8a711b93b

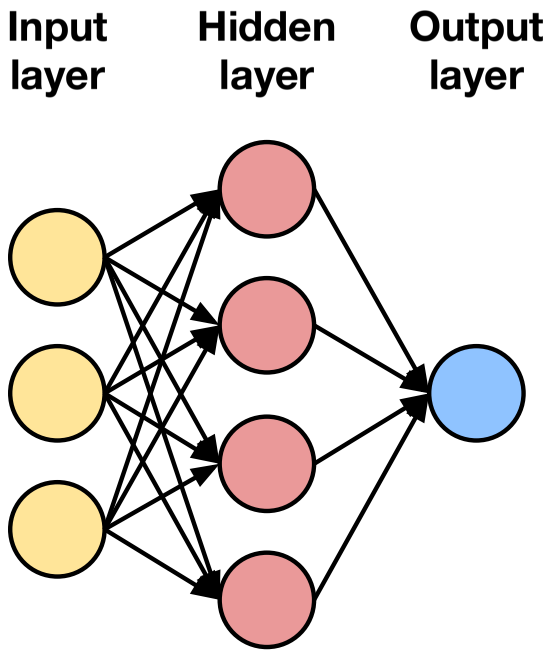
Neural Networks

Neural networks

We'll start with a *fully connected* neural network.

1. Single layer
2. Single neuron
3. Multiple layers
4. Input and output

Later, we'll cover other types of layers (convolution, max-pool, …)



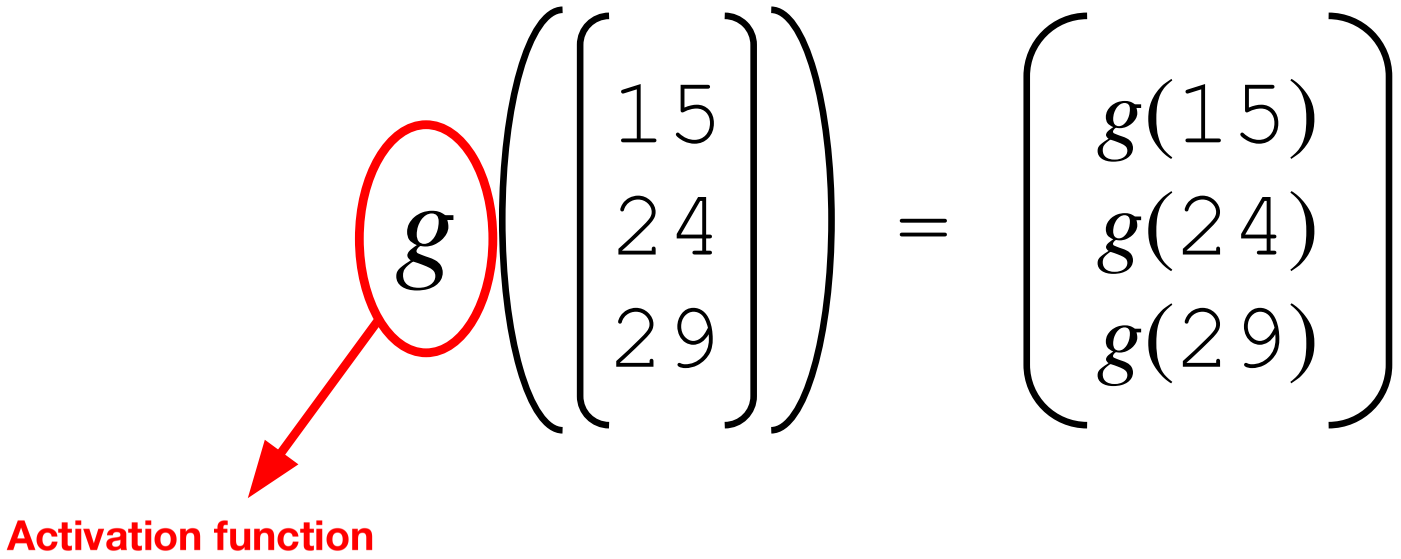
What does a single layer in a neural network do?

First, it involves some matrix operations...

$$\begin{pmatrix} 2 & 4 & 2 \\ 1 & 3 & 7 \\ 0 & 7 & 3 \end{pmatrix} \begin{pmatrix} 1 \\ 3 \\ 2 \end{pmatrix} + \begin{pmatrix} -3 \\ 0 \\ 2 \end{pmatrix} = \begin{pmatrix} 15 \\ 24 \\ 29 \end{pmatrix}$$

What does a single layer in a neural network do?

Then, the intermediate values are passed through a nonlinear function...

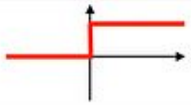
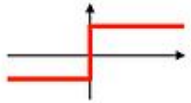
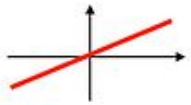
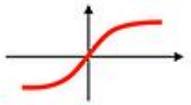
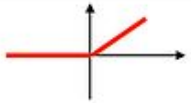
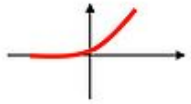


Activation functions

There exist a number of activation functions, some of which were designed with neurons in mind

What's the purpose?

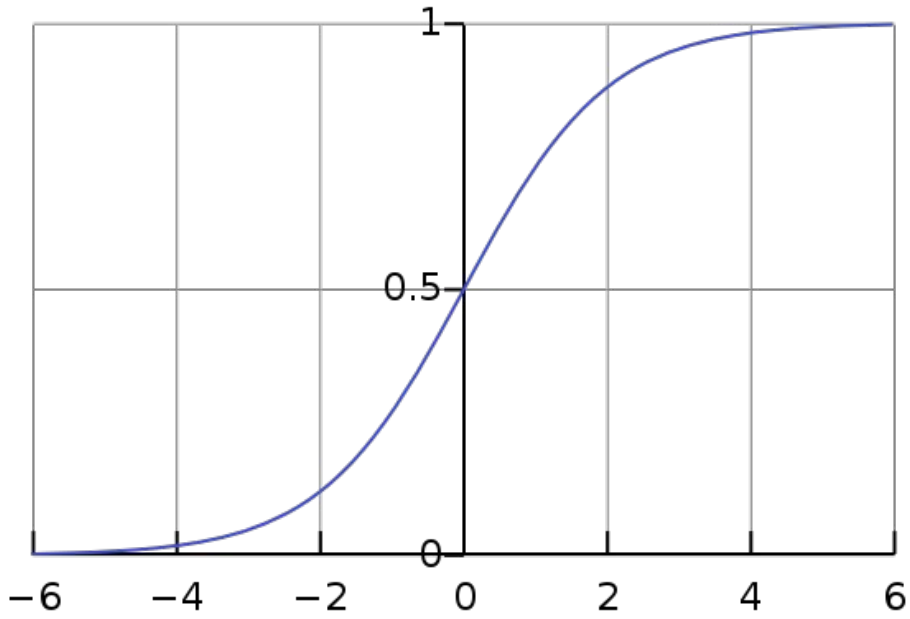
- Most phenomena are not linear, so we introduce some nonlinearities to the network

Activation function	Equation	Example	1D Graph
Unit step (Heaviside)	$\phi(z) = \begin{cases} 0, & z < 0, \\ 0.5, & z = 0, \\ 1, & z > 0, \end{cases}$	Perceptron variant	
Sign (Signum)	$\phi(z) = \begin{cases} -1, & z < 0, \\ 0, & z = 0, \\ 1, & z > 0, \end{cases}$	Perceptron variant	
Linear	$\phi(z) = z$	Adaline, linear regression	
Piece-wise linear	$\phi(z) = \begin{cases} 1, & z \geq \frac{1}{2}, \\ z + \frac{1}{2}, & -\frac{1}{2} < z < \frac{1}{2}, \\ 0, & z \leq -\frac{1}{2}, \end{cases}$	Support vector machine	
Logistic (sigmoid)	$\phi(z) = \frac{1}{1 + e^{-z}}$	Logistic regression, Multi-layer NN	
Hyperbolic tangent	$\phi(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$	Multi-layer Neural Networks	
Rectifier, ReLU (Rectified Linear Unit)	$\phi(z) = max(0, z)$	Multi-layer Neural Networks	
Rectifier, softplus	$\phi(z) = \ln(1 + e^z)$	Multi-layer Neural Networks	

"A visual proof that neural nets can compute any function": http://neuralnetworksanddeeplearning.com/chap4.html

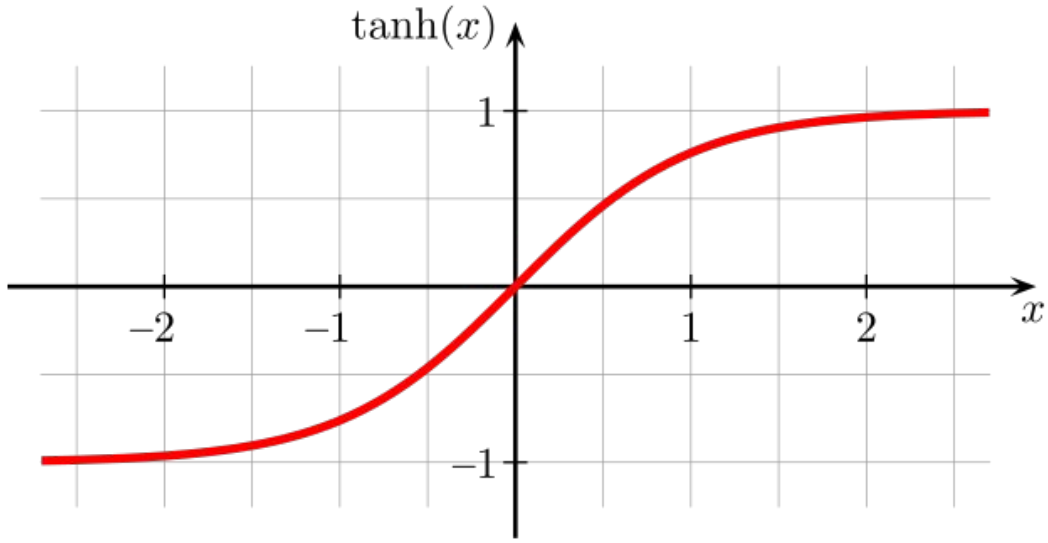
Sigmoid (logistic) activation function

$$\text{sigmoid}(x) = \frac{1}{1 + e^{-x}}$$



Hyperbolic tangent activation function

$$\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$



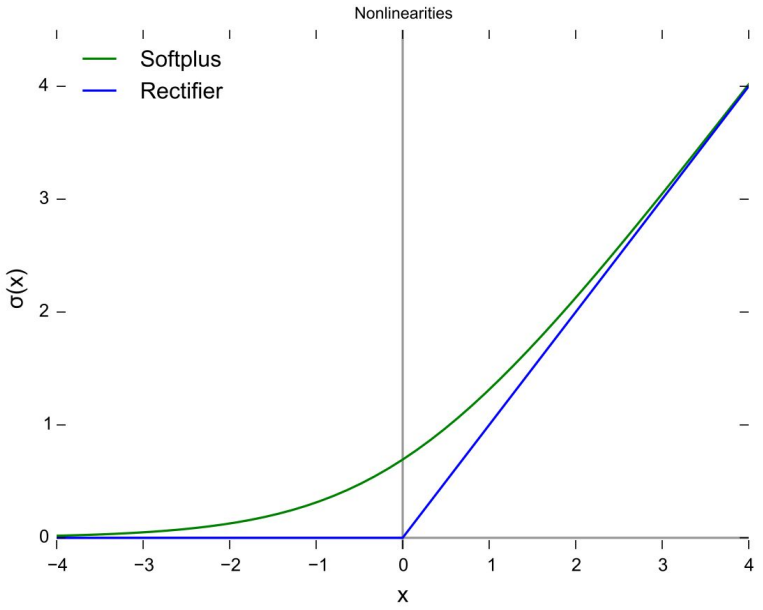
ReLU activation function

Stands for **Re**ctified **L**inear **U**nit

$$\mathrm{ReLU}(x) = \max(0, x)$$

A smooth version of ReLU is softplus

$$\mathrm{softplus}(x) = \ln(1 + e^x)$$



Poll: Activation functions

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As its input goes to infinity, the output of the logistic function goes to...

