MACHINE LEARNING IN PHYSICS
FOUNDATIONS 1

Harrison B. Prosper

PHY 6938 Fall 2024

Goals of this Course

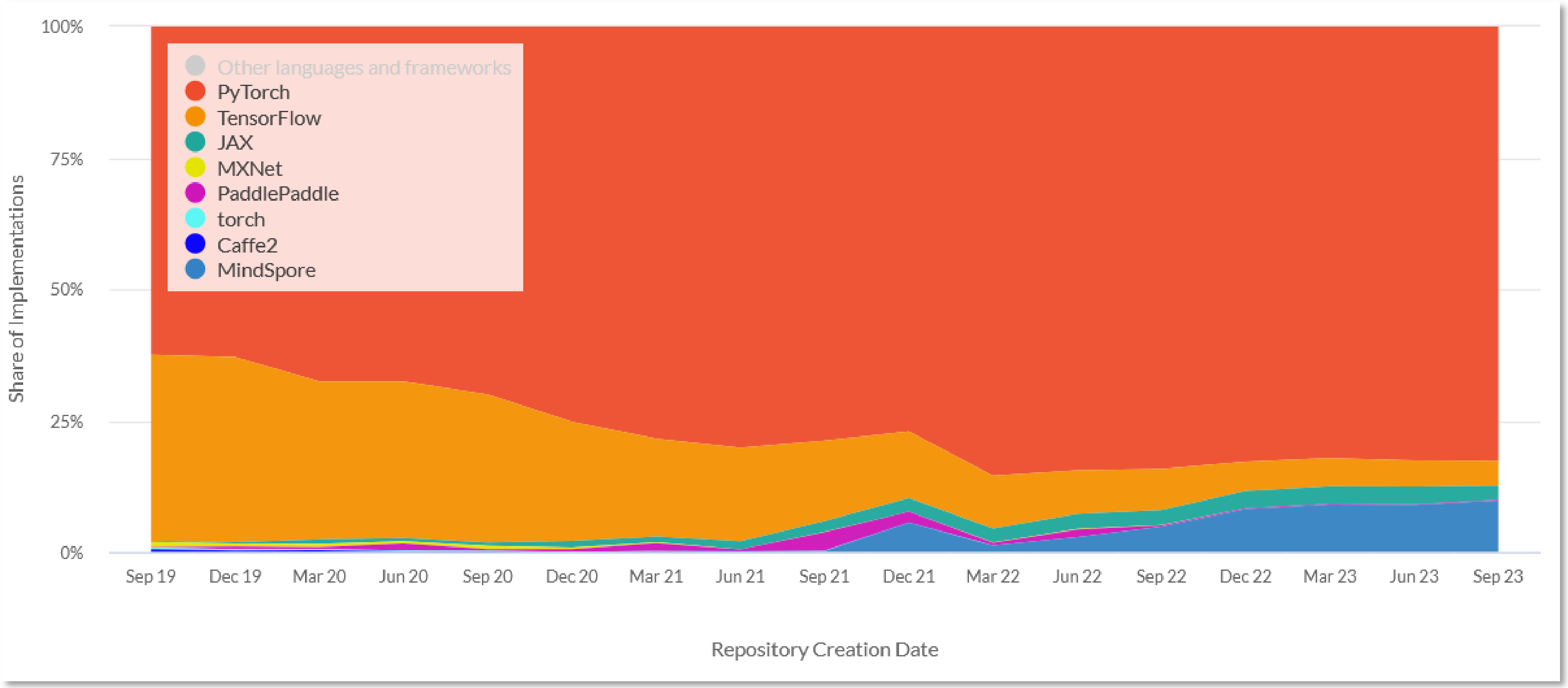
1. Gain a good understanding of the mathematical basis of machine learning (ML).

