

#### **CHECK-IN**

## INTRODUCTION TO MACHINE LEARNING (PART 3

OF 5)

THURSDAY, JANUARY 18 AT 2:00PM



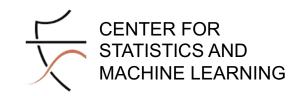
https://cglink.me/2gi/c19387701115114149

- 1 Open the My PrincetonU app.
- (2) Select a Hub
- (3) Click on QR Code scanner.
- 4 Scan this QR Code and you are checked-in!







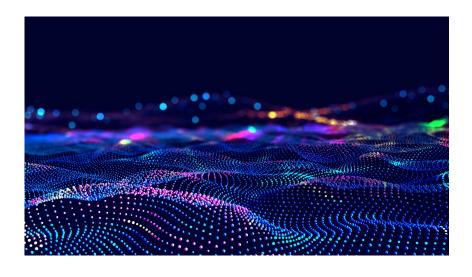


## Introduction to Machine Learning



Wintersession 2024 Jan 16-18, 22-23

Gage DeZoort
Julian Gold
Jake Snell



With materials from:
Brian Arnold, Jonathan Halverson, Christina Peters, Savannah Thias, and Amy Winecoff



## Course Outline

Date	Instructor	Topic
Day 1 Tue. 1/16	Jake Snell	Machine Learning Overview and Simple Models
Day 2 Wed. 1/17	Jake Snell	Model Evaluation and Improving Performance
Day 3 Thu. 1/18	Julian Gold	Introduction to Neural Networks
Day 4 Mon. 1/22	Gage DeZoort	Survey of Neural Network Architectures
Day 5 Tue. 1/23	Gage DeZoort Julian Gold Jake Snell	<ul><li>Hackathon!</li><li>Computer Vision</li><li>Diffusion Models</li><li>Large Language Models</li></ul>



#### **Artificial Intelligence**

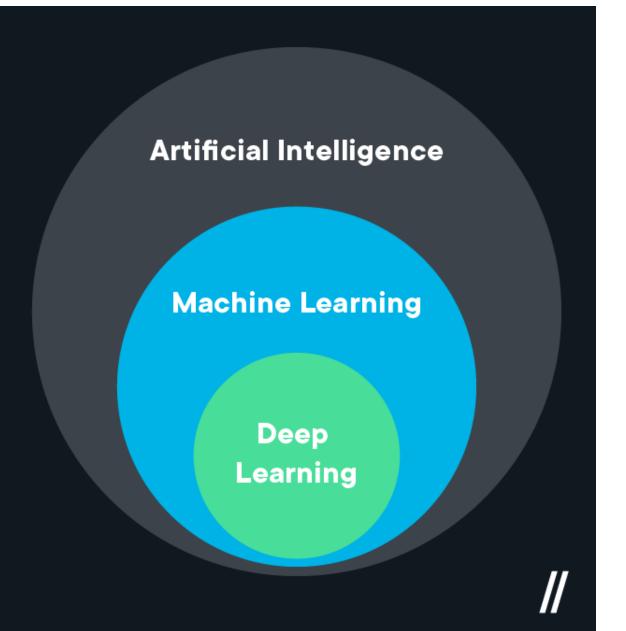
A science devoted to making machines think and act like humans.

#### Machine Learning

Focuses on enabling computers to perform tasks without explicit programming.

#### **Deep Learning**

A subset of machine learning based on artificial neural networks.