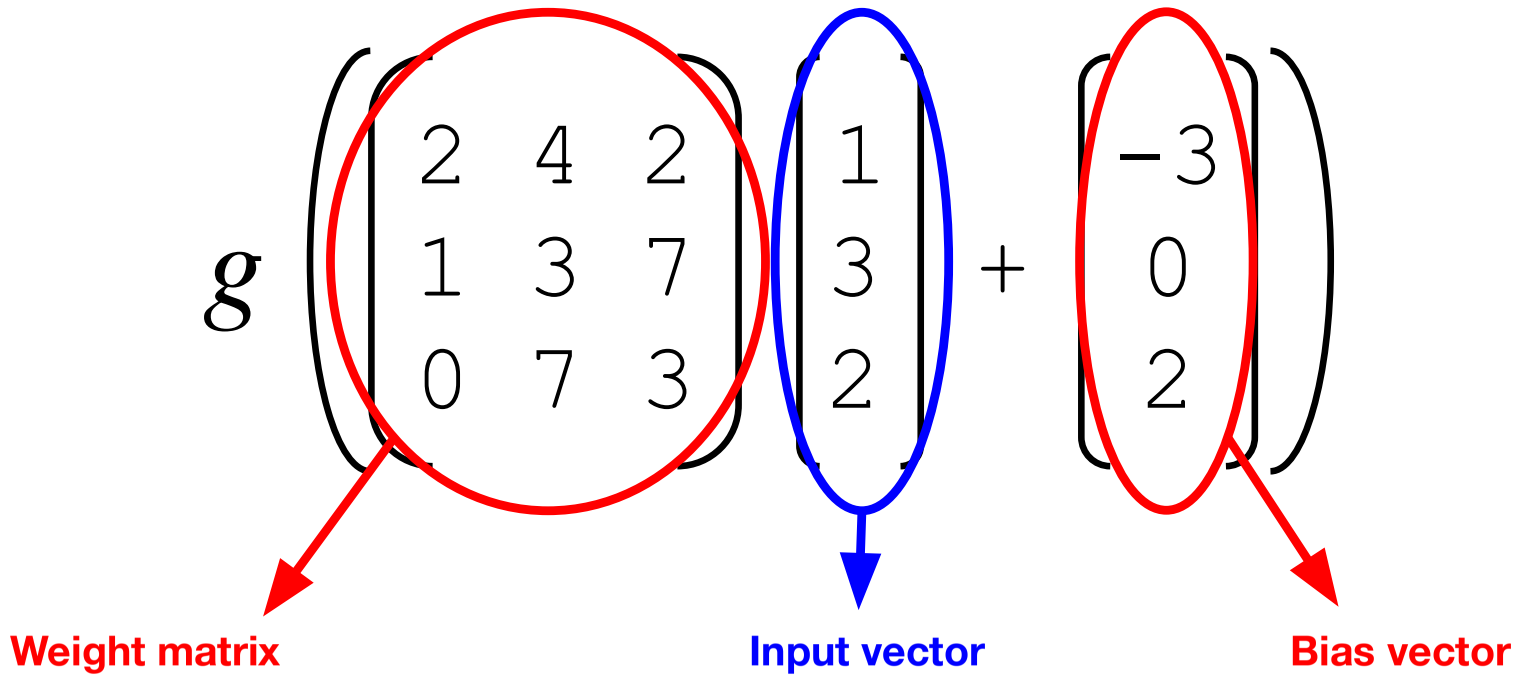
$$\lim_{x \to \infty} \frac{1}{1 + e^{-x}} =$$

A. 0 B. 0.5 C. 1 D. Infinity

Activation functions FAQ

1. Why these activation functions? Why not x^2 or other nonlinear functions?
   a. History of the field
   b. Normalizing layer outputs, concerns with backpropagation (to be discussed)
2. How does one choose among the various options for activation functions?
   a. You don't have to choose -- architectures have already been designed
   b. Sigmoid, tanh, and ReLU are popular choices, with ReLU being the most common. ReLU has fewer vanishing gradient problems than the other 2 (see Session 3). If you're developing your own architecture, you should use your validation set to experiment with choice of activation function.

Recall: a single layer is matrix multiplication followed by a nonlinearity



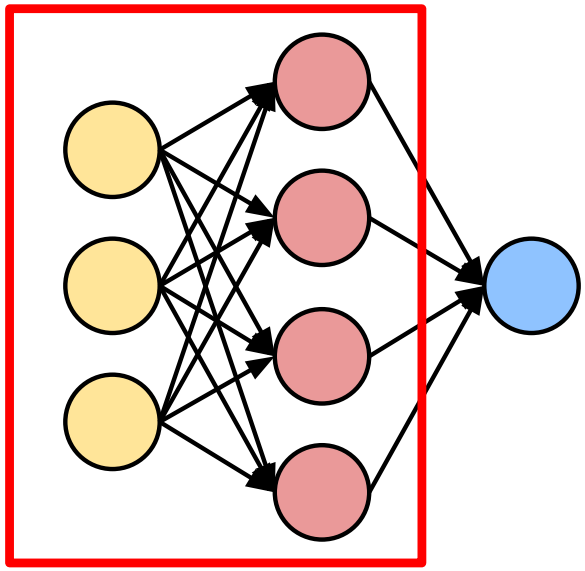
What are the matrix and vectors?

$$g\left(\begin{bmatrix} 2 & 4 & 2 \\ 1 & 3 & 7 \\ 0 & 7 & 3 \end{bmatrix}\begin{bmatrix} 1 \\ 3 \\ 2 \end{bmatrix} + \begin{bmatrix} -3 \\ 0 \\ 2 \end{bmatrix}\right)$$

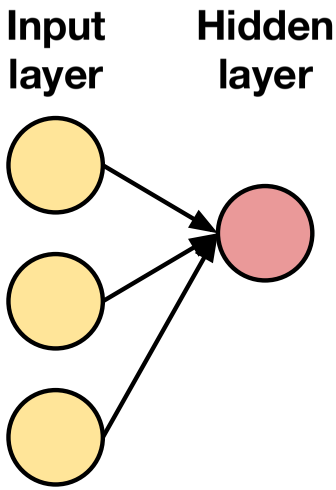
Trainable parameters

A more compact notation

$$g(\mathbf{W}\vec{x} + \vec{b})$$



What does a single neuron do?



Each circle is one element of an input or hidden layer

Each edge is a weight

$$g(\vec{w}_1^{\top}\vec{x} + b_1)$$

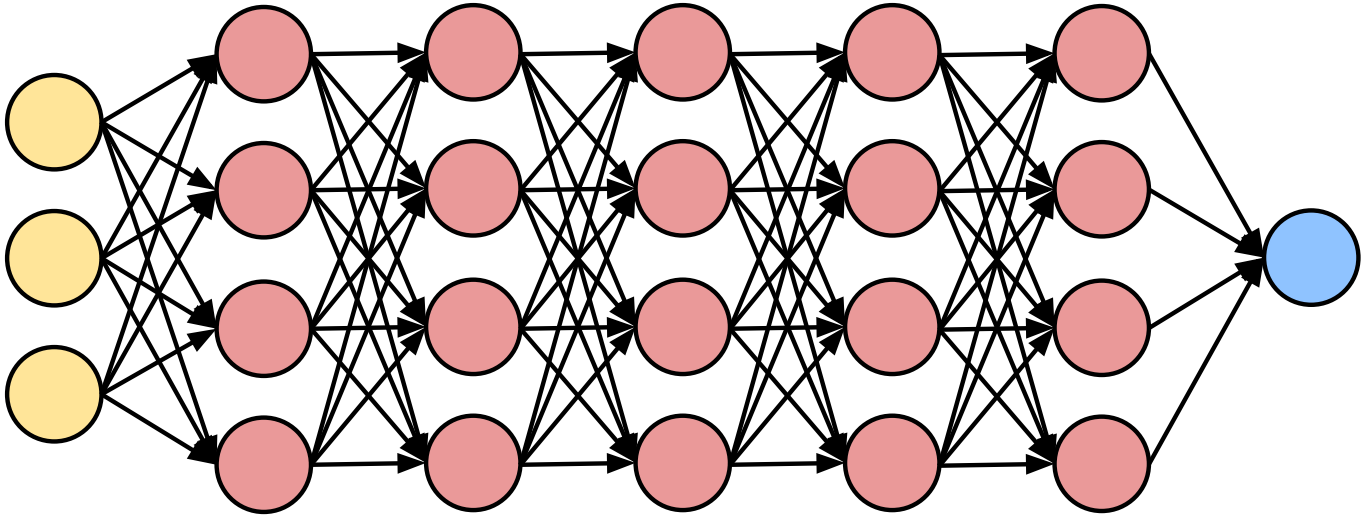
Weights for each neuron

$$\mathbf{W} = \begin{pmatrix} 2 & 4 & 2 \\ 1 & 3 & 7 \\ 0 & 7 & 3 \end{pmatrix} = \begin{pmatrix} w_1^\top \\ w_2^\top \\ w_3^\top \end{pmatrix}$$

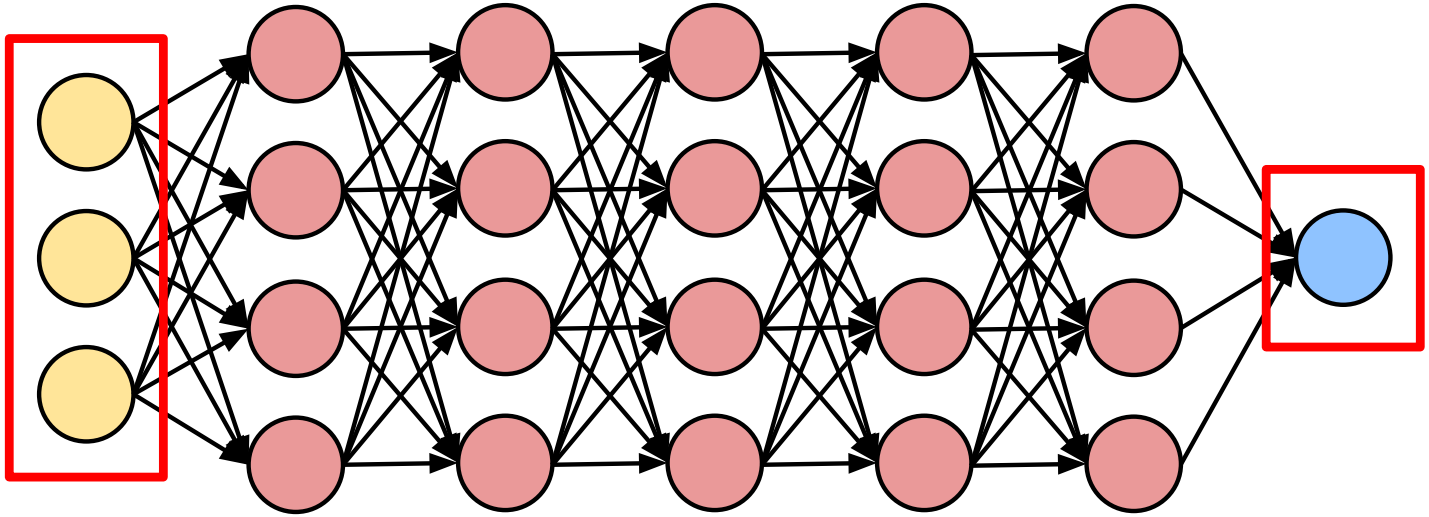
A fully connected layer with weight matrix $\mathbf{W} \in \mathbb{R}^{m \times n}$ is a function from $\mathbb{R}^n$ to $\mathbb{R}^m$

Stacking multiple layers

It becomes a *deep* neural network when you use many layers



What are the inputs and outputs?



