Dive into Deep Learning in 1 Day

1 Basics · 2 Convnets · 3 Computation · 4 Sequences

ODSC 2019

Alex Smola
http://courses.d2l.ai/odsc2019/

Outline

- Installation
- Linear Algebra and Deep Numpy
- Autograd
- Softmax Classification
- Optimization
- Multilayer Perceptron


Installation

Tools

- Python
- Jupyter
- Reveal (for notebook slides)

```
conda create --name mxnet
conda activate mxnet
conda install python==3.7 pip jupyter rise
pip install mxnet-cu100 --pre
pip install git+https://github.com/d2l-ai/d2l-en@numpy2
git clone https://github.com/d2l-ai/1day-notebooks.git
```

mxnet.np

NumPy

mxnet.np

Deep NumPy

numpy.d2l.ai

Typical Deep Learning Workflow

- Get data and load it (e.g. in Pandas)
  - Preprocess it in NumPy
  - Convert to framework specific format
- Train model
  - Build model in specific format (TF, PyTorch, Gluon)
  - Optimize
- Convert predictions into NumPy
  - Plot and serve

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- Convert predictions into NumPy
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Do you remember all the peculiarities?

Matrix Multiplication in NumPy

```
import numpy as np
from time import time
```

```
# testing NumPy
n = 1024
x = np.random.normal(0, 1, (n, n))
y = np.random.normal(0, 1, (n, n))
```

Random normal matrix

```
# single invocation
def single():
    z = np.dot(x,y)
timer(single)

def multiple():
    for i in range(1000):
        z = np.dot(x,y)
timer(multiple, True)
```

Matrix-matrix multiplication

```
0.065011 seconds
53.658205 seconds
4.002153 Gigaflops
```

Numbers from old 2015 MacBook Pro
(runs on GPU, too)

aws

Matrix Multiplication in PyTorch

```python
import numpy as np
from time import time
```

```python
# testing NumPy
n = 1024
x = np.random.normal(0, 1, (n, n))
y = np.random.normal(0, 1, (n, n))
```

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def single():
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def multiple():
    for i in range(1000):
        z = np.dot(x,y)
timer(multiple, True)
```

```
0.065011 seconds
53.658205 seconds
4.002153 Gigaflops
```

```python
import torch
```

Random normal matrix

```python
x = torch.randn(n,n)
y = torch.randn(n,n)
```

```python
# single invocation
def single():
    z = torch.mm(x,y)
timer(single)

def multiple():
    for i in range(1000):
        z = torch.mm(x,y)
timer(multiple, True)
```

Matrix-matrix multiplication

```
0.029826 seconds
22.214673 seconds
9.666960 Gigaflops
```

aws

Matrix Multiplication in TensorFlow

```python
import numpy as np
from time import time
```

```python
# testing NumPy
n = 1024
x = np.random.normal(0, 1, (n, n))
y = np.random.normal(0, 1, (n, n))
```

```python
# single invocation
def single():
    z = np.dot(x,y)
timer(single)

def multiple():
    for i in range(1000):
        z = np.dot(x,y)
timer(multiple, True)
```

```
0.065011 seconds
53.658205 seconds
4.002153 Gigaflops
```

Random normal matrix

```python
import tensorflow
```

```python
x = tf.random.normal([n, n])
y = tf.random.normal([n, n])
```

```python
# single invocation
def single():
    z = tf.matmul(x,y)
timer(single)

def multiple():
    for i in range(1000):
        z = tf.matmul(x,y)
timer(multiple, True)
```

Matrix-matrix multiplication

```
0.028445 seconds
19.343846 seconds
11.101638 Gigaflops
```

Matrix Multiplication in …

```
import numpy as np
from time import time
```

```
# testing NumPy
n = 1024
x = np.random.normal(0, 1, (n, n))
y = np.random.normal(0, 1, (n, n))
```

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# single invocation
def single():
    z = np.dot(x,y)
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def multiple():
    for i in range(1000):
        z = np.dot(x,y)
timer(multiple, True)
```

```
0.065011 seconds
53.658205 seconds
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```

- MXNet Gluon
- Caffe2
- CNTK
- Chainer
- Paddle
- Keras

Matrix Multiplication in …

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Confusing

Deep NumPy

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0.065011 seconds
53.658205 seconds
4.002153 Gigaflops
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```
from mxnet import np as np
```

```
# testing Deep NumPy
x = np.random.normal(0, 1, (n, n))
y = np.random.normal(0, 1, (n, n))
```

```
# single invocation
def single():
    z = np.dot(x,y)
timer(single)

def multiple():
    for i in range(100):
        z = np.dot(x,y)
timer(multiple)

def multiple_touch():
    for i in range(1000):
        z = np.dot(x,y)
    z.wait_to_read()
timer(multiple_touch, True)
```

Barrier

```
0.000663 seconds
0.008336 seconds
18.248058 seconds
11.768286 Gigaflops
```

Frontend for Deep NumPy (on MXNet)

- `np (numpy drop-in replacement)`
  - 100% NumPy compatible* (arguments for device context)
  - Asynchronous evaluation
- `autograd`
- `npx (numpy extensions)`
  - Devices
  - Convolutions and other DL operators
- `nn (neural networks)`
  - Layers, optimizers, loss functions … (MXNet Gluon)