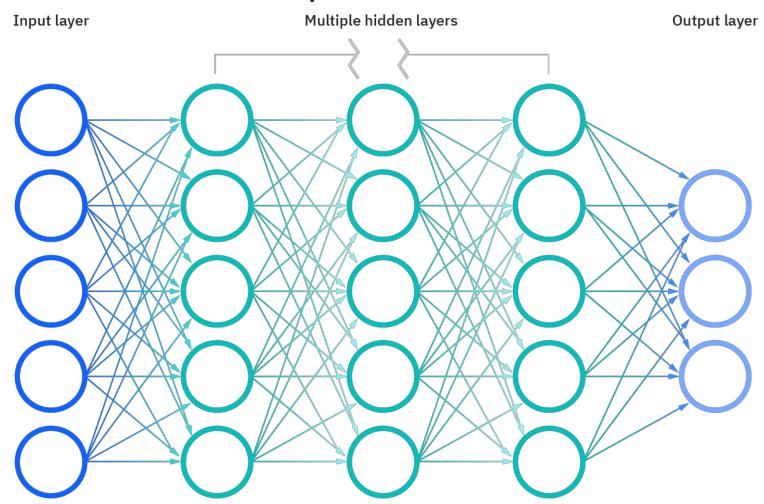


#### WHY USE DL?

- Data with complex (highly non-linear) relationships
- Big data many examples to leverage
- High-dimensional data
- Data with complicated structure (images, video, language, social networks etc.)

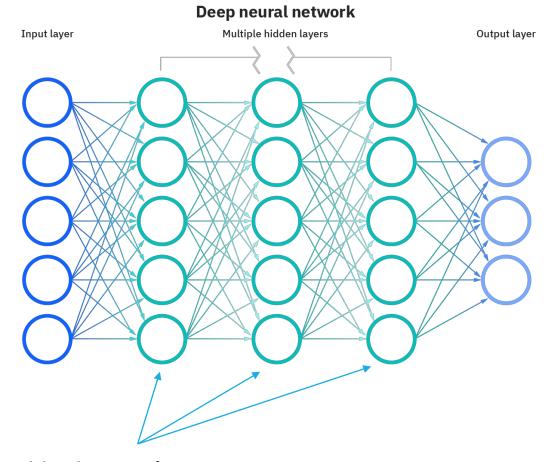


#### Deep neural network



## DEEP NEURAL NETWORKS

- A class of ML algorithms based on artificial neural networks (ANNs)
  - Neural network → networks of neurons responding to stimuli
  - "Deep" → multiple layers of neurons interacting in sequence

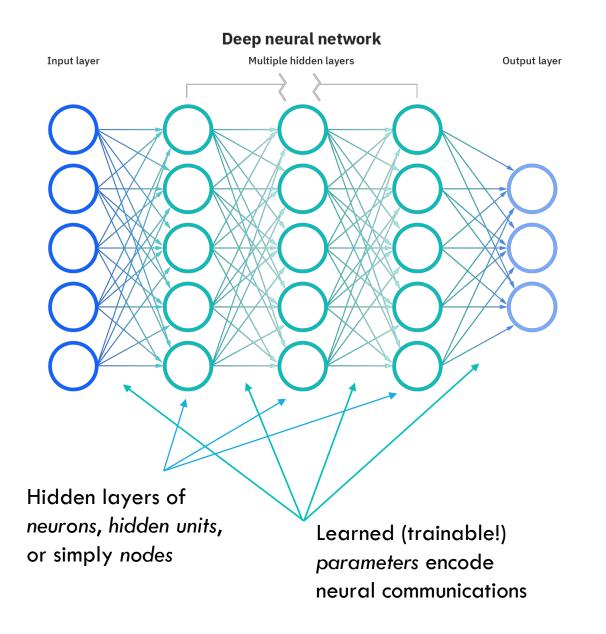


Hidden layers of neurons, hidden units, or simply nodes

#### DEEP NEURAL NETWORKS

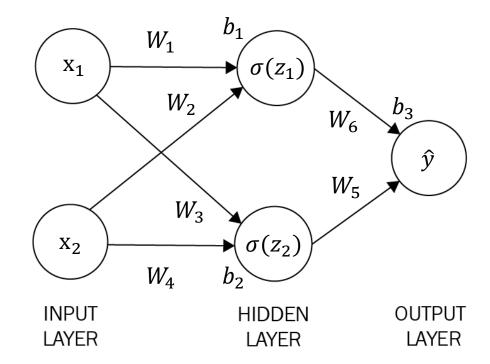
- A class of ML algorithms based on artificial neural networks (ANNs)
  - Neural network → networks of neurons responding to stimuli
  - "Deep" → multiple layers of neurons interacting in sequence
- Practically speaking, DNNs are nonlinear models designed to leverage complicated relationships in data

$$f(x \mid parameters) = output$$
Adjustable, e.g. fit to data in supervised learning