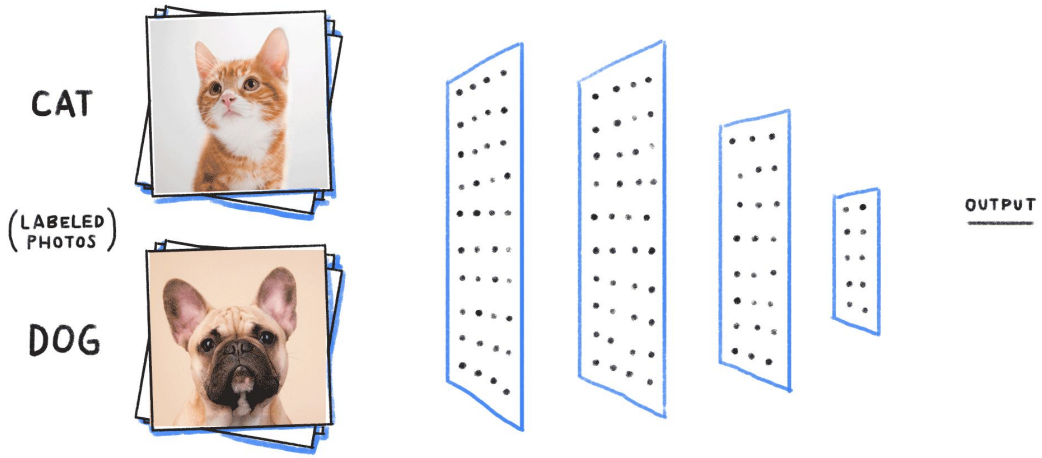
Defining the problem

- You want to predict some output **y** given input **x**
- If **y** is a discrete output (e.g. image classes), then it's a *classification problem*
- If **y** is a continuous variable (e.g. price), then it's a *regression problem*

$$y = \mathrm{DNN}(\vec{x})$$

Defining the problem

- If **y** is a discrete output, you can use one-hot encoding
- If **y** is a continuous variable, it can be output by the network directly



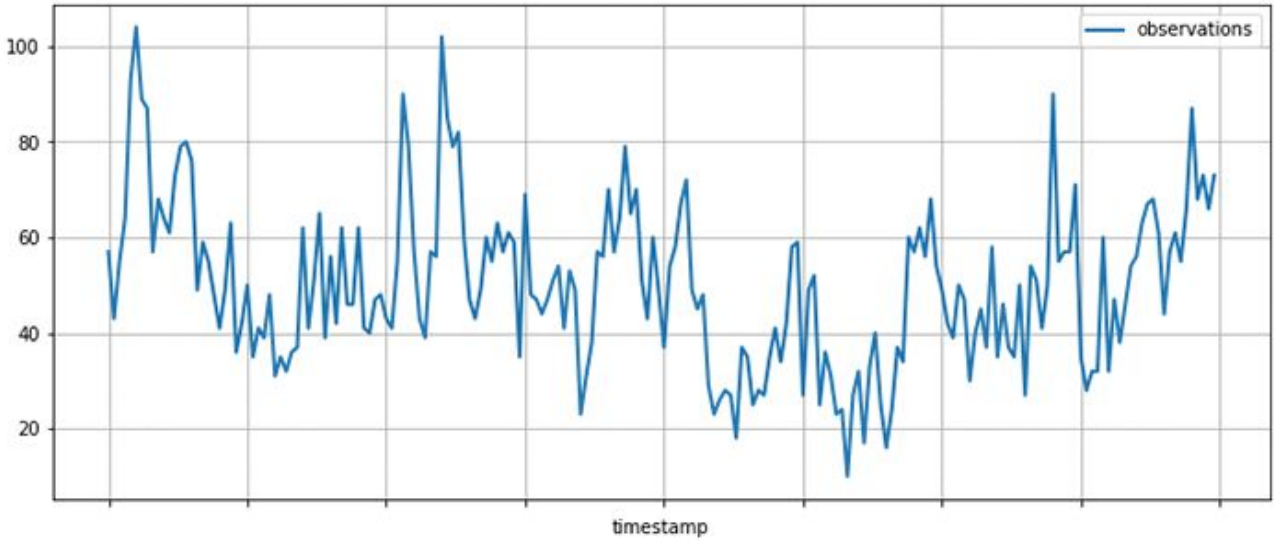
Classes = {cat, dog}

$$y = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{“cat”} \qquad y = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad \text{“dog”}$$

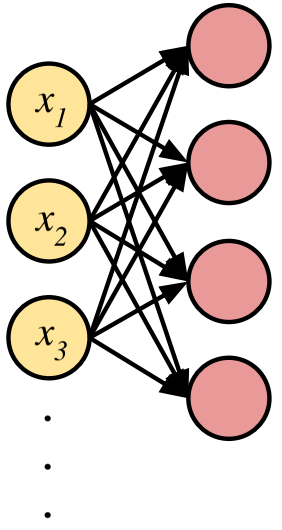
https://becominghuman.ai/building-an-image-classifier-using-deep-learning-in-python-totally-from-a-beginners-perspective-be8dbaf22dd8

Defining the problem

- If **x** is a discrete output, you can use one-hot encoding
- If **x** is a continuous variable, it can be input to the network directly



$$x = \begin{pmatrix} 59 \\ 42 \\ 63 \\ 93 \\ 102 \\ 88 \\ 86 \\ 58 \\ \dots \end{pmatrix}$$

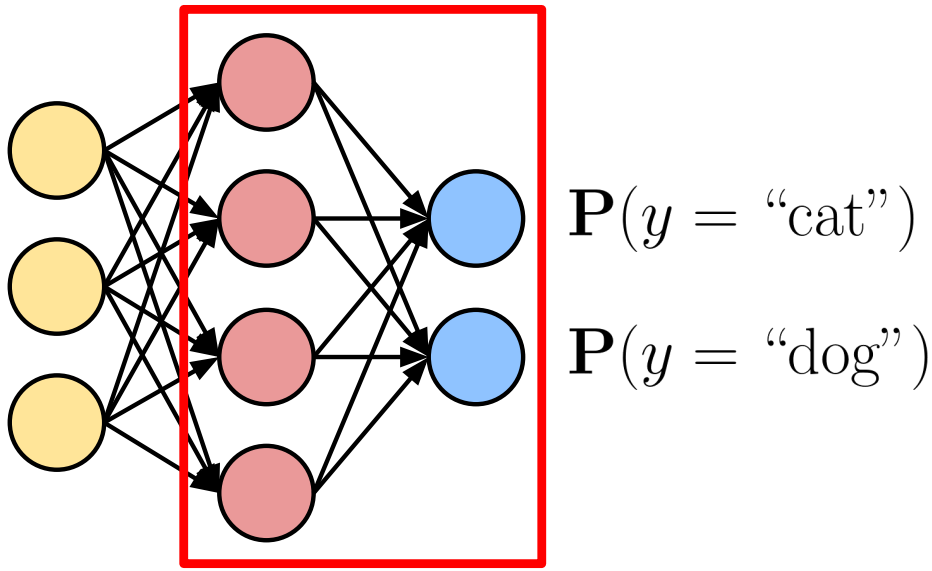


Last layer activation function

For classification, each neuron in the output represents one output class

You want the output to represent the probability that the input belongs to each class

What constraints must the output satisfy?



Last layer activation function

What constraints must the output satisfy?

- Probabilities are positive
- Probabilities sum to 1

$$\mathbf{P}(y = \text{“cat”}) \geq 0$$
$$\mathbf{P}(y = \text{“dog”}) \geq 0$$

$$\mathbf{P}(y = \text{“cat”}) + \mathbf{P}(y = \text{“dog”}) = 1$$

Softmax activation function

$$\text{softmax}(\mathbf{z})_i = \frac{e^{z_i}}{\sum_{j=1}^{n} e^{z_j}}$$

Ensures positivity

Normalizes sum to 1

$$\mathbf{z} = \begin{pmatrix} 1.1 \\ 0.4 \\ -8.2 \\ -0.9 \\ 3.7 \end{pmatrix} \qquad e^{\mathbf{z}} = \begin{pmatrix} e^{1.1} \\ e^{0.4} \\ e^{-8.2} \\ e^{-0.9} \\ e^{3.7} \end{pmatrix} \qquad \frac{e^{\mathbf{z}}}{\sum_{j=1}^{n} e^{z_j}} = \begin{pmatrix} e^{1.1}/\sum_j e^{\mathbf{z}_j} \\ e^{0.4}/\sum_j e^{\mathbf{z}_j} \\ e^{-8.2}/\sum_j e^{\mathbf{z}_j} \\ e^{-0.9}/\sum_j e^{\mathbf{z}_j} \\ e^{3.7}/\sum_j e^{\mathbf{z}_j} \end{pmatrix} = \begin{pmatrix} 0.07 \\ 0.03 \\ 0.00 \\ 0.01 \\ 0.89 \end{pmatrix}$$

Up Next:

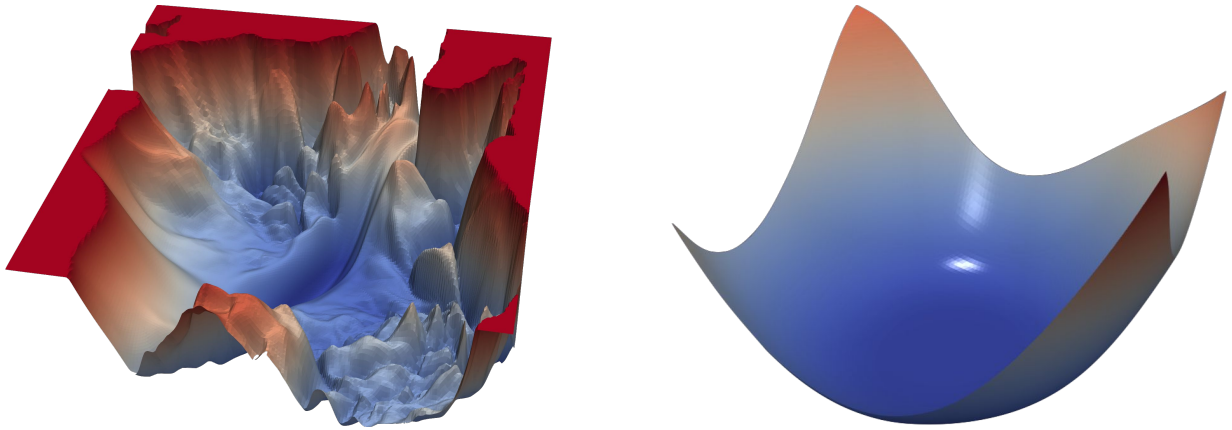
Training neural networks

ICME Summer Workshops 2021

Introduction to Deep Learning

Session 2: 9:45—11:00 AM
Instructor: Sherrie Wang

icme-workshops.github.io/deep-learning



Li *et al.* "Visualizing the Loss Landscape of Neural Nets" (2018)

Workshop Schedule

Day 1

Session 1 (Today 8:00—9:30 AM)

- Introduction
- Examples of deep learning
- Math review
- Neural network basics

Session 2 (Today 9:45—11:00 AM)

- Loss functions
- Gradient descent
- Backpropagation
- Walkthrough of an example

Day 2

Session 3 (Tomorrow 8:00—9:30 AM)

- Overfitting and underfitting
- Convolutional neural networks
- Recurrent neural networks

Session 4 (Tomorrow 9:45—11:00 AM)

- Other architectures
- Deep learning libraries
- Walkthrough of an example
- Failures of deep learning

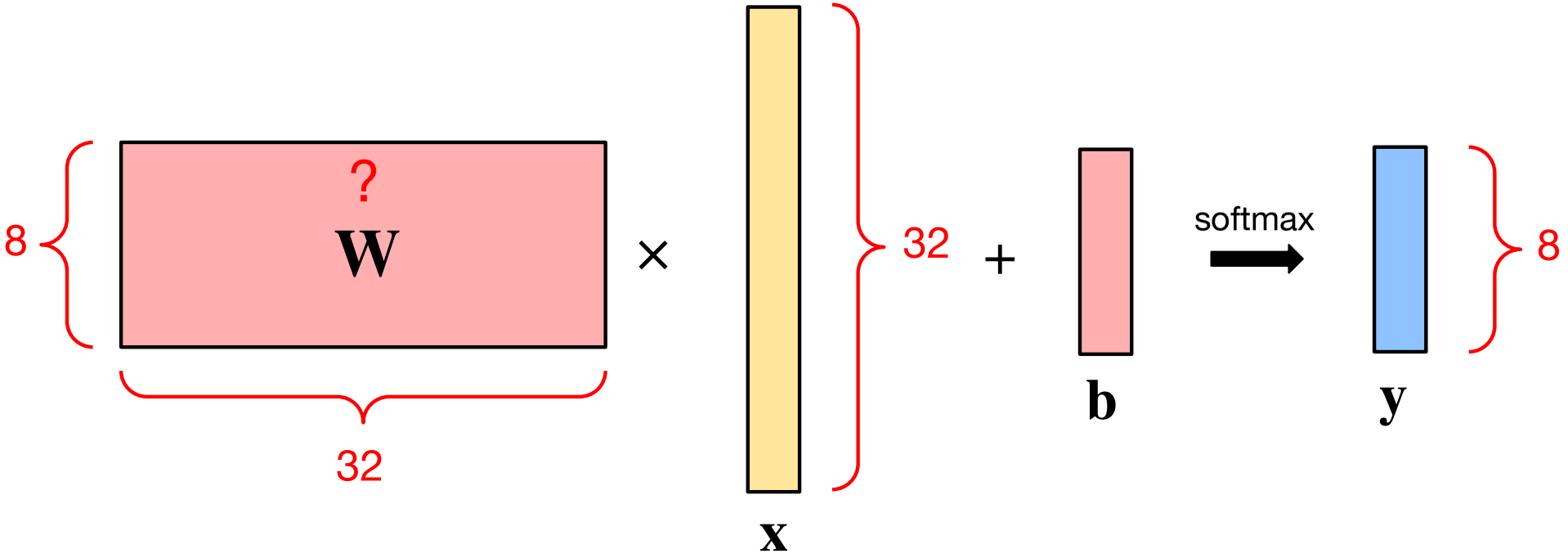
Poll: Weight matrix

Go to **tinyurl.com/dlworkshop2021**

Suppose we have a neural network with 1 fully connected hidden layer. The input is a 32-dimensional vector. The output is a probability distribution across 8 classes. The weight matrix of the hidden layer should have dimension...