NumPy notebook

Automatic Differentiation

Automatic Differentiation

$$z = \left(\langle \mathbf{x}, \mathbf{w} \rangle - y\right)^2$$

Computing derivatives by hand is hard

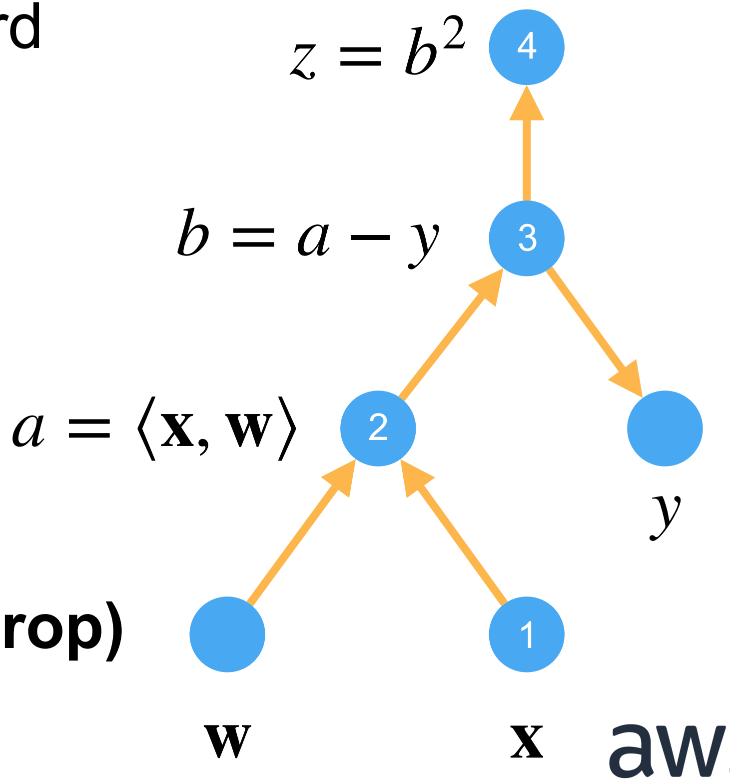
Computers can automate this

Compute graph

- Build explicitly (TensorFlow, MXNet Symbol)
- **Build implicitly by tracing** (Chainer, PyTorch, DeepNumpy)

Chain rule (evaluate e.g. via backprop)

$$\frac{\partial y}{\partial x} = \frac{\partial y}{\partial u_n} \frac{\partial u_n}{\partial u_{n-1}} \cdots \frac{\partial u_2}{\partial u_1} \frac{\partial u_1}{\partial x}$$



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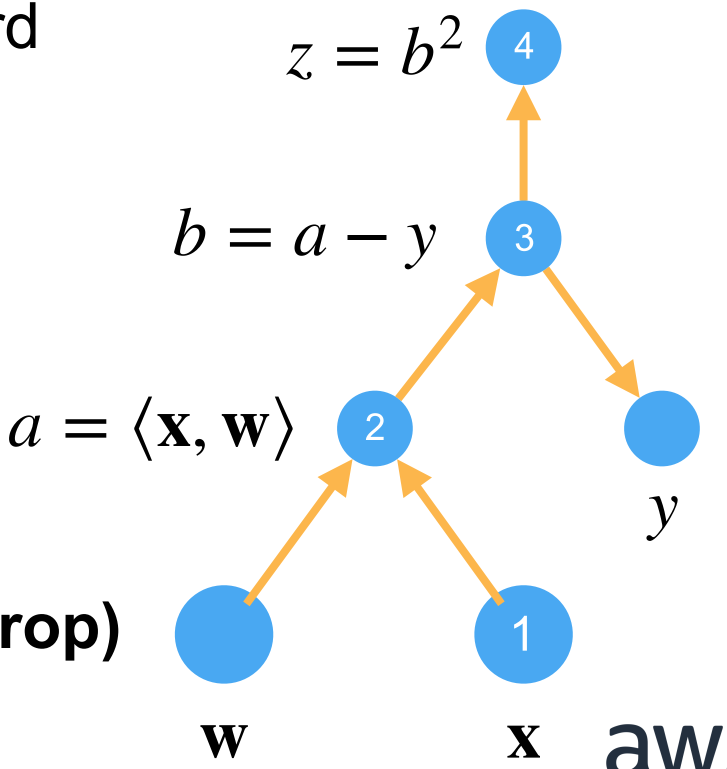