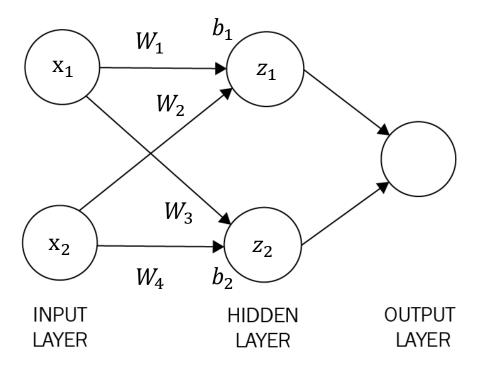
- **Example**: Classification problem with  $x_i \in \mathbb{R}^2$   $y_i \in \{0,1\}$
- Let's draw a test data point and pass it through a simple ANN:

$$x = (x_1, x_2) \qquad \qquad y = 1$$



- Single hidden layer with 2 neurons
- Key Ingredients:
  - Trainable weights  $W_1, W_2, W_3, W_4, W_5, W_6$  and biases  $b_1, b_2, b_3$
  - Non-linear activation functions (called non-linearities)  $\sigma(z)$

The simplest artificial neural network - Practical Convolutional Neural Networks [Book] (oreilly.com)



#### 1. Compute preactivations at each neuron

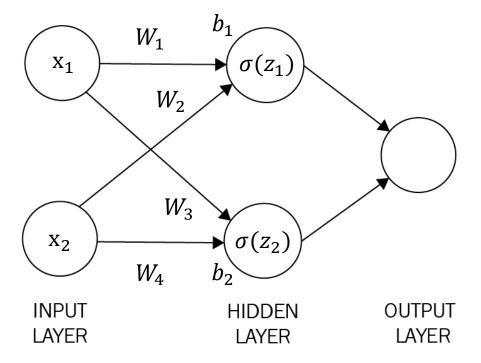
$$z_1 = w_1 x_1 + w_2 x_2 + b_1$$
  
$$z_2 = w_3 x_1 + w_4 x_2 + b_2$$

Or, in matrix notation:

$$\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} w_1 & w_2 \\ w_3 & w_4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

the weight matrix mixes up the inputs and feeds them to the each neuron the bias vector adds constants to the mixed inputs

Note: this is a linear operation!!



1. Compute preactivations at each neuron

$$\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} w_1 & w_2 \\ w_3 & w_4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

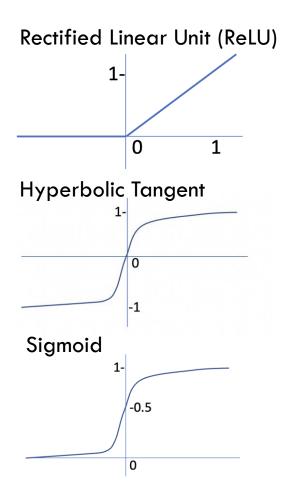
2. Calculate how much the neuron activates given the strength of the preactivation

 $\sigma(z) \rightarrow$  activation function

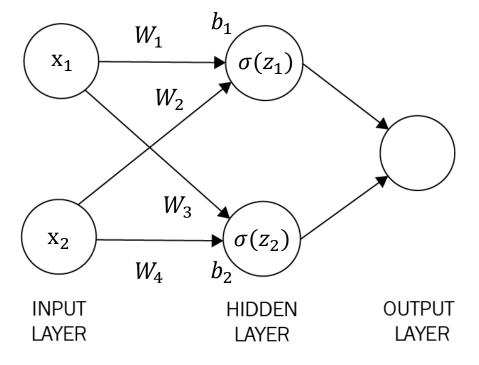
$$\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \to \begin{pmatrix} \sigma(z_1) \\ \sigma(z_2) \end{pmatrix}$$