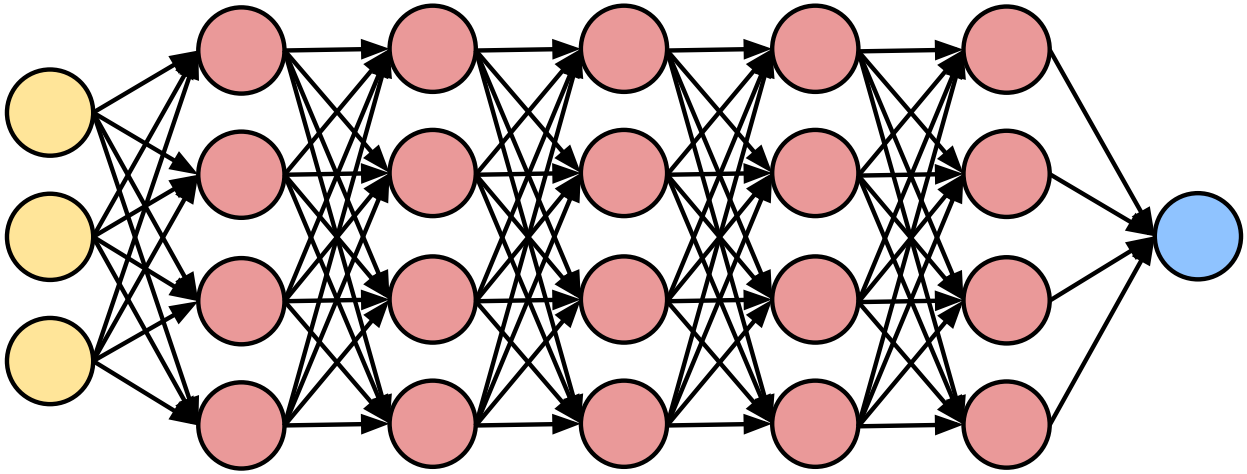
A. 32x1 B. 8x32 C. 32x8 D. 32x32

Poll: Weight matrix



Loss Functions

Training neural networks



$$g\left(\begin{bmatrix} 2 & 4 & 2 \\ 1 & 3 & 7 \\ 0 & 7 & 3 \end{bmatrix}\begin{bmatrix} 1 \\ 3 \\ 2 \end{bmatrix} + \begin{bmatrix} -3 \\ 0 \\ 2 \end{bmatrix}\right)$$

Trainable parameters

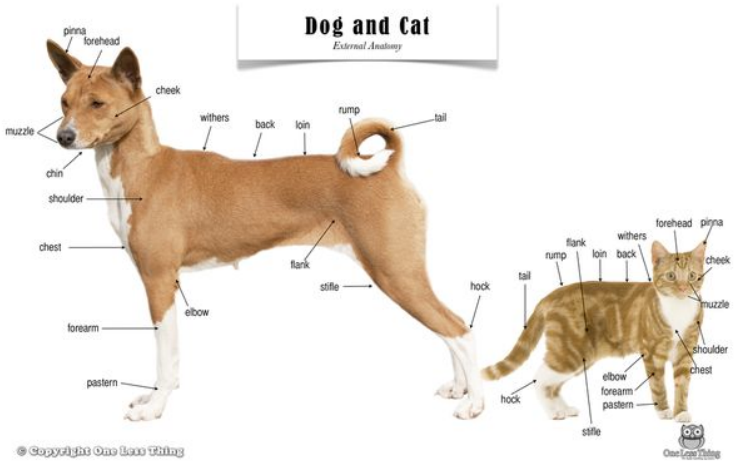
Trained how?

Training neural networks

Machine learning: builds a model based on “training data” in order to make predictions without being explicitly programmed to do so

Not machine learning

Human says: “dogs are like this, and cats are like this…”



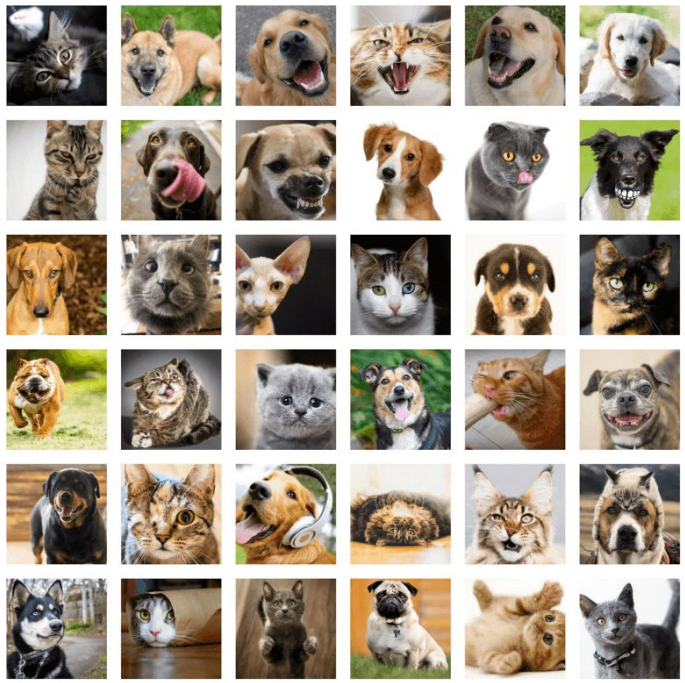
Machine learning

“Here’s a bunch of pictures of cats and dogs. Figure out how to sort them.”

https://mc.ai/deep-learning-vs-machine-learning-a-simple-explanation/

Training neural networks

Dataset



training

Weights & biases

$$\begin{pmatrix} 2 & 4 & 2 \\ 1 & 3 & 7 \\ 0 & 7 & 3 \end{pmatrix} \quad \begin{pmatrix} -3 \\ 0 \\ 2 \end{pmatrix}$$

https://mc.ai/deep-learning-vs-machine-learning-a-simple-explanation/

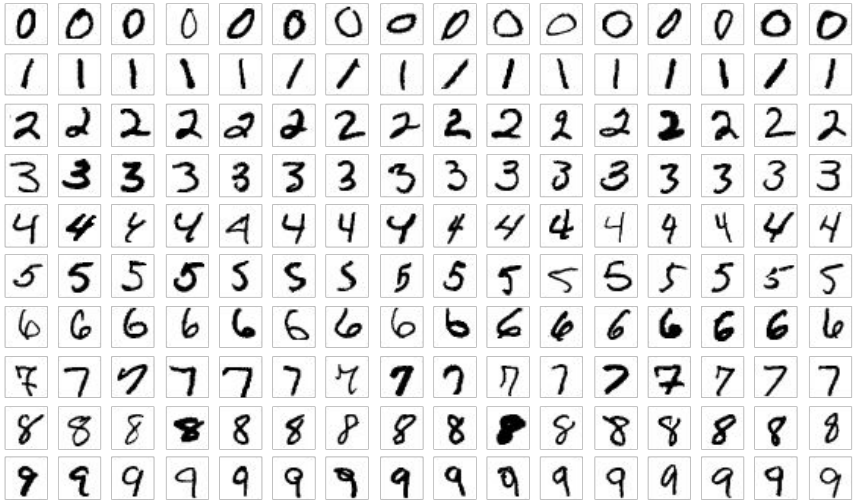
Supervised learning

Dataset has labels
(Created by humans)

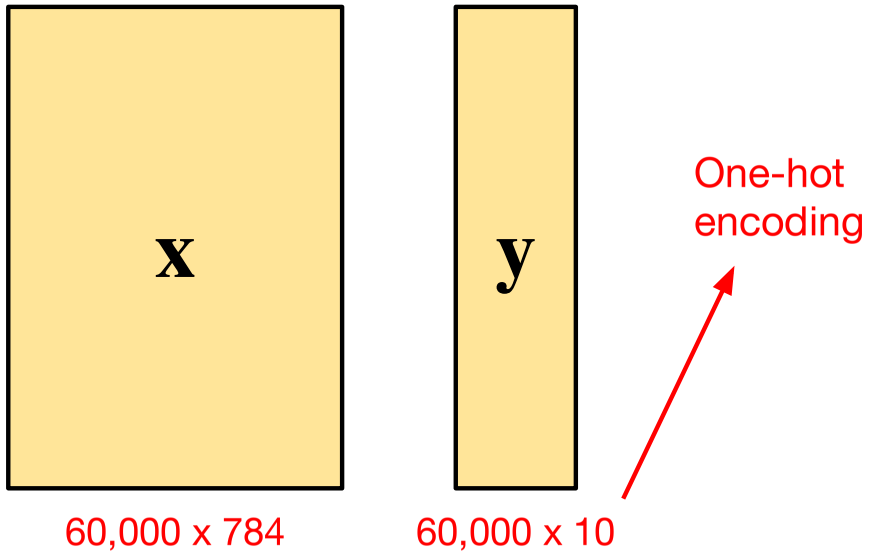
https://blogs.sas.com/content/subconsciousmusings/2017/09/25/machine-learning-concepts-styles-machine-learning/

Supervised learning

MNIST Dataset (Handwritten digits)



Each image is 28 x 28 pixels



The goal of training

Intuitively, we want to tweak the weights of the neural network until the network predicts the correct output for most of the examples in the training set.

Neural network #1

$$\text{softmax}\left(\begin{bmatrix} 2 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix}\right) = \begin{bmatrix} 0.98 \\ 0.02 \end{bmatrix}$$

Weights Input Prediction

Neural network #2

$$\text{softmax}\left(\begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix}\right) = \begin{bmatrix} 0.12 \\ 0.88 \end{bmatrix}$$

Weights Input Prediction

True label $\mathbf{y} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ We prefer network #1 to #2

Optimization formulation

We will frame this as an optimization problem:

$$\max_{\mathbf{W}_i, \mathbf{b}_i} \text{accuracy}(\text{DNN}(\mathbf{W}_i, \mathbf{b}_i))$$

Accuracy is the fraction of training examples that the model predicts correctly

Optimization formulation

Accuracy is not a continuous function, so it is hard to directly optimize for maximum accuracy.

So we use **loss functions**.

Think of losses as continuous proxies to accuracy, so that we can formulate it as an optimization problem and solve it.

Loss functions

$$\text{True label } \mathbf{y} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad \text{Predicted probabilities} = \begin{pmatrix} 0.2 \\ 0.7 \\ 0.1 \end{pmatrix}$$

In English, we want to **reward the neural network** for predicting class 2 with higher probability than classes 1 and 3, while incentivizing it to become even better at making this distinction

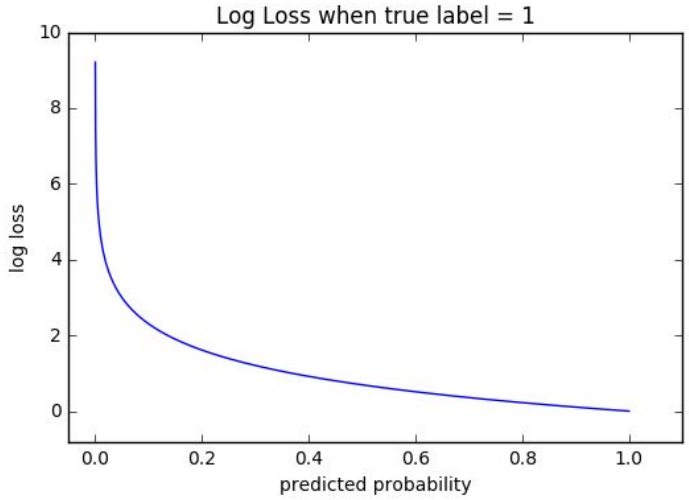
Cross entropy loss

Predicted probabilities = $\begin{pmatrix} 0.2 \\ 0.7 \\ 0.1 \end{pmatrix}$ $-\log(0.7) = 0.35$

Predicted probabilities = $\begin{pmatrix} 0.6 \\ 0.1 \\ 0.3 \end{pmatrix}$ $-\log(0.1) = 2.3$

Cross entropy loss

$$\mathrm{CE}(\mathbf{y}, \hat{\mathbf{y}}) = -\sum_i y_i \log \hat{y}_i$$



Cost function

Cost = Average loss over training examples

$$\min_{\mathbf{W}_i, \mathbf{b}_i} \text{cost}(\text{DNN}(\mathbf{W}_i, \mathbf{b}_i))$$