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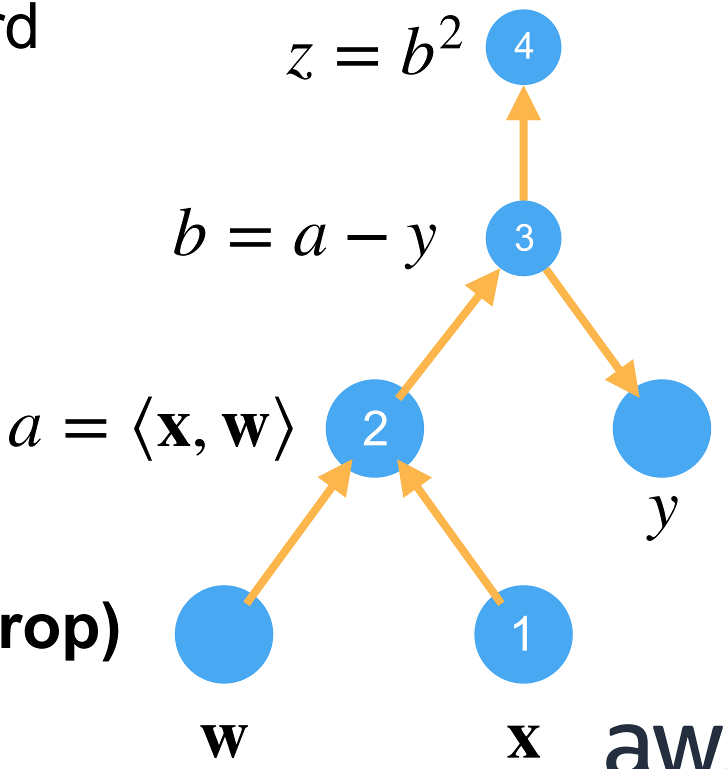

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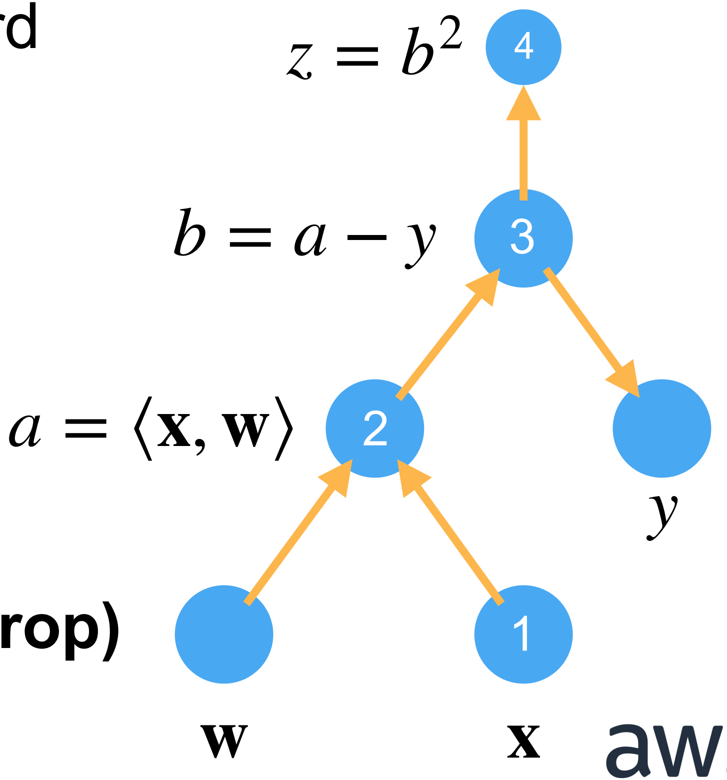

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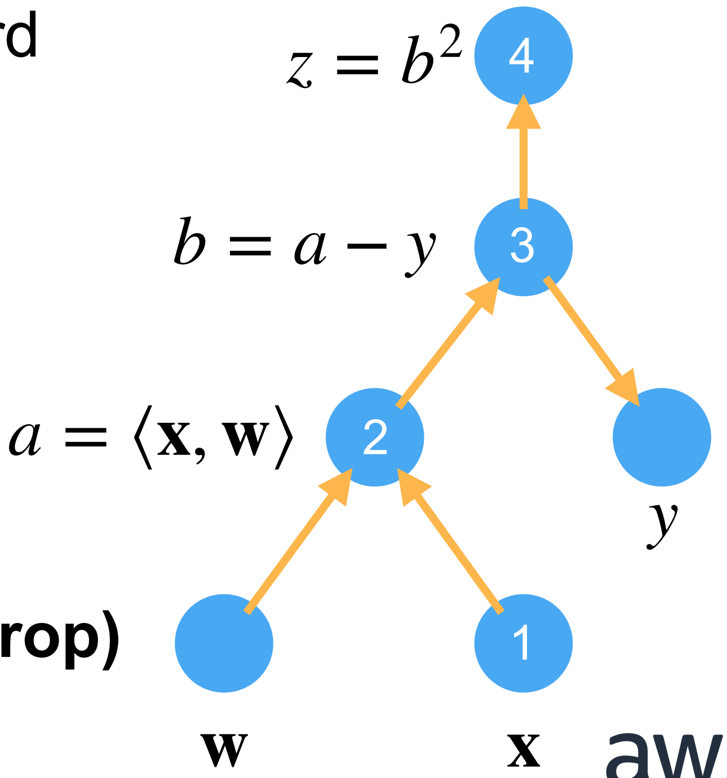