2. Gain experience building ML models using **PyTorch** to solve data science problems in physics.

3. Gain experience with different ML models.

4. Gain an appreciation of the power of ML models as well as their (current) limitations.

Why PyTorch?



https://viso.ai/deep-learning/pytorch-vs-tensorflow/

The Birth of Artificial Intelligence

A PROPOSAL FOR THE

DARTMOUTH SUMMER RESEARCH PROJECT

ON ARTIFICIAL INTELLIGENCE

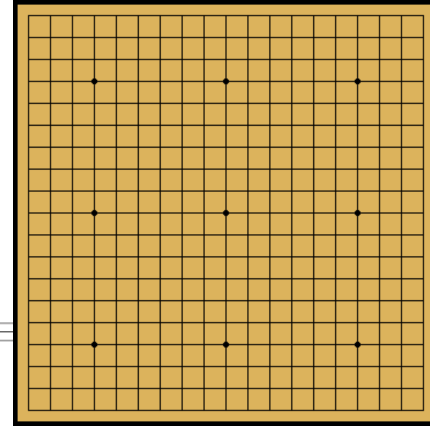
J. McCarthy, Dartmouth College
M. L. Minsky, Harvard University
N. Rochester, I. B. M. Corporation
C. E. Shannon, Bell Telephone Laboratories

1956

What is Artificial Intelligence?

Artificial Intelligence
Algorithms that cause machines to exhibit *human*- or *superhuman*-level intelligence.