Often written $\min_{\mathbf{W}_i, \mathbf{b}_i} \mathcal{J}(\mathbf{W}_i, \mathbf{b}_i)$

The objective function is now a continuous function of the weights and biases

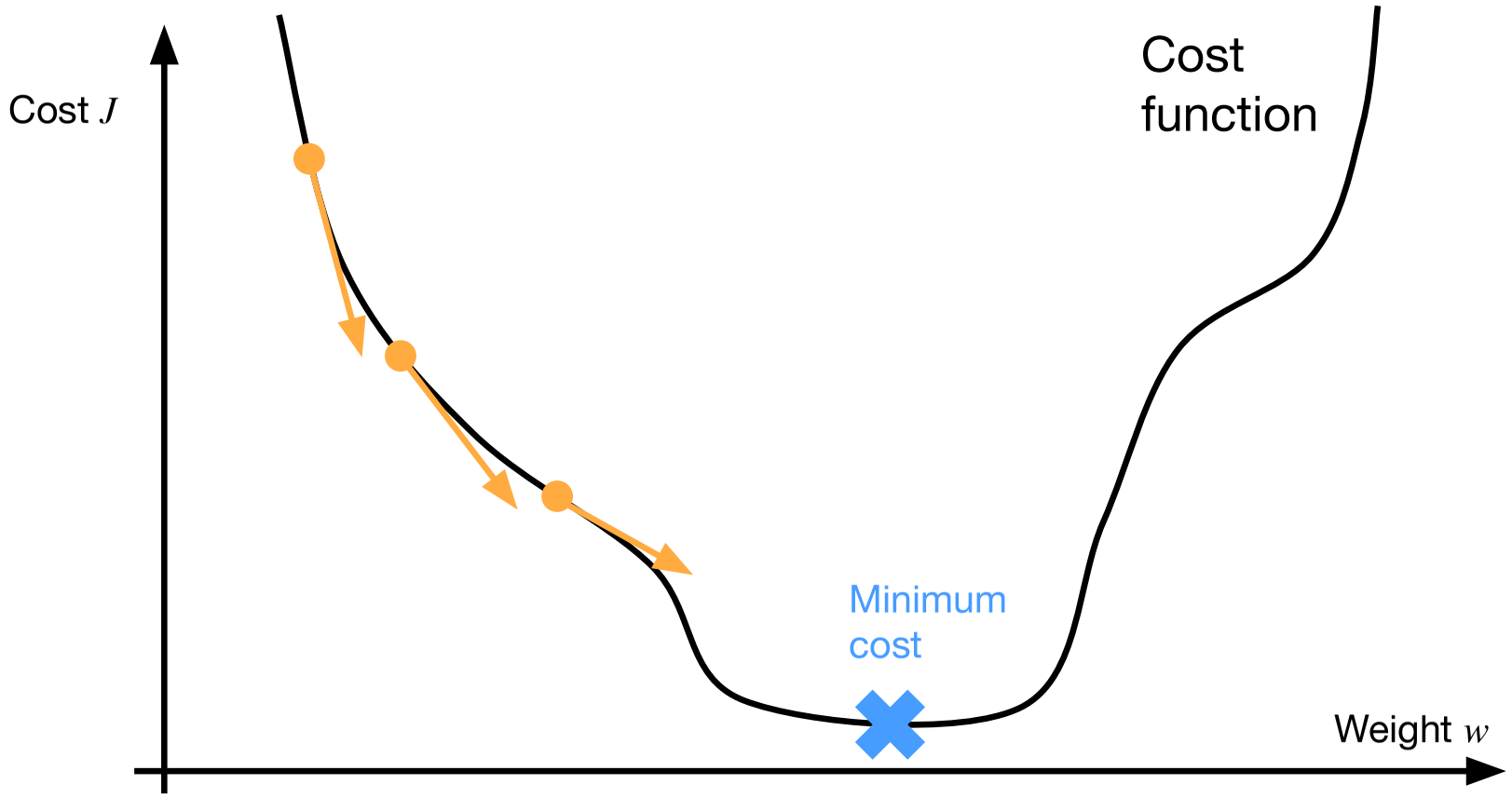
Gradient Descent

How do we solve the optimization problem?

The purpose of reformulating the problem in terms of a cost function is so that we can use gradient-based methods

1. Start with random weights
2. Compute the gradient with respect to the cost function
3. Update the weights so that the cost function decreases
4. Repeat steps 2-3

Gradient descent

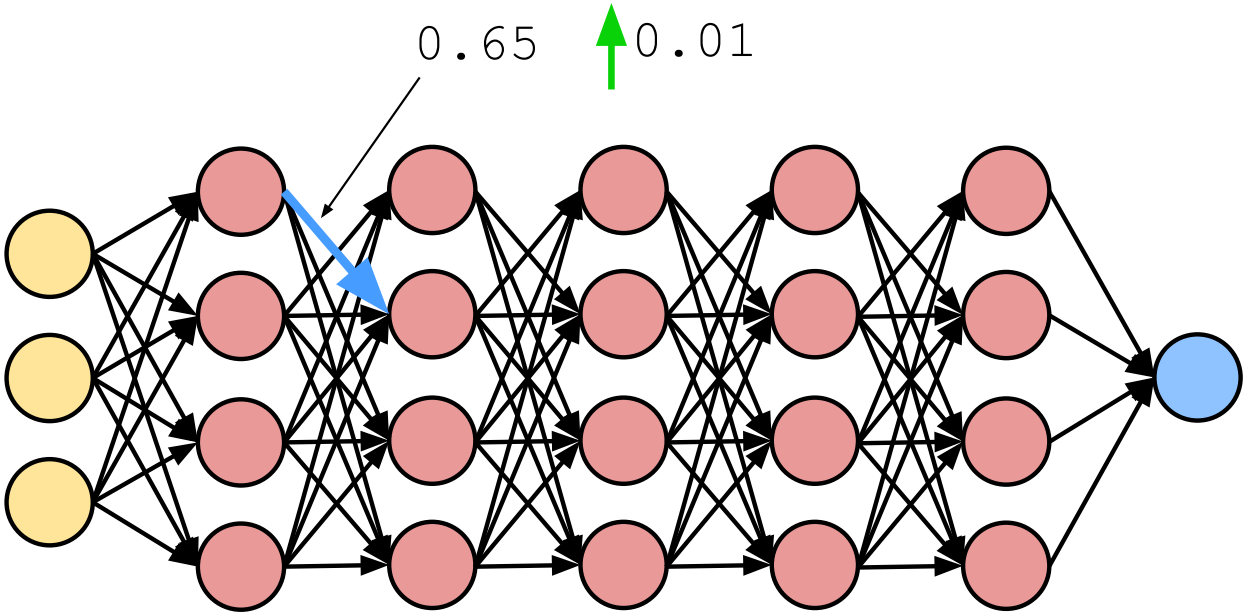


What are gradients?

1. It is a vector whose elements are the partial derivatives associated with every weight and bias in the neural network
2. The partial derivative on a weight = how many units the cost function will change by if the weight is changed by one unit
3. This assumes that the unit of change is small (technically infinitesimally small)

$$\nabla f(x, y, z) = \begin{bmatrix} \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \\ \frac{\partial f}{\partial z} \end{bmatrix}$$

What are gradients?



J = 4.50

0.05

Gradient = $\frac{\partial \mathcal{J}}{\partial w_i} = \frac{-0.05}{0.01} = -5$

What are gradients?

Suppose you have a function $\mathrm{F}(x,y,z)$

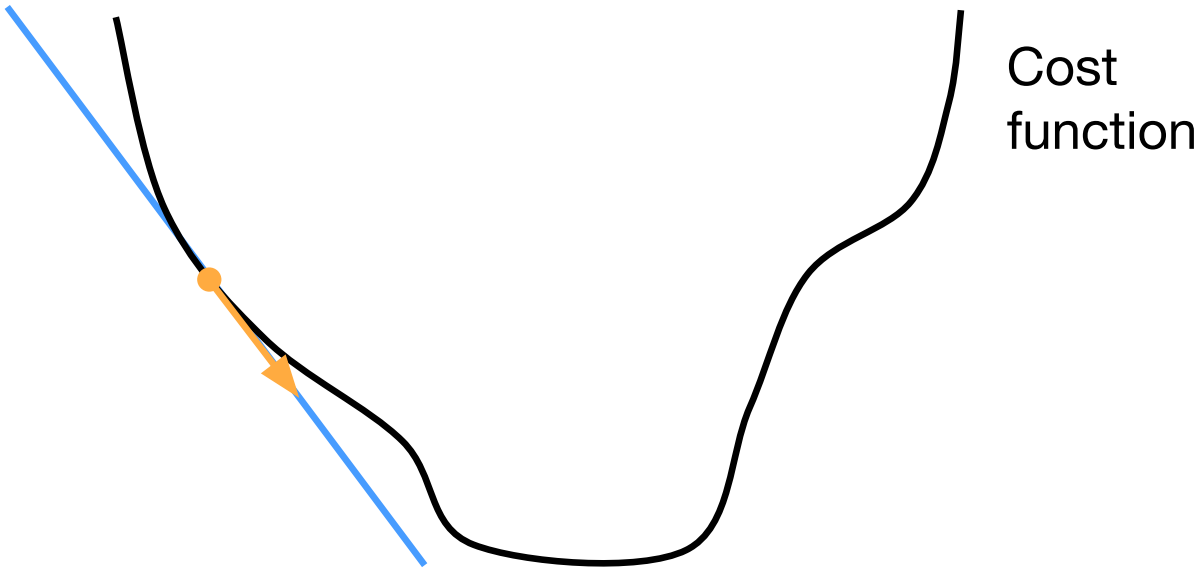
Then we have partial derivatives F_x, F_y, and F_z

$$F(x+\Delta x, y, z) \approx F(x, y, z) + F_x \Delta x$$
$$F(x, y+\Delta y, z) \approx F(x, y, z) + F_y \Delta y$$
$$F(x, y, z+\Delta z) \approx F(x, y, z) + F_z \Delta z$$

Linear approximation to the cost function

We can build a linear approximation to the function $\mathrm{F}(x,y,z)$ using the gradients

$$F(x+\Delta x, y+\Delta y, z+\Delta z) \approx F(x, y, z)+F_x\Delta x+F_y\Delta y+F_z\Delta z$$



Gradient descent

1. Go downhill according to the linear approximation of the cost function
2. But not by too much, as the approximation may not be accurate far away
3. This means updating each weight in proportion to the gradient:

$$w' = w - \alpha g$$

Learning rate

Backpropagation

How to compute gradients

- Numerically approximating gradients is too slow and computationally expensive
- The neural network is a well-defined mathematical function, so we should be able to differentiate it and calculate the derivatives using the **Chain Rule**

...like this?

$$
\begin{aligned}
&\frac{d}{dx}\sqrt{\sqrt{(x-1)(x+2)}+1} \\
&= \frac{d}{dx}\left\{[(x-1)(x+2)]^{1/2}+1\right\}^{1/2} \\
&= \frac{1}{2}\left\{[(x-1)(x+2)]^{1/2}+1\right\}^{1/2-1}\frac{d}{dx}\left\{[(x-1)(x+2)]^{1/2}+1\right\} \\
&= \frac{1}{2}\left\{[(x-1)(x+2)]^{1/2}+1\right\}^{1/2-1}\frac{1}{2}[(x-1)(x+2)]^{1/2-1}\frac{d}{dx}[(x-1)(x+2)] \\
&= \frac{1}{2}\left\{[(x-1)(x+2)]^{1/2}+1\right\}^{1/2-1}\frac{1}{2}[(x-1)(x+2)]^{1/2-1}\left\{\left[\frac{d}{dx}(x-1)\right](x+2)+(x-1)\left[\frac{d}{dx}(x+2)\right]\right\}
\end{aligned}
$$

- This also too tedious, so we use an algorithm called **backpropagation**

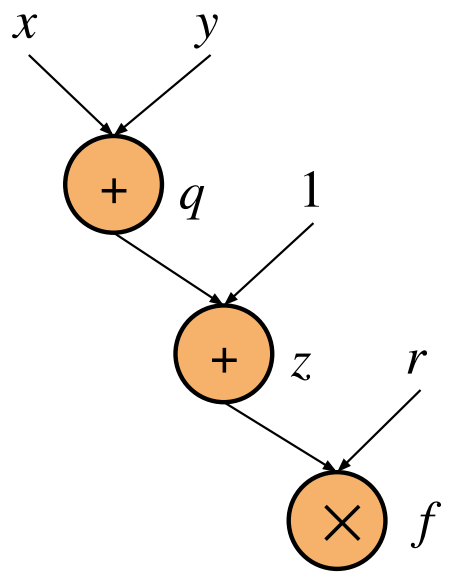
Computational graph

A way to organize mathematical expressions

Mathematical expressions

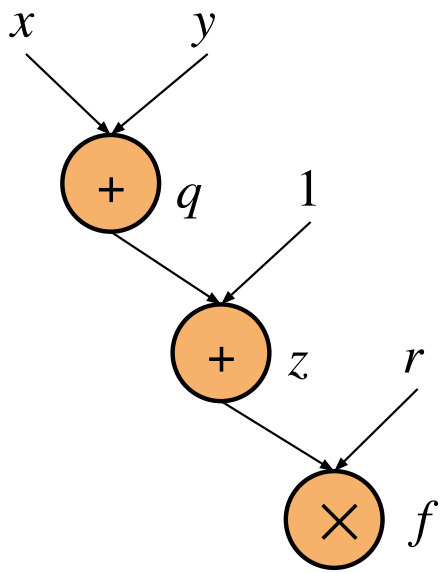
$$x + y = q$$
$$q + 1 = z$$
$$z \times r = f$$

Computational graph



Each circle denotes an **operation**

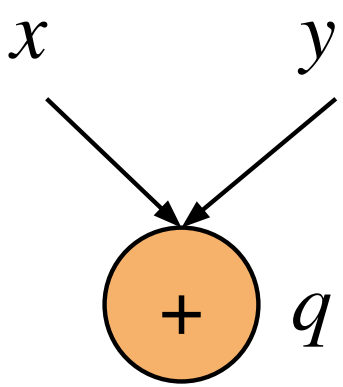
Gradients on computational graphs



Suppose we want to know $\frac{\partial f}{\partial x}$.