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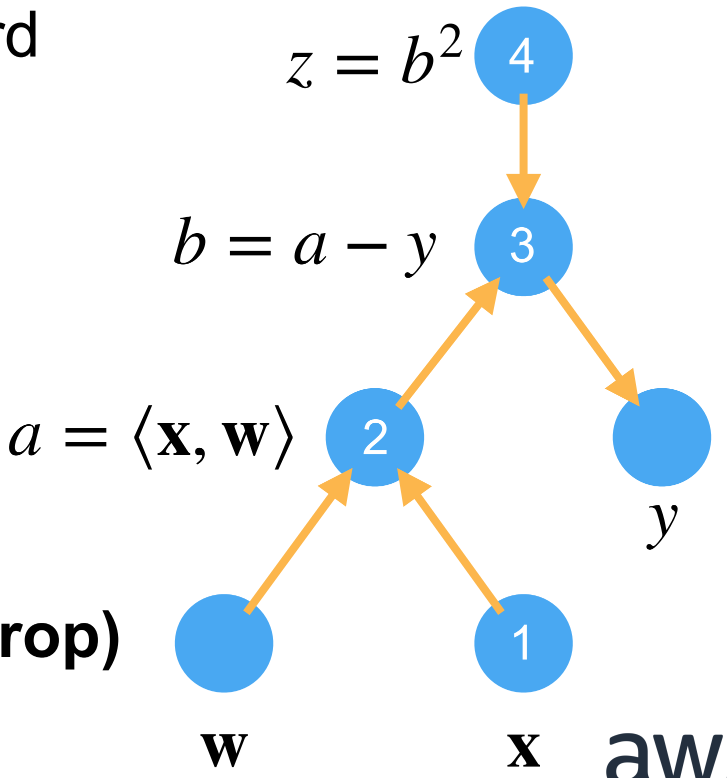

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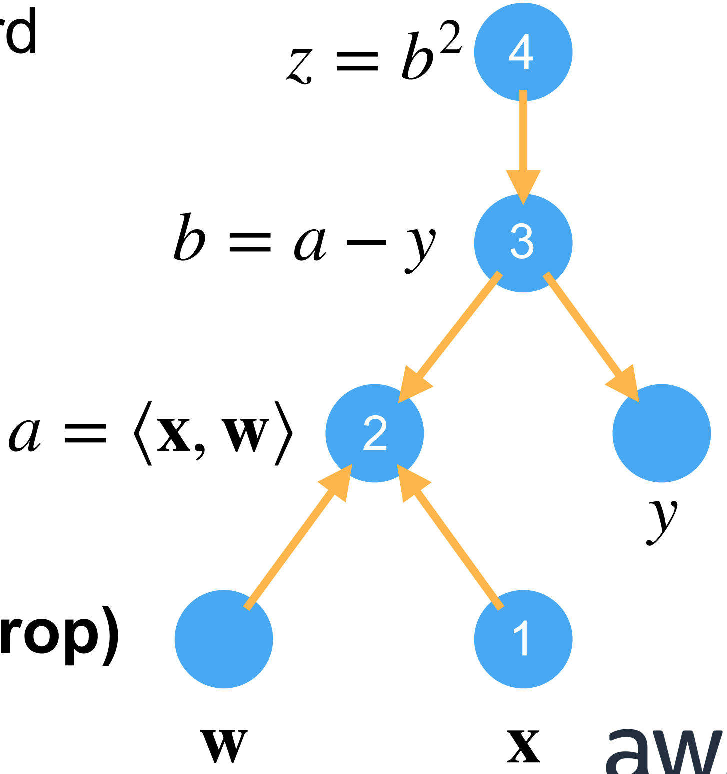