#### NON-LINEAR ACTIVATION FUNCTIONS

- Non-linear activation functions allow us to learn complex relationships by "intervening" between linear operations
- In practice, they allow neurons to switch "on" and "off" to varying degrees



← Most popular choice; simple to compute (fast training), no "saturating" regions with tiny gradients



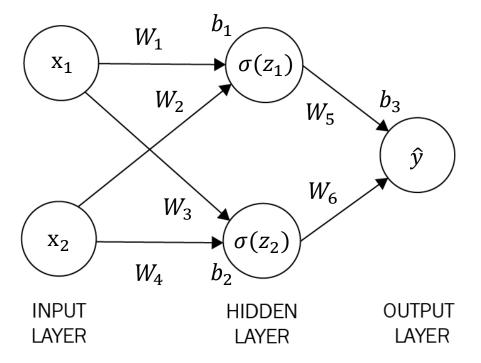
1. Compute preactivations at each neuron

$$\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} w_1 & w_2 \\ w_3 & w_4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

2. Calculate how much the neuron activates given the strength of the preactivation

$$\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \to \begin{pmatrix} \sigma(z_1) \\ \sigma(z_2) \end{pmatrix}$$

#### HOW IT WORKS



1. Compute preactivations at each neuron

$$\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} w_1 & w_2 \\ w_3 & w_4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

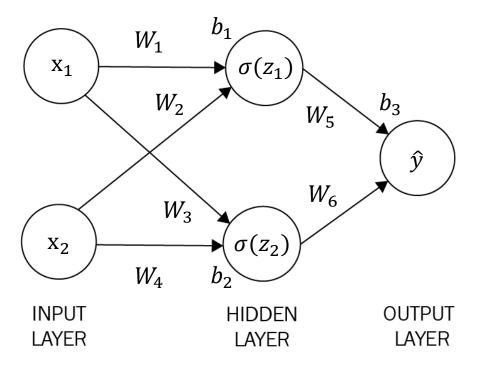
2. Calculate how much the neuron activates given the strength of the preactivation

$$\begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \to \begin{pmatrix} \sigma(z_1) \\ \sigma(z_2) \end{pmatrix}$$

3. Calculate model outputs

$$\hat{y} = (w_5 \quad w_6) \begin{pmatrix} \sigma(z_1) \\ \sigma(z_2) \end{pmatrix} + b_3$$

## HOW IT WORKS



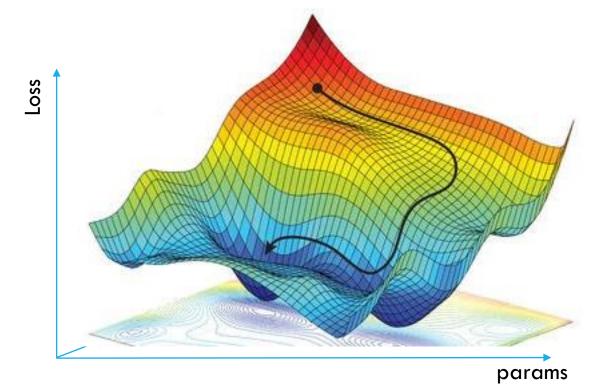
#### Forward Pass Predictions

- 1. Compute preactivations at each neuron
- 2. Calculate how much the neuron activates given the strength of the pre-activation (Repeat 1 and 2 to some fixed depth)
- 3. Calculate model outputs

When we define an NN, we fix an architecture by specifying:

- Number of hidden layers (here 1)
- Dimension of the hidden layers (here 2)
- Activation functions
- Random initial values for weights and biases

#### TRAINING A NN



The loss function may be very complicated in practice!