We can find this by chaining together derivatives at each operation.

Gradients on computational graphs

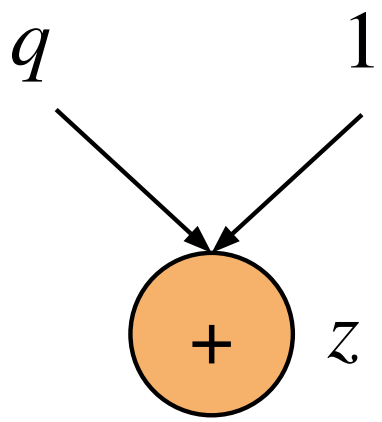


Let's take one piece of the computational graph at a time.

$$x + y = q$$

$$\frac{\partial q}{\partial x} = 1 \quad \frac{\partial q}{\partial y} = 1$$

Gradients on computational graphs



$$q + 1 = z$$

$$\frac{dz}{dq} = 1$$

Chain Rule

$$\frac{\partial z}{\partial x} = \frac{dz}{dq}\frac{\partial q}{\partial x} = 1$$

Gradients on computational graphs

$$f = x \times z$$

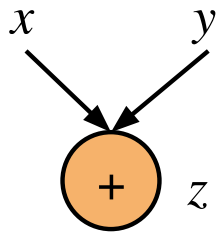
$$x = \frac{\partial f}{\partial x} \quad z = \frac{\partial f}{\partial z}$$

Chain Rule

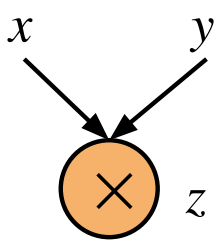
$$x = \frac{\partial f}{\partial q}\frac{\partial q}{\partial x} \quad = \frac{\partial f}{\partial z}\frac{\partial z}{\partial p}\frac{\partial p}{\partial q}\frac{\partial q}{\partial x}$$

In backprop, gradients are highly local

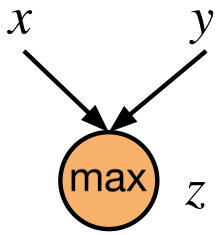
Three common operations in neural networks:



$$\frac{\partial f}{\partial x} = 1 \quad \frac{\partial f}{\partial y} = 1$$



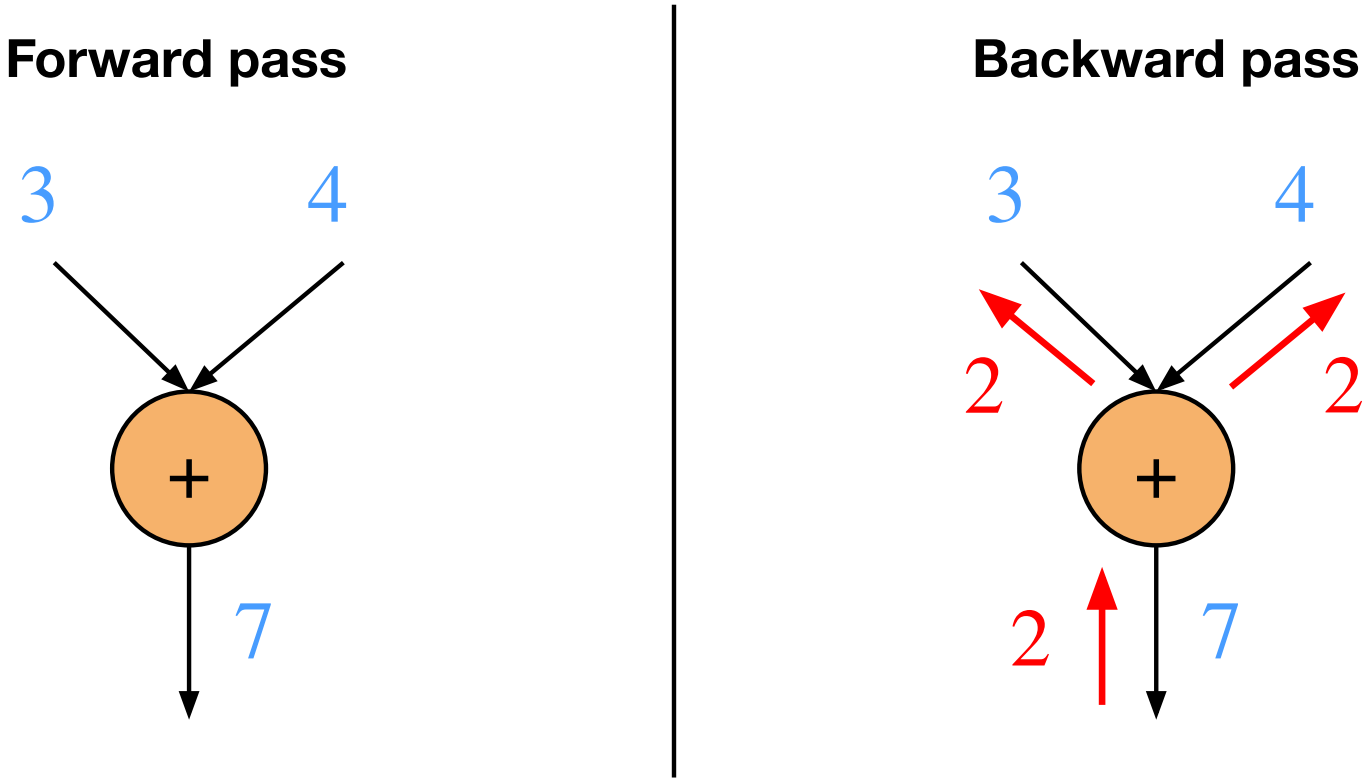
$$\frac{\partial f}{\partial x} = y \quad \frac{\partial f}{\partial y} = x$$



$$\frac{\partial f}{\partial x} = \mathbf{1}\{x \geq y\}$$

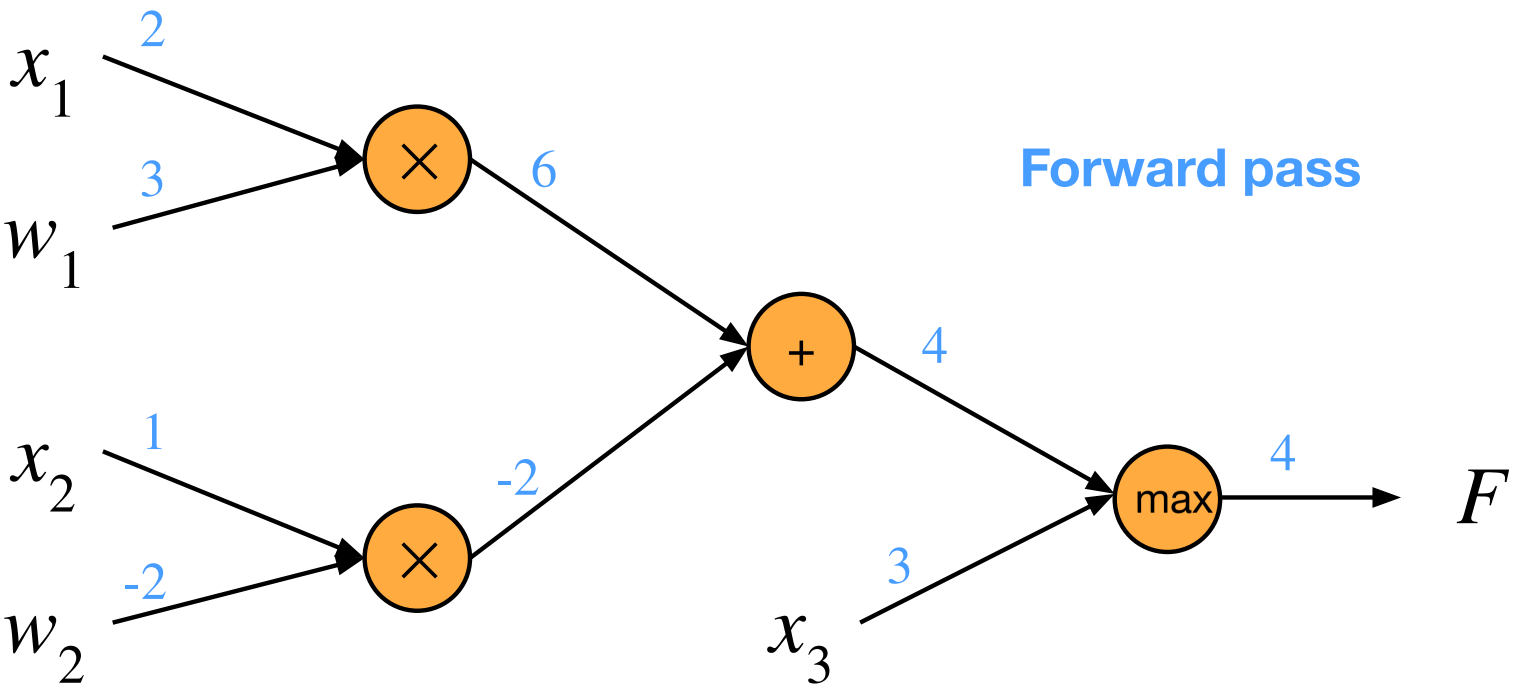
$$\frac{\partial f}{\partial y} = \mathbf{1}\{y \geq x\}$$