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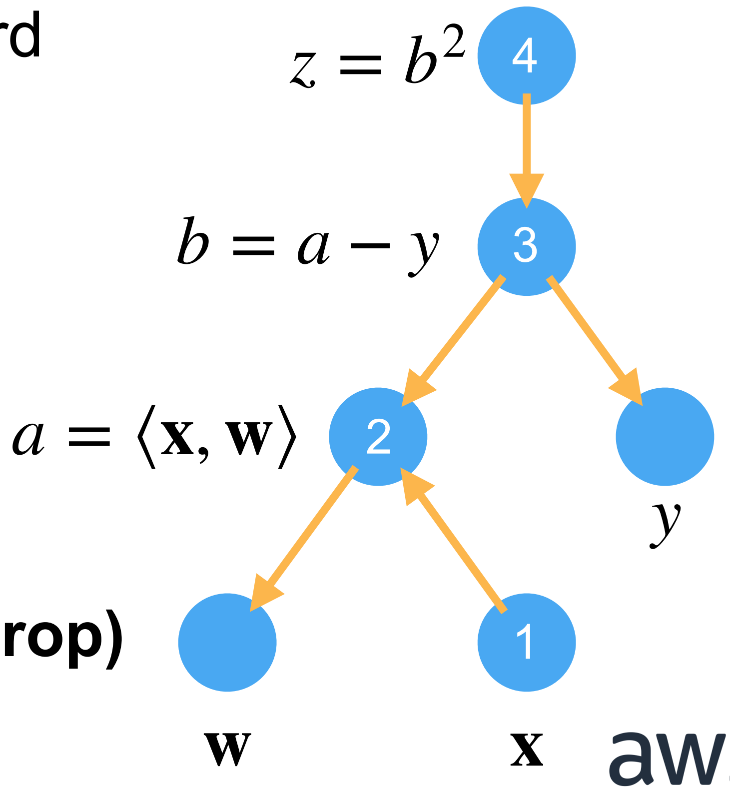
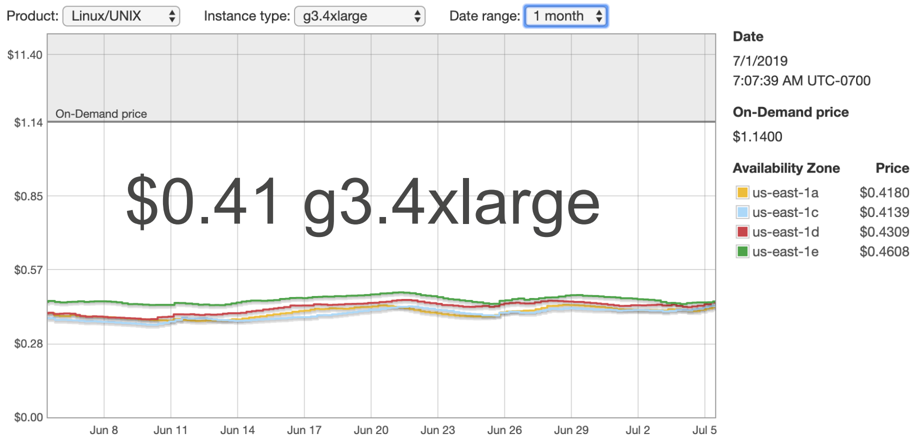
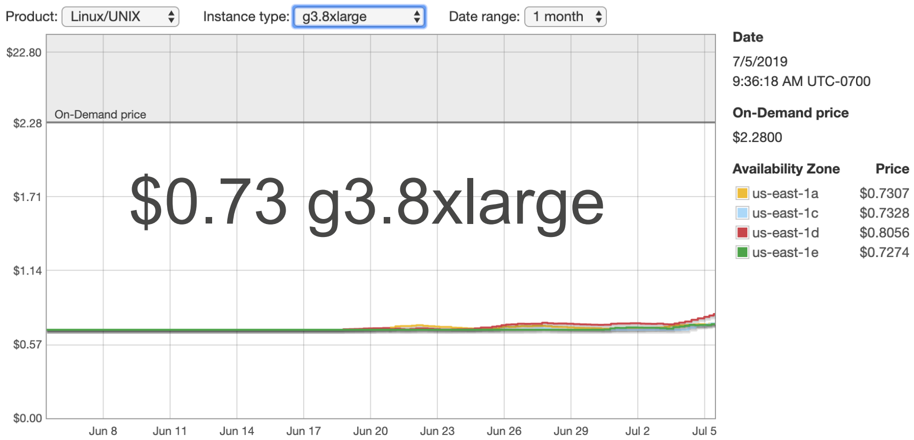
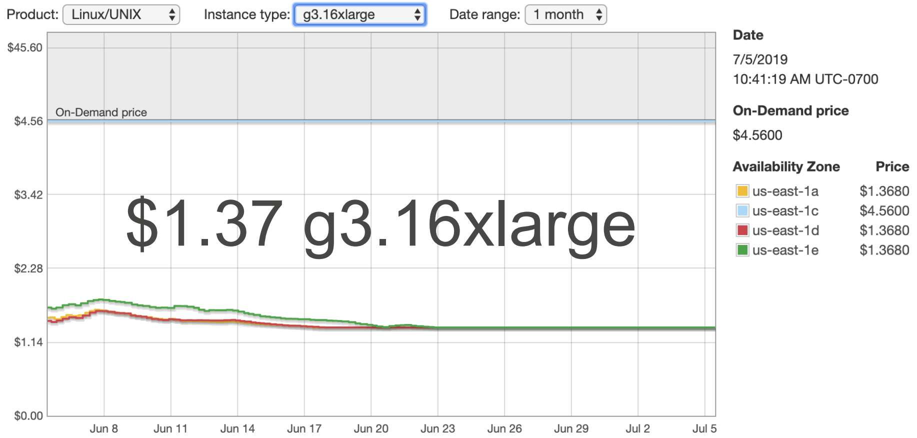