Training a  $NN \rightarrow$  find "optimal" weights, biases

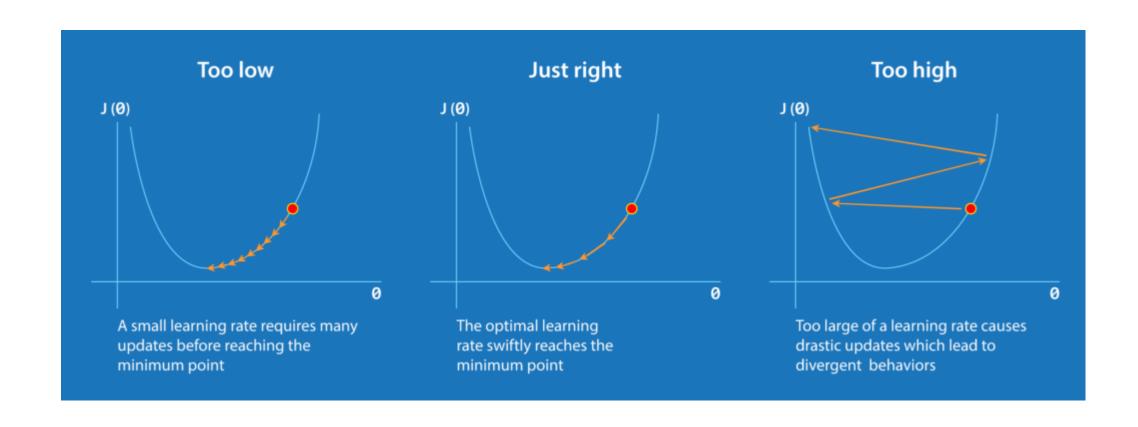
- Start by defining a loss function  $L(y, \hat{y})$
- Compute the gradient of  $L(y, \hat{y})$  with respect to each weight and bias
- Update the weights and biases via **gradient descent**:

$$W_{1}^{(k+1)} = W_{1}^{(k)} - \gamma \frac{\partial L}{\partial W_{1}} \Big|_{W_{1}^{(k)}}$$
$$b_{1}^{(k+1)} = b_{1}^{(k)} - \gamma \frac{\partial L}{\partial b_{1}} \Big|_{b_{1}^{(k)}}$$

etc.

 $\gamma \rightarrow$  learning rate

## LEARNING RATES



## TRAINING A NN

What we want:  $\frac{\partial L}{\partial W}$ ,  $\frac{\partial L}{\partial b}$ 

Generically, "gradients"

# Backward Pass (Backpropagation)

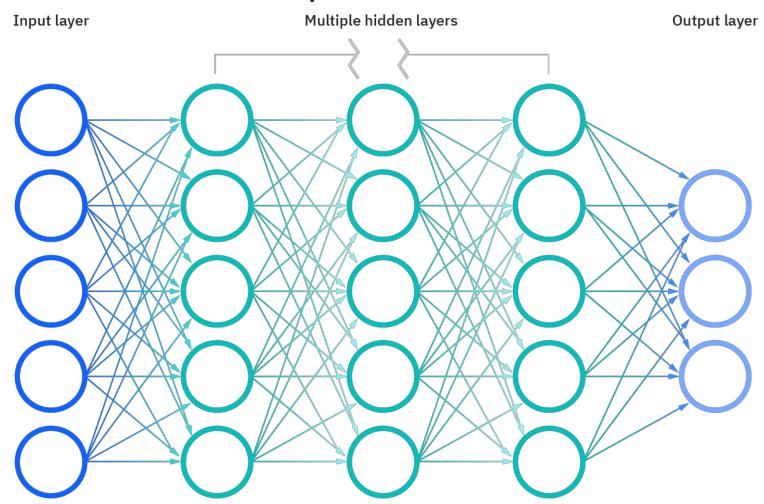
Apply the chain rule to calculate derivatives of the loss with respect to the weights/biases

$$f^{(3)}$$
  $y$   $\frac{\partial z}{\partial w}$   $f^{(2)}$   $=\frac{\partial z}{\partial y} \frac{\partial y}{\partial x} \frac{\partial x}{\partial w}$   $=f^{(3)'}(y)f^{(2)'}(x)f^{(1)'}(w)$ 