A small example with numbers



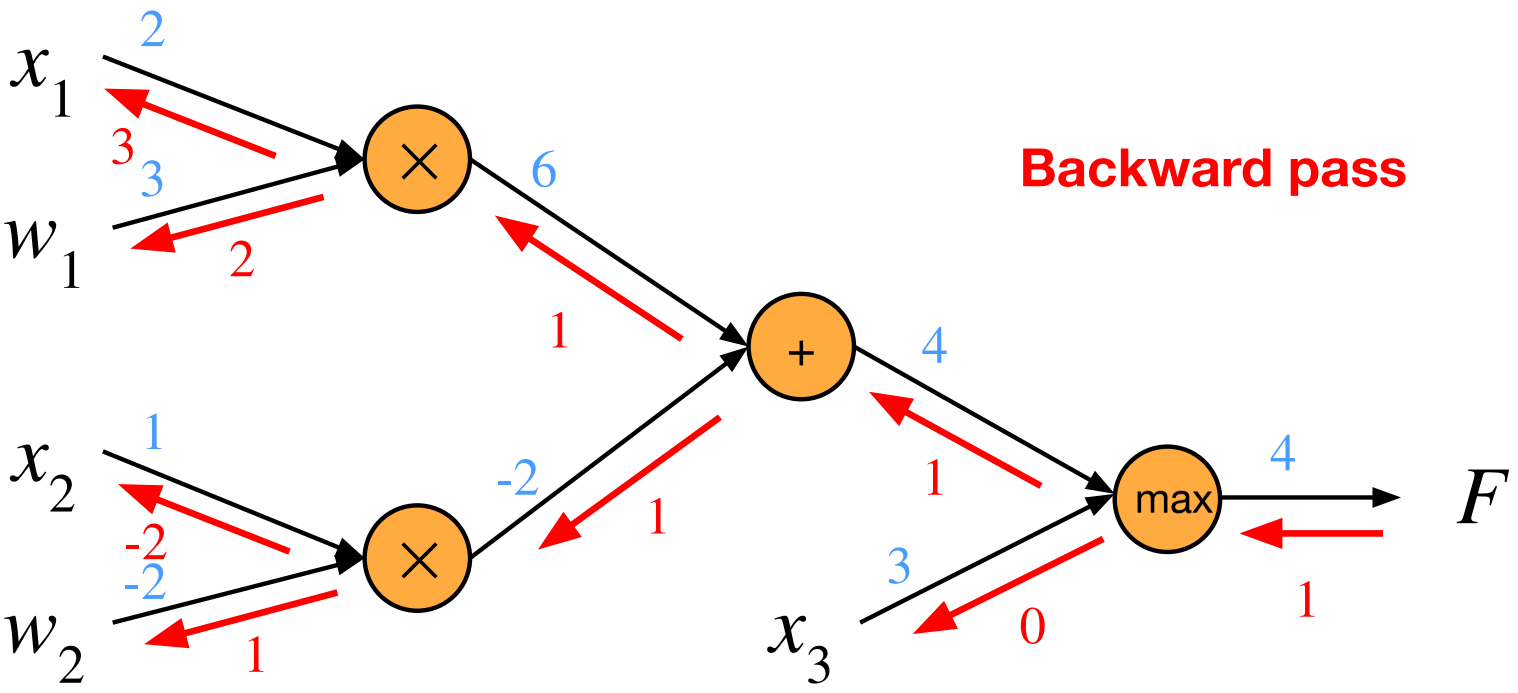
A larger example with numbers

$$F(x_1, x_2, x_3) = \max(w_1 x_1 + w_2 x_2, x_3)$$



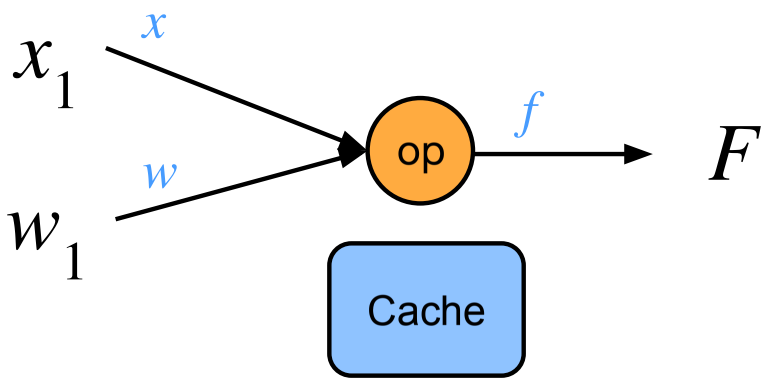
A larger example with numbers

$$F(x_1, x_2, x_3) = \max(w_1 x_1 + w_2 x_2, x_3)$$

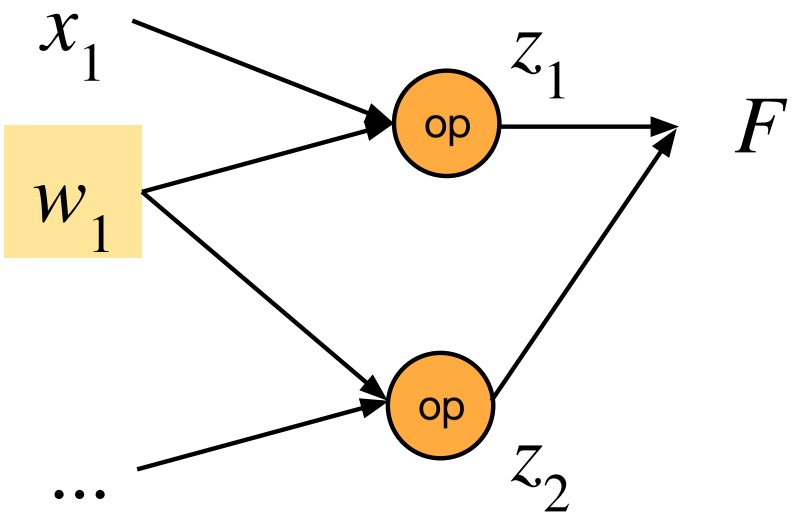


Note 1: Cache forward pass variables

During the backward pass, variable values from the forward pass are often needed



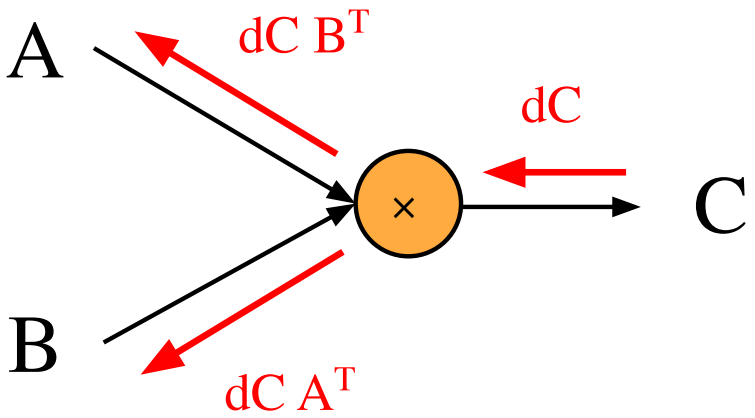
Note 2: Gradients add when a variable appears multiple times



$$\frac{\partial F}{\partial w_1} = \frac{\partial F}{\partial z_1}\frac{\partial z_1}{\partial w_1} + \frac{\partial F}{\partial z_2}\frac{\partial z_2}{\partial w_1}$$

Multivariable Chain Rule

Note 3: Backprop through matrix multiplication



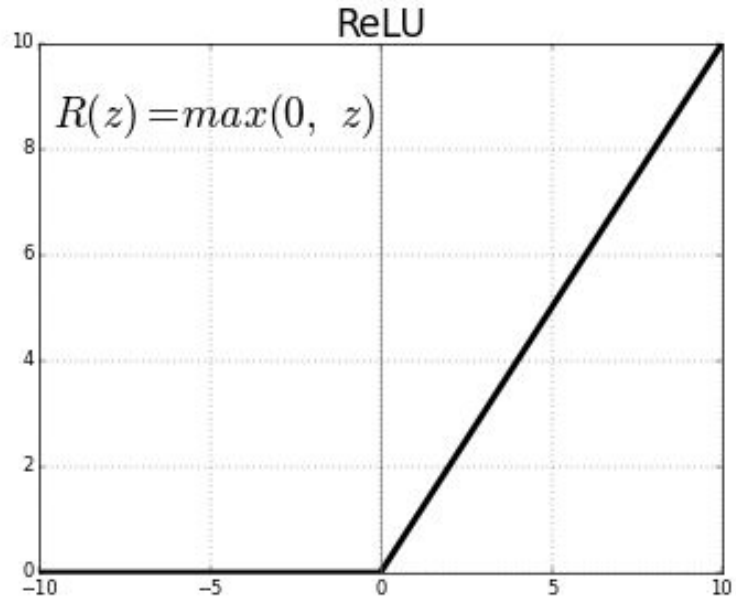
$$AB = C$$

$$dA = dC \times B^\top$$

$$dB = dC \times A^\top$$

Check matrix dimensions to verify

Poll: What happens when the gradient passes through the ReLU function?



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A. It stays the same
B. It is multiplied by a constant
C. It becomes zero
D. It either stays the same or is zeroed
E. None of the above

Gradient descent

$$w' = w - \alpha g$$

The cost function is the average of the loss function over all training examples.

This means we have to forward and backward pass through all training examples before we take one step of gradient descent.

Stochastic gradient descent

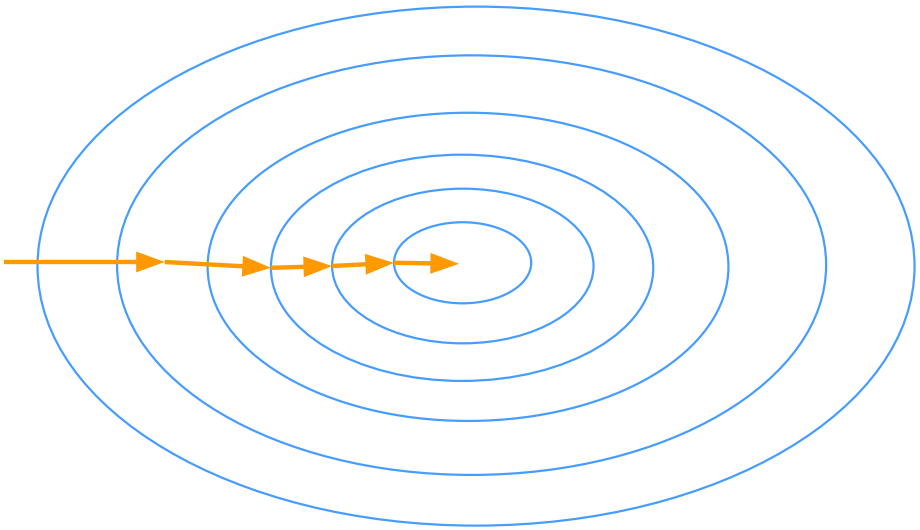
In SGD, we estimate the gradient by evaluating it over only a small subset of the training examples.

The size of this subsample is the **batch size**, which becomes another hyperparameter.

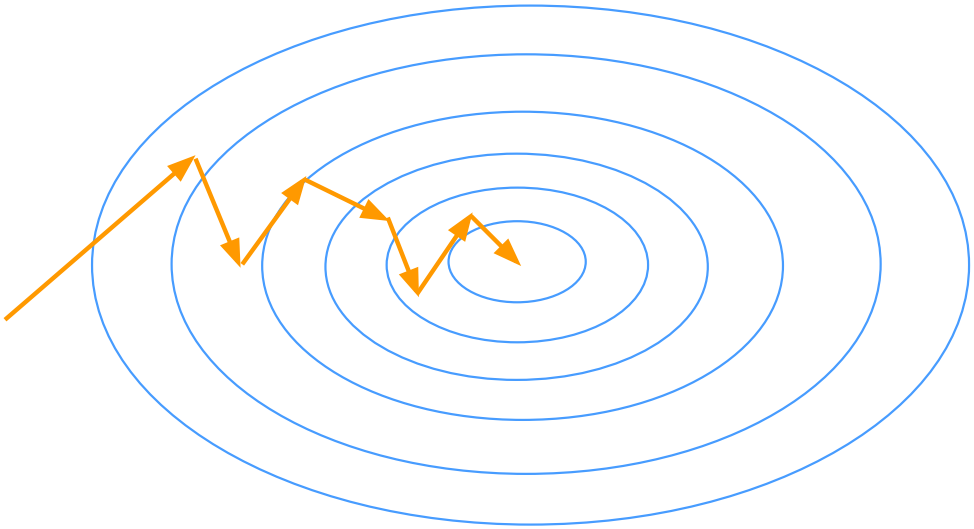
We use a different subsample for each gradient step, so as to go through all the training examples. Going through the entire training set once is called one **epoch** of training.