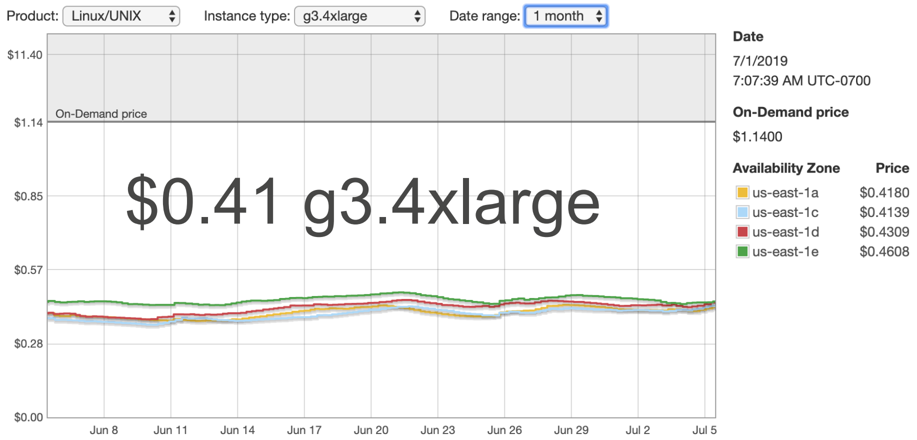
AutoGrad notebook

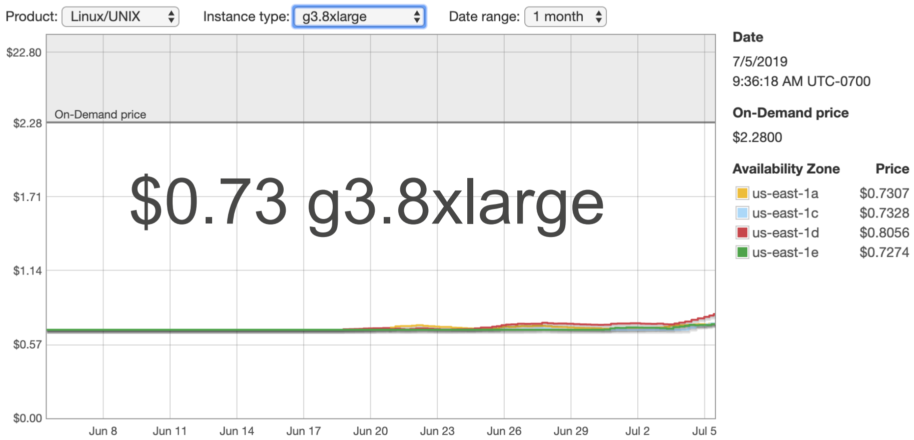


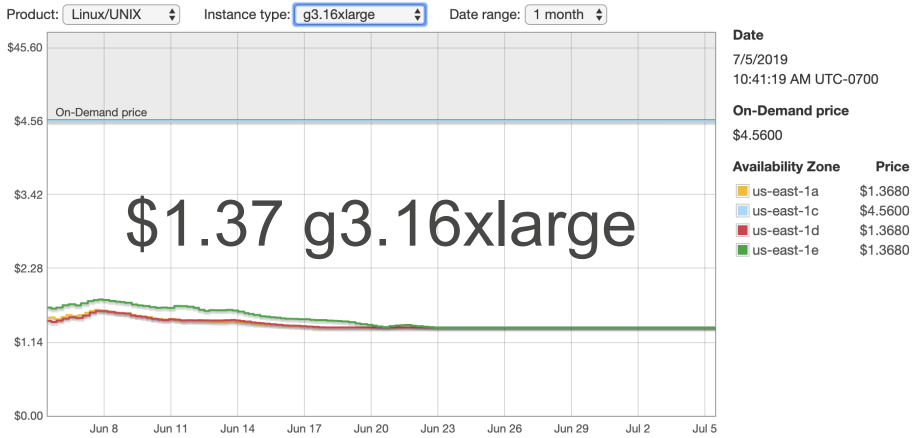




Can we estimate prices (time, server, region)?







Can we estimate prices (time, server, region)?

$$p = w_{\text{time}} \cdot t + w_{\text{server}} \cdot s + w_{\text{region}}[r]$$

Linear Model

- n-dimensional inputs $\mathbf{x} = [x_1, x_2, \ldots, x_n]^T$
- Linear model

$$\hat{y} = w_1 x_1 + w_2 x_2 + \ldots + w_n x_n + b$$

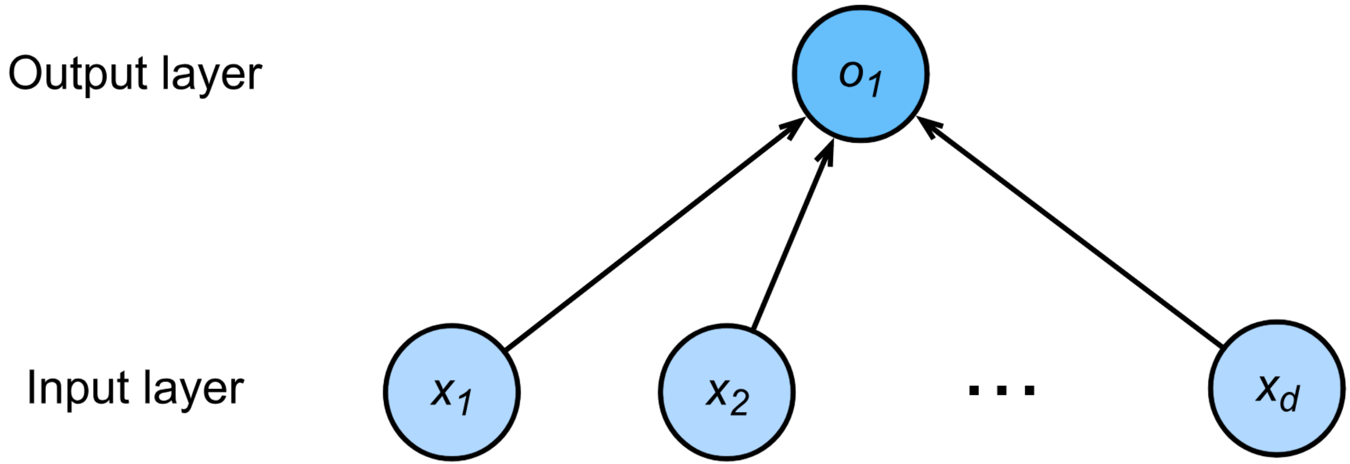
- Weights and bias $\mathbf{w} = [w_1, w_2, \ldots, w_n]^\top$ and b
- Vectorized version

$$\hat{y} = \langle \mathbf{w}, \mathbf{x} \rangle + b$$

- Loss function (to measure goodness of fit)

$$l(y, \hat{y}) = (y - \hat{y})^2$$

Linear Model as a Single-layer Neural Network



We can stack multiple layers to get deep neural networks

Training and Test Data

- Collect multiple data points to fit parameters (spot instance prices in the past 6 months)
- Training data - the more the better

$$\mathbf{X} = \left[\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_n\right]^T \qquad \mathbf{y} = \left[y_0, y_1, \ldots, y_n\right]^T$$