ARTICLE



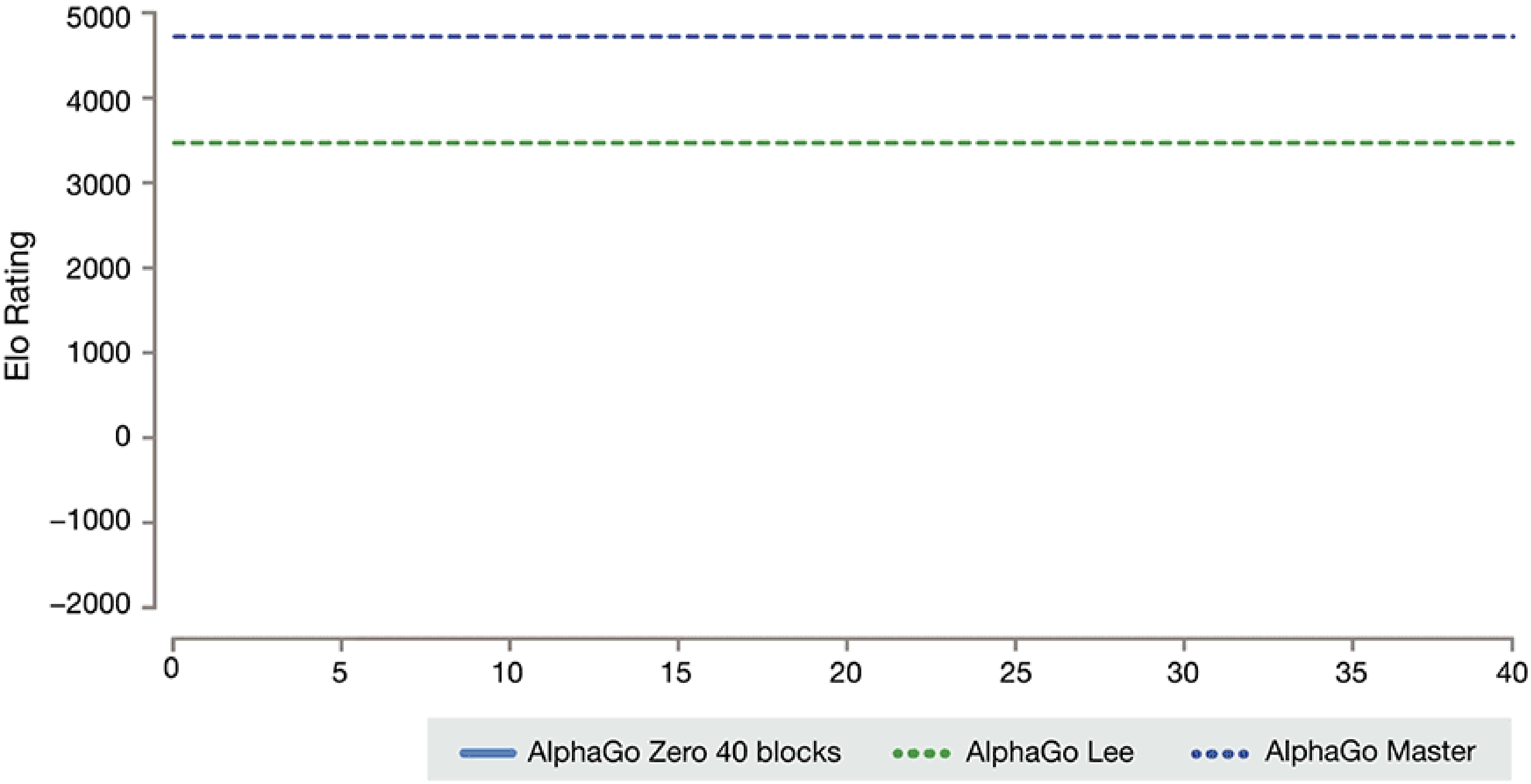
doi:10.1038/nature24270

Mastering the game of Go without human knowledge

David Silver[1]*, Julian Schrittwieser[1]*, Karen Simonyan[1]*, Ioannis Antonoglou[1], Aja Huang[1], Arthur Guez[1], Thomas Hubert[1], Lucas Baker[1], Matthew Lai[1], Adrian Bolton[1], Yutian Chen[1], Timothy Lillicrap[1], Fan Hui[1], Laurent Sifre[1], George van den Driessche[1], Thore Graepel[1] & Demis Hassabis[1]

A long-standing goal of artificial intelligence is an algorithm that learns, *tabula rasa*, superhuman proficiency in challenging domains. Recently, AlphaGo became the first program to defeat a world champion in the game of Go. The tree search in AlphaGo evaluated positions and selected moves using deep neural networks. These neural networks were trained by supervised learning from human expert moves, and by reinforcement learning from self-play. Here we introduce an algorithm based solely on reinforcement learning, without human data, guidance or domain knowledge beyond game rules. AlphaGo becomes its own teacher: a neural network is trained to predict AlphaGo's own move selections and also the winner of AlphaGo's games. This neural network improves the strength of the tree search, resulting in higher quality move selection and stronger self-play in the next iteration. Starting *tabula rasa*, our new program AlphaGo Zero achieved superhuman performance, winning 100–0 against the previously published, champion-defeating AlphaGo.

https://deepmind.com/blog/alphago-zero-learning-scratch/



Symbolic Mathematics

In December 2019, Guillaume Lample and François Charton* (Meta fka Facebook AI Research, Paris) claimed: “*We achieve results that outperform commercial Computer Algebra Systems such as Matlab or Mathematica*.”

Lample

Charton

* G. Lample and F. Charton, Deep Learning for Symbolic Mathematics, arXiv: 1912.01412v1

MACHINE
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Science and Technology

CrossMark

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PAPER

SYMBA: symbolic computation of squared amplitudes in high energy physics with machine learning

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Keywords: physics, high energy physics, machine learning

Abstract

The cross section is one of the most important physical quantities in high-energy physics and the most time consuming to compute. While machine learning has proven to be highly successful in numerical calculations in high-energy physics, analytical calculations using machine learning are still in their infancy. In this work, we use a sequence-to-sequence model, specifically, a transformer, to compute a key element of the cross section calculation, namely, the squared amplitude of an interaction. We show that a transformer model is able to predict correctly 97.6% and 99% of squared amplitudes of quantum chromodynamics and quantum electrodynamics processes, respectively, at a speed that is up to orders of magnitude faster than current symbolic computation frameworks. We discuss the performance of the current model, its limitations and possible future directions for this work.

What is Machine Learning?

Artificial Intelligence
Algorithms that cause machines to exhibit human- or *super-human* level intelligence.

Machine Learning
Algorithms for modeling data.

What is Machine Learning?