Stochastic gradient descent

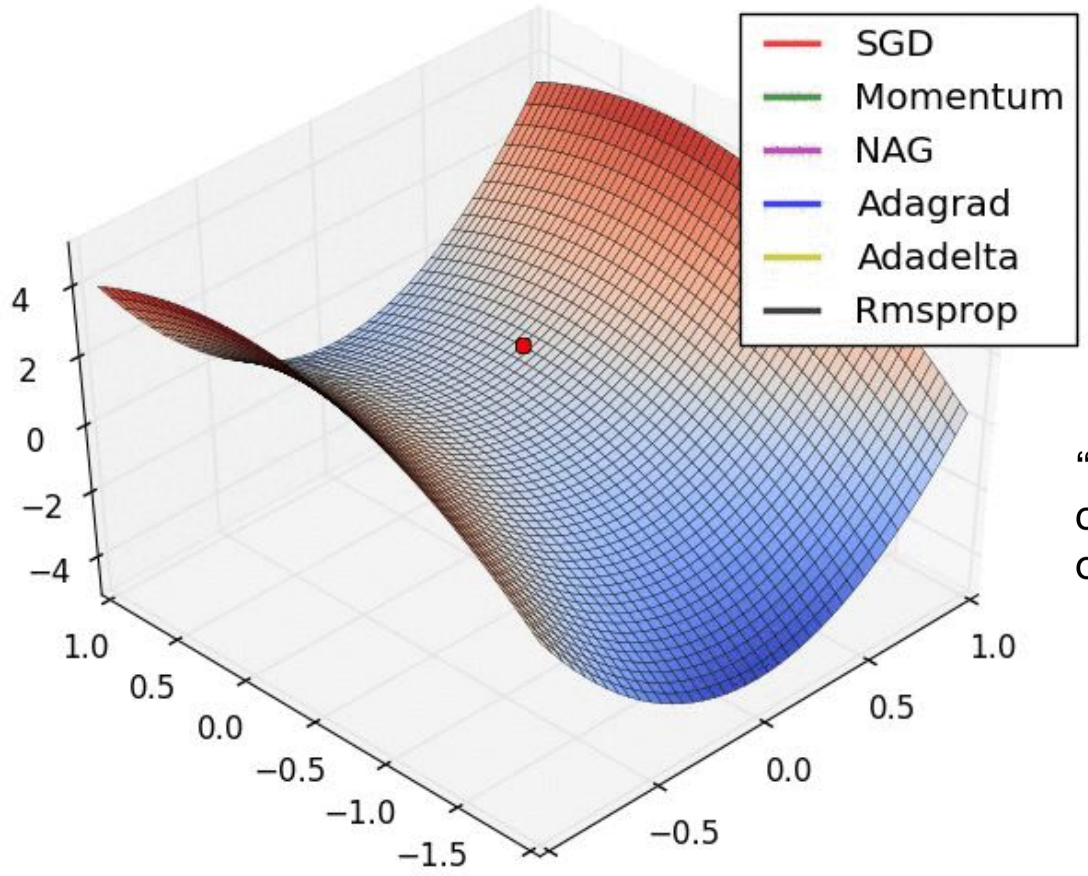
Gradient descent



Stochastic gradient descent



Other optimization algorithms



“Adam” is a very commonly used optimizer

When to stop training neural network?

Until *convergence*, when the loss no longer changes much.

In practice, often for a fixed number of epochs.

What data do we train on?

Training, validation, and test sets

To evaluate the performance of the model, set aside a portion of the dataset.

Training set: used to train the weights of the neural network.

Validation set: used to tune the network hyperparameters and perform architecture search.

Test set: reserved until the end, used only once to evaluate the final weights and hyperparameters of the model.

https://towardsdatascience.com/train-test-split-and-cross-validation-in-python-80b61beca4b6

Poll: Data splits

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Suppose I want to try training my neural network with different learning rates {0.1, 0.01, 0.001, 0.0001}. Which split should I use to evaluate which learning rate is best?

A. Train B. Validation C. Test

Training loop

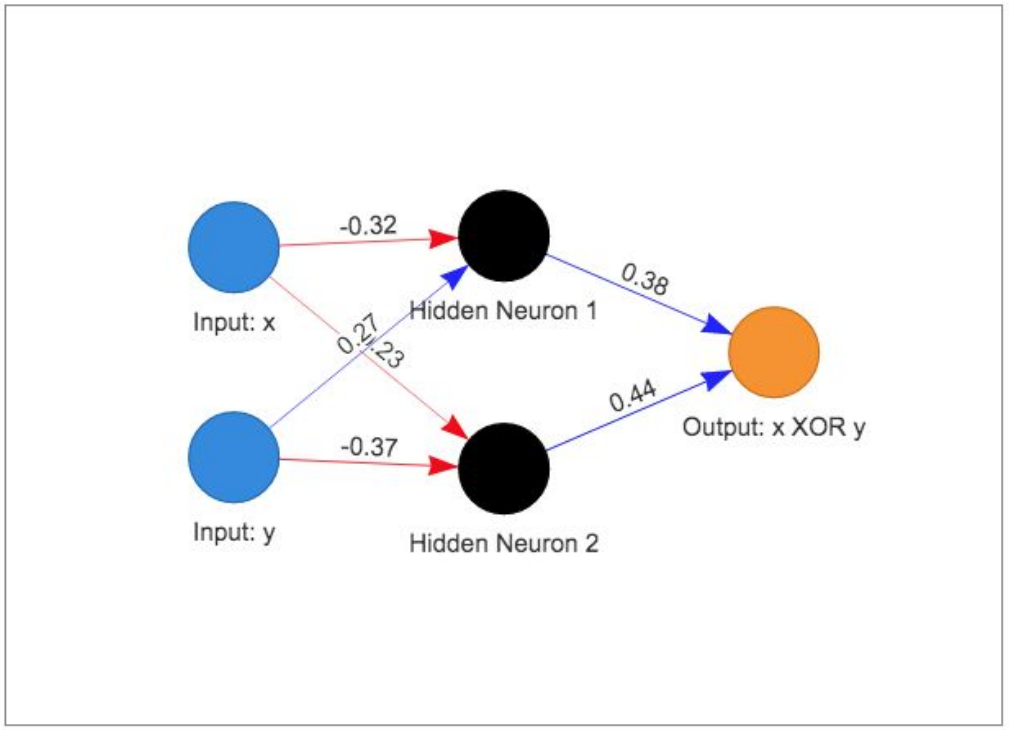
1. Sample a batch of data
2. Forward pass through all examples in the batch
3. Compute loss
4. Backpropagate through all examples
5. Compute final gradient on batch and update weights
6. Repeat

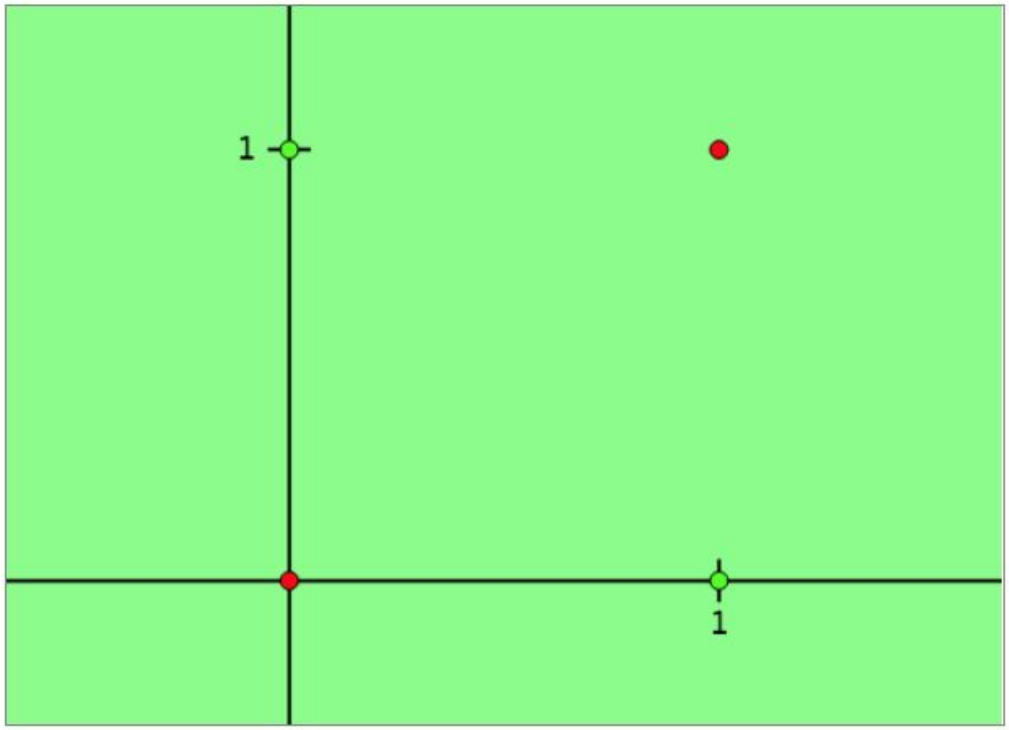
Workflow

1. Split your data into train/val/test
2. Choose architecture
3. Choose hyperparameters: learning rate, batch size, etc
4. Train neural network until convergence, evaluating on validation set each epoch
5. Check if training is overfitting or underfitting
6. Modify architecture and hyperparameters as needed, repeat

A complete example

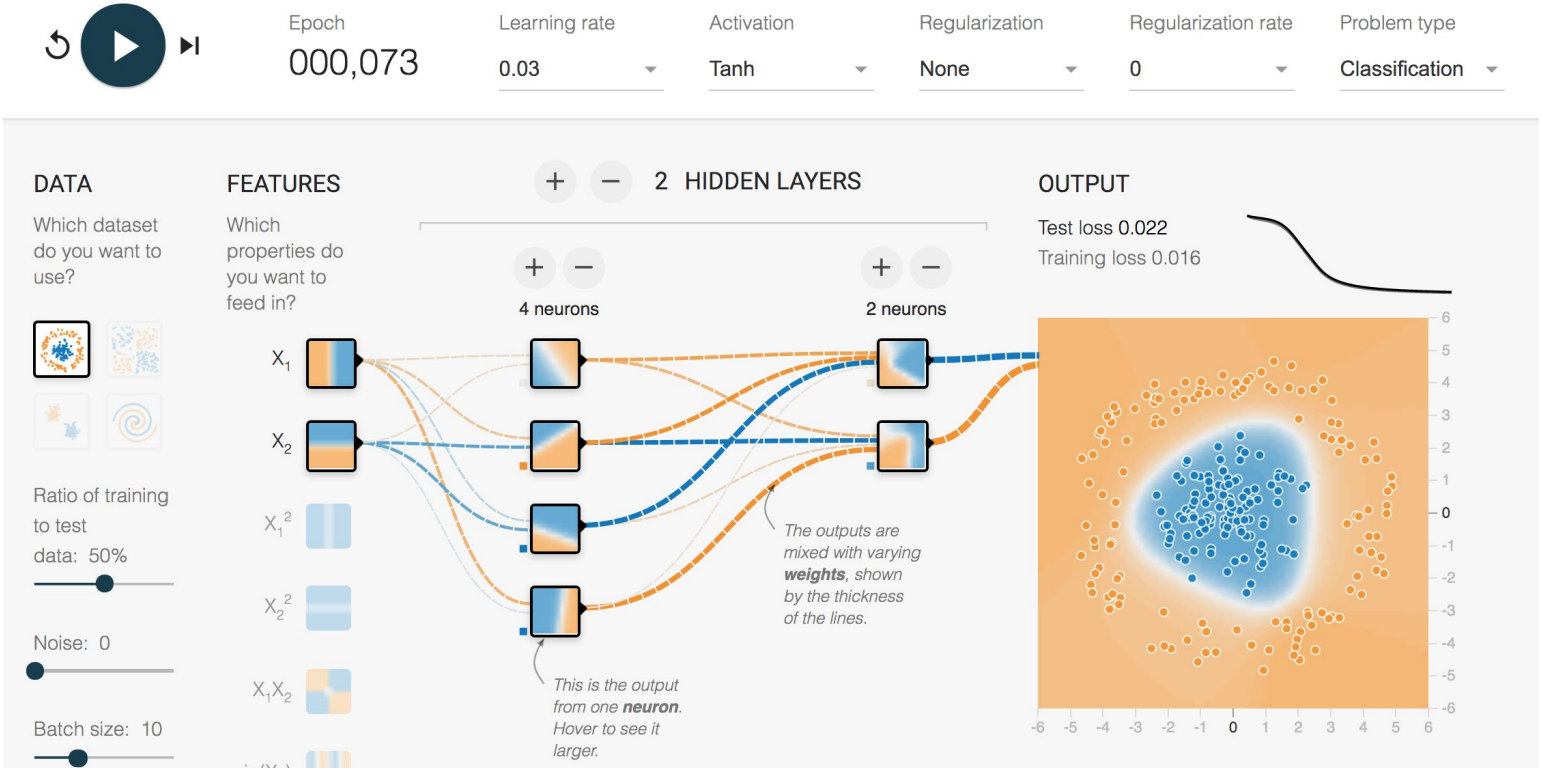
https://phiresky.github.io/neural-network-demo/





TensorFlow playground

https://playground.tensorflow.org



That's it for today! See you tomorrow!

Day 1

Session 1 (Today 8:00—9:30 AM)

- Introduction
- Examples of deep learning
- Math review
- Neural network basics

Session 2 (Today 9:45—11:00 AM)

- Loss functions
- Gradient descent
- Backpropagation
- Walkthrough of an example

Day 2

Session 3 (Tomorrow 8:00—9:30 AM)

- Overfitting and underfitting
- Convolutional neural networks
- Recurrent neural networks

Session 4 (Tomorrow 9:45—11:00 AM)

- Other architectures
- Deep learning libraries
- Walkthrough of an example
- Failures of deep learning