- Test data - when we actually want to try it out

$$\mathbf{X}' = \left[\mathbf{x}'_0, \mathbf{x}'_1, \ldots, \mathbf{x}'_{n'}\right]^T$$

We do not observe labels at time of prediction (after all, that's what we use ML for)

Training

- Objective is to minimize (regularized) training loss

$$\boxed{\operatorname*{argmin}_{w} \frac{1}{n} \sum_{i=1}^{n} l(y_i, \hat{y}_i)}$$

- Plugging in expansion $\hat{y} = \langle \mathbf{w}, \mathbf{x} \rangle + b$ yields objective

$$\frac{1}{n} \sum_{i=1}^{n} (y_i - \langle \mathbf{w}, \mathbf{x}_i \rangle - b)^2 = \boxed{\frac{1}{n} \left\| \mathbf{y} - \mathbf{X}\mathbf{w} - b \right\|^2}$$

Linear Regression notebook

Logistic Regression

Regression vs. Classification

Regression estimates a continuous value

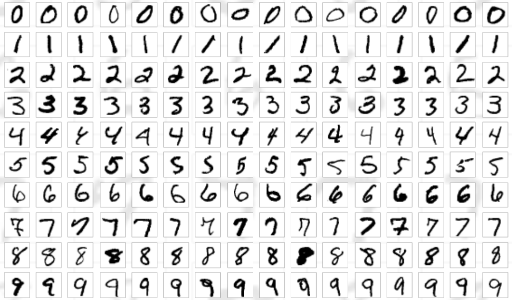
Classification predicts a discrete category

Regression vs. Classification

Regression estimates a continuous value

Classification predicts a discrete category

MNIST: classify hand-written digits (10 classes)



Regression vs. Classification

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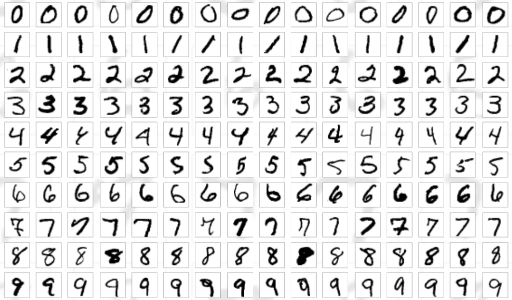
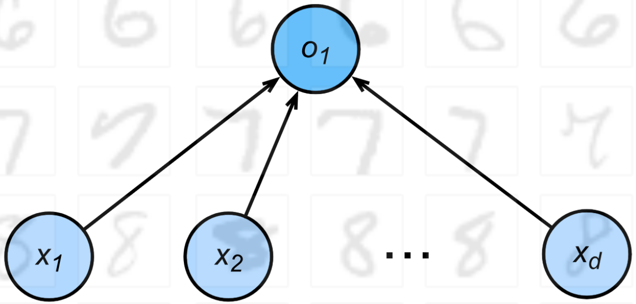


ImageNet: classify nature objects (1000 classes)

From Regression to Multi-class Classification

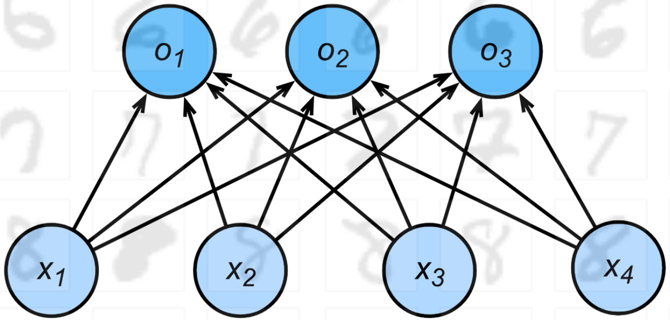
Regression

- Single continuous output
- Natural scale in $\mathbb{R}$
- Loss given e.g. in terms of difference $y - f(x)$



Classification

- Multiple classes, typically multiple outputs
- Score *should* reflect confidence …



From Regression to Multi-class Classification

Square Loss

- One hot encoding per class

$$\mathbf{y} = [y_1, y_2, \ldots, y_n]^\top$$

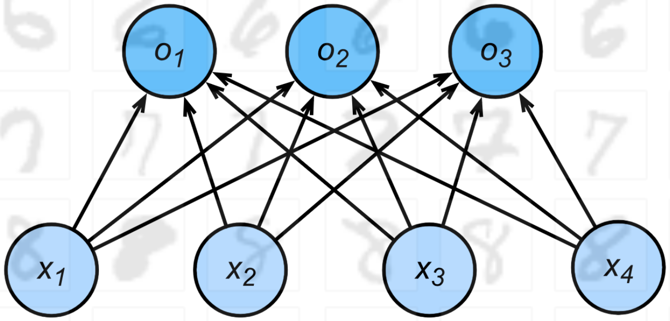
$$y_i = \begin{cases} 1 \text{ if } i = y \\ 0 \text{ otherwise} \end{cases}$$