Supervised Learning

Data: (x, y)

y are labels

Task: $x \rightarrow y$

Use cases:

- Classification, regression, etc.

Unsupervised Learning

Data: x

no labels

Task: find structure in, and/or model, data

Use cases:

- Clustering, data compression, solving differential equations, etc.

What is Machine Learning?

Generative Learning

Data: x

may or may not be associated with labels

Task: $x \to p(x) \to x$

Use cases:

- fast simulators, image/text generation, etc.

Reinforcement Learning

Data: (x, a, r)

x state of the environment

a action taken on environment

r reward arising from action

Task: find optimal $x \to a$

Use cases:

- Game playing, robotics, accelerator controls, etc.

What is Deep Learning?

Artificial Intelligence
Algorithms that cause machines to exhibit human- or *super-human*-level intelligence.

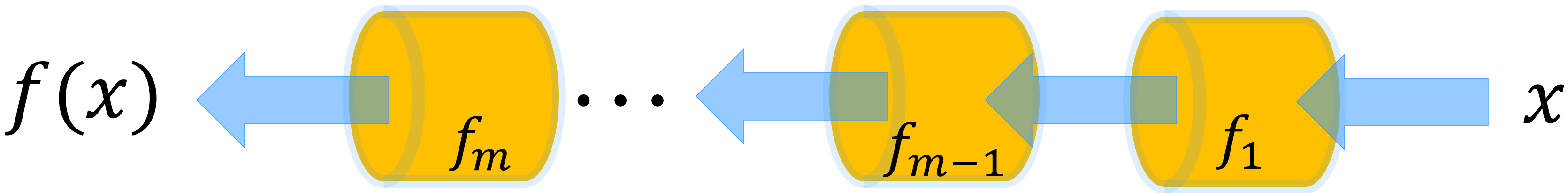
Machine Learning
Algorithms for modeling data

Deep Learning
ML using (large) neural networks

What is Deep Learning?

Deep learning is the science and art of fitting functions to data using functions formed by *composing* sequences of nonlinear parameterized functions, $f_1(*, \omega_1), f_2(*, \omega_2), \dots, f_m(*, \omega_m)$,

$$
\begin{aligned}
f(x) &= f_m \circ f_{m-1} \circ \cdots f_1 \\
&= f_m(f_{m-1}(\dots f_1(x)) \dots)
\end{aligned}
$$



Each of these functions is referred to as a **layer**. The ChatGPT3 function has **96** layers and **175 billion** parameters!

What is Deep Learning? Example

Here is a simple example of a quark/gluon classifier:

$$f(x) = \text{softmax}\left(\text{dropout}(\text{linear}(\text{flatten}\left(\boldsymbol{g}(\boldsymbol{c}\left(\boldsymbol{h}(\boldsymbol{c}(x))\right))\right)))\right)$$

Here is an algorithm-level view:

$$y = \boldsymbol{c}(x) \qquad y = \text{flatten}(y)$$
$$y = \boldsymbol{h}(y) \qquad y = \text{linear}(y)$$
$$y = \boldsymbol{c}(y) \qquad y = \text{dropout}(y)$$
$$y = \boldsymbol{g}(y) \qquad f = \text{softmax}(y)$$