## **PSEUDOCODE**

```
for each training epoch:
   for each (input, truth) in train_data:
        prediction = NN(train_data)
        loss = loss_function(prediction, truth)
        gradients = compute_gradients(loss)
        new_params = grad_descent(gradients, NN.parameters, lr)
        model.update(new_params)
```

#### Deep neural network



# SHOULD YOU USE DL FOR YOUR PROJECT?

#### Why DL?

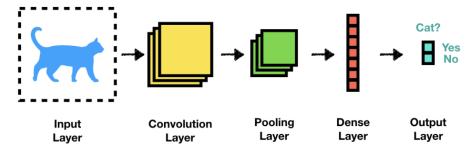
- Produce predictions in multiple feed-forward stages > powerful feature extraction:
  - Less need for data pre-processing
  - Ability to leverage large amounts of data ("big data")
- Handle more complicated data representations like images, sentences, and graphs
- Can be designed to perform complicated (multi-stage) tasks end-to-end

#### Why not DL?

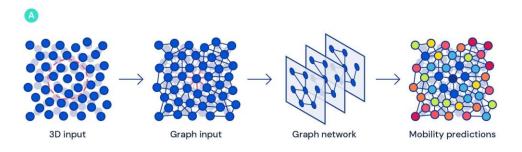
- Developing and training large DL models is computationally expensive (slow, resource intensive) and often requires specialized computing hardware
- It usually takes a lot of data to train DL models

#### MORE ARCHITECTURES

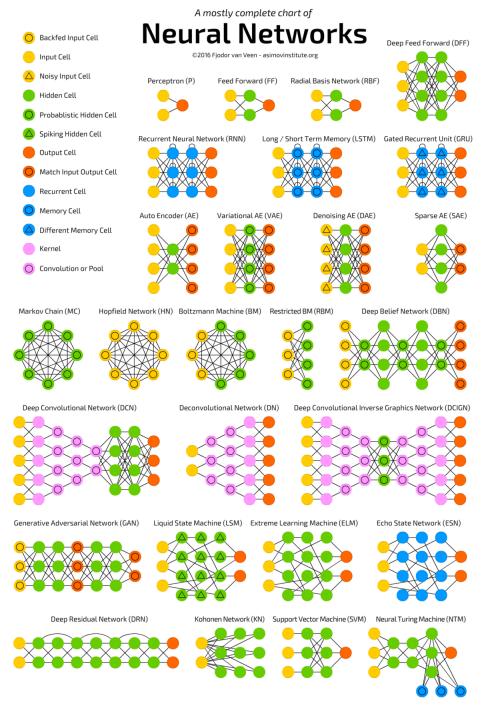
- NNs are the building blocks for more complicated architectures, e.g.
  - Convolutional Neural Networks are frequently applied to images or other grid data
  - Recurrent Neural Networks are applied to sequences like sentences
  - Graph Neural Networks operate on networks of objects (nodes) connected by their relationships (edges)
  - Generative Adversarial Networks are used to generate new data (e.g. photographs) similar to a reference set



Convolutional Neural Network: A Step By Step Guide | by Shashikant | Towards Data Science



Towards understanding glasses with graph neural networks (deepmind.com)



A bit outdated, but fun to see the creativity...

The mostly complete chart of Neural Networks, explained | by Andrew Tch | Towards Data Science



#### Time for some NN practice!

Please navigate to Day 3!

PrincetonUniversity/intro machine learning (github.com)