- Train with squared loss
- Largest output wins

$$\hat{y} = \operatorname*{argmax}_i o_i$$

Classification

- Multiple classes, typically multiple outputs
- Score *should* reflect confidence …



From Regression to Multi-class Classification

Calibrated Scale

- Output matches probabilities (nonnegative, sums to 1)

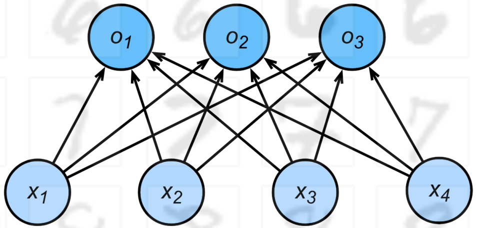
$$p(y \mid o) = \mathrm{softmax}(o)$$
$$= \frac{\exp(o_y)}{\sum_i \exp(o_i)}$$

- Negative log-likelihood

$$-\log p(y \mid y) = \log \sum_i \exp(o_i) - o_y$$

Classification

- Multiple classes, typically multiple outputs
- Score *should* reflect confidence …



Softmax and Cross-Entropy Loss

- Negative log-likelihood (for given label y)

$$-\log p(y \mid o) = \log \sum_i \exp(o_i) - o_y$$

- Cross-Entropy Loss (for probability distribution y)

$$l(y, o) = \log \sum_i \exp(o_i) - y^\top o$$

- **Gradient**

Difference between true and estimated probability

$$\partial_o l(y, o) = \frac{\exp(o)}{\sum_i \exp(o_i)} - y$$

aws

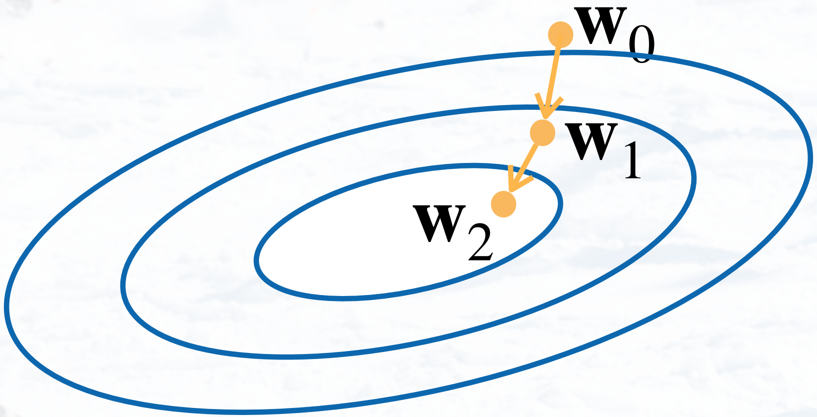
Logistic Regression Notebook


momentum
negative gradient
Stochastic Gradient Descent

Gradient Descent

Choose a starting point $\mathbf{w}_0$

Repeat to update weight

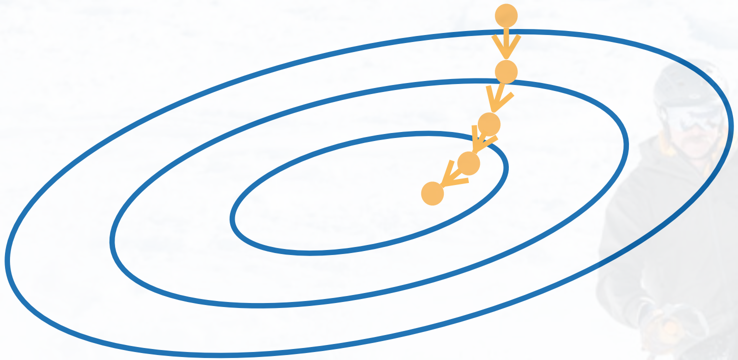


$$\mathbf{w}_t = \mathbf{w}_{t-1} - \eta \partial_w l(w_{t-1})$$

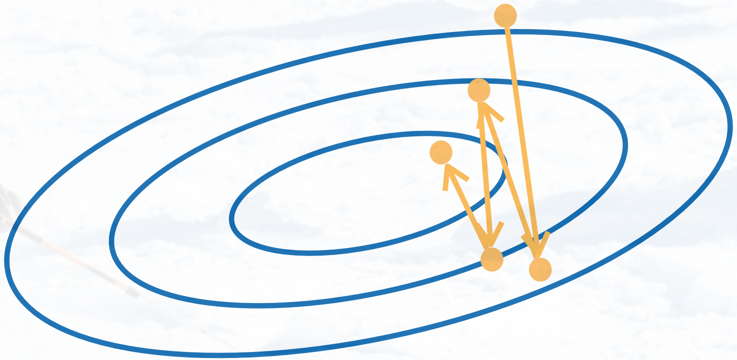
- Gradient direction indicates increase in value
- Learning rate adjusts step length

Goldilocks Learning Rate

Too small



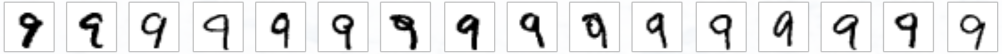
Too big



numpy.d2l.ai

Stochastic Gradient Descent (SGD)

- Computing the gradient over all data is too slow
- Redundancy in data (e.g. many similar digits)