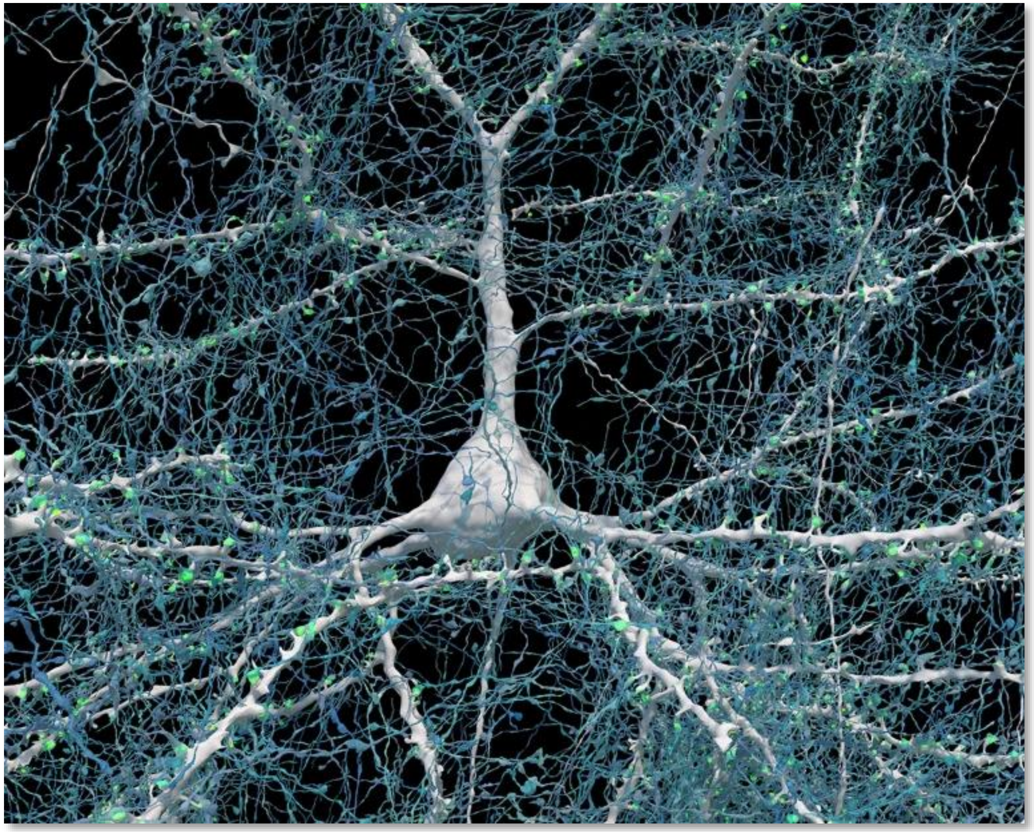
And here is a code-level view:

```
Sequential(
  (0): Conv2d(1, 4, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
  (1): MaxPool2d(kernel_size=(2, 2), stride=2, padding=0, dilation=1, ceil_mode=False)
  (2): ReLU()
  (3): Conv2d(4, 4, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
  (4): MaxPool2d(kernel_size=(2, 2), stride=2, padding=0, dilation=1, ceil_mode=False)
  (5): ReLU()
  (6): Flatten(start_dim=1, end_dim=-1)
  (7): Linear(in_features=64, out_features=2, bias=True)
  (8): Dropout(p=0.2, inplace=False)
  (9): Softmax(dim=1)
)
number of parameters: 318
```

BASIC BUILDING BLOCK:

THE PERCEPTRON

The Brain's Computational Unit



https://www.nature.com/articles/d41586-024-01387-9

Artificial Comp. Unit: The Perceptron

$$y = g(xA^T + b)$$

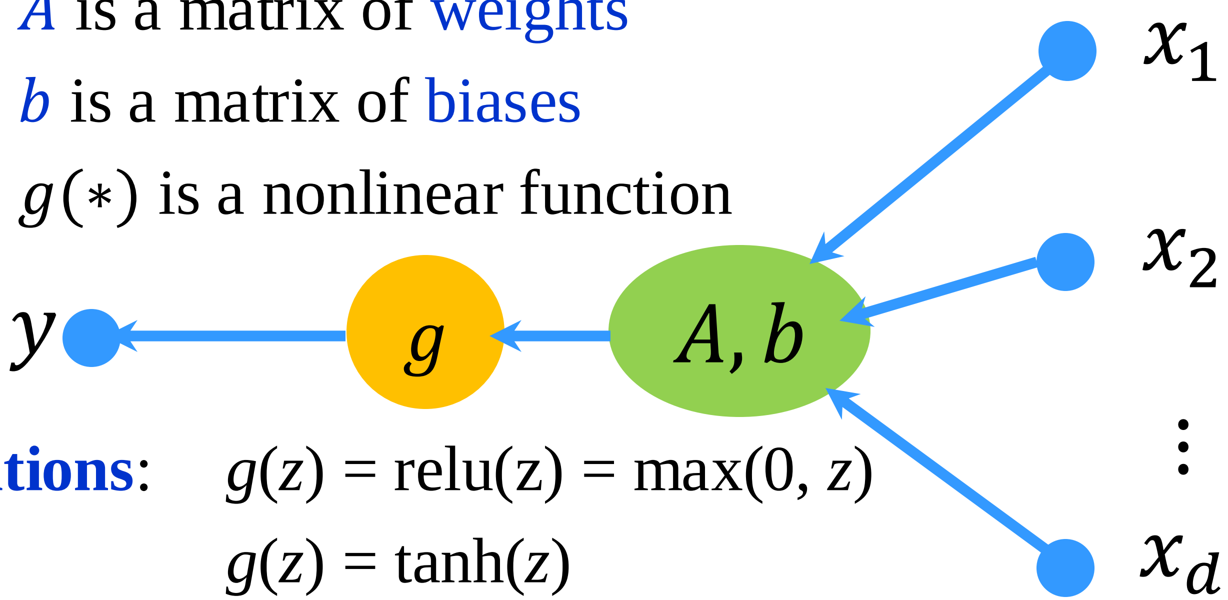
(Frank Rosenblatt, 1958)

x is a (row) matrix of input data

A is a matrix of weights

b is a matrix of biases

$g(*)$ is a nonlinear function



Activations: $g(z) = \text{relu}(z) = \max(0, z)$

$g(z) = \tanh(z)$

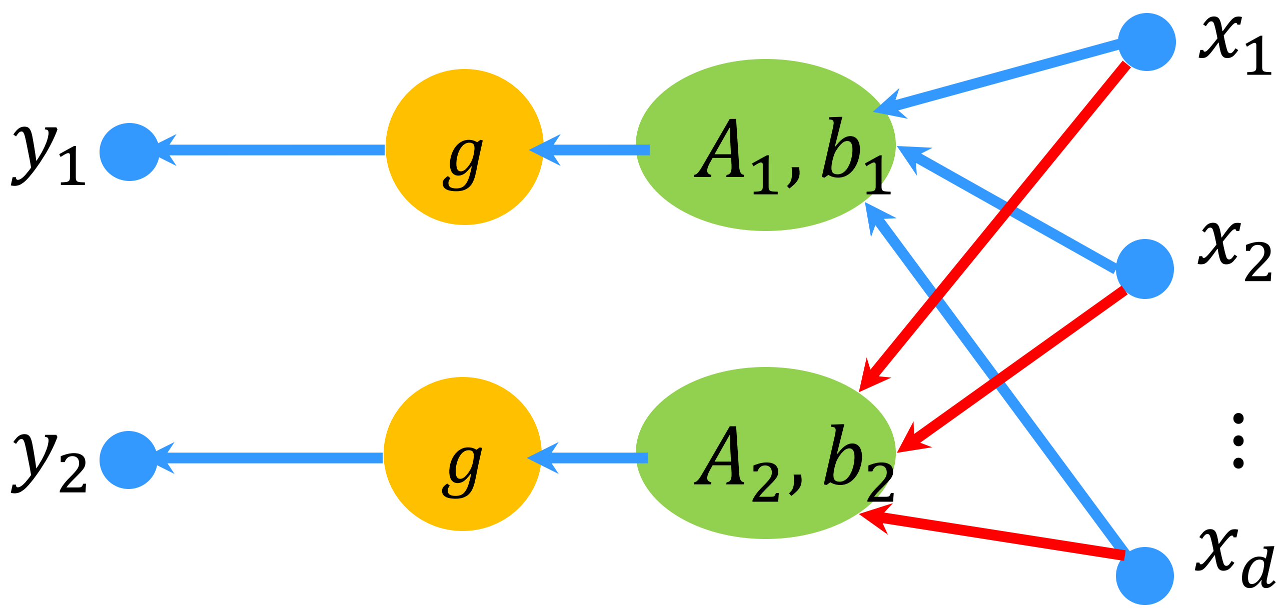
$g(z) = \text{sigmoid}(z) = 1 / (1 + \exp(-z))$

https://news.cornell.edu/stories/2019/09/professors-perceptron-paved-way-ai-60-years-too-soon

Artificial Comp. Unit: The Perceptron

Building a *2-node* layer:

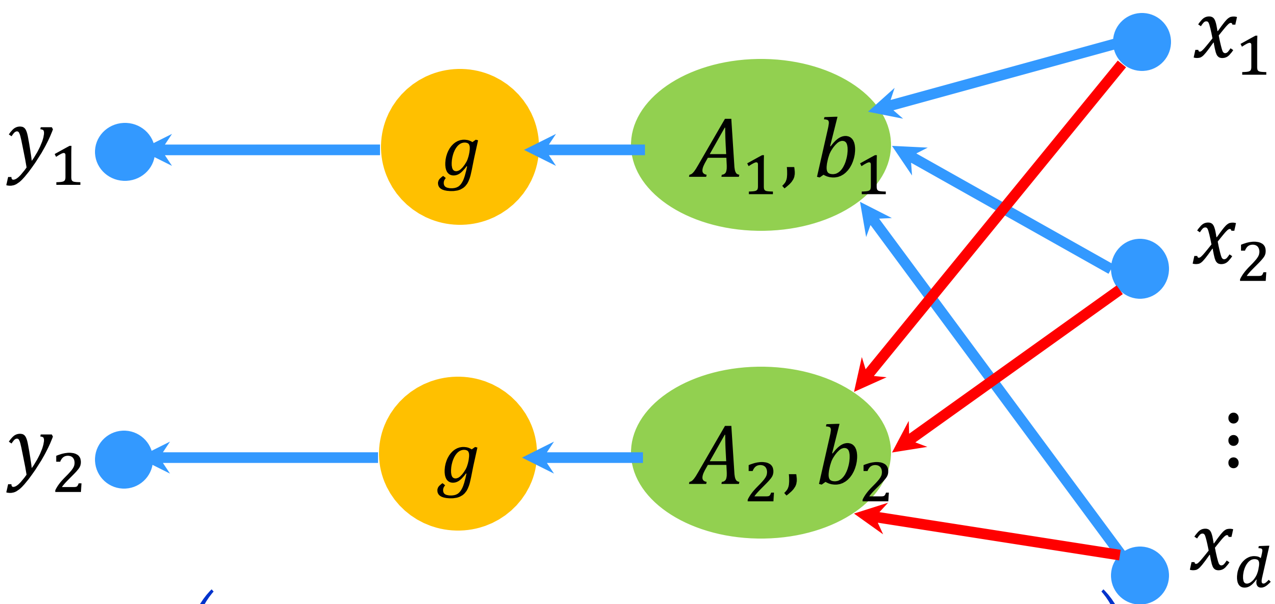
$$y_1 = g(xA_1^T + b_1),\ y_2 = g(xA_2^T + b_2)$$



This can be written as $y = g(z),\ z = x\boldsymbol{A}^T + \boldsymbol{b}$

The Perceptron: Example

$x = (-2, 1, 4), \qquad A = \begin{pmatrix} 2 & -3 & 1 \\ 1 & 2 & 3 \end{pmatrix}, \qquad b = (-5, -4)$



$$y = \text{relu}\left((-2,1,4) \begin{pmatrix} 2 & -3 & 1 \\ 1 & 2 & 3 \end{pmatrix}^{\mathrm{T}} + (-5, -4) \right)$$

Summary

- **General Approaches**
  - Supervised, unsupervised, generative, and reinforcement learning.
- **Deep Learning**
  - Uses functions constructed through deep composition.
- **The Perceptron**
  - Basic computational unit: matrix multiplication and addition and (typically) an element-wise nonlinear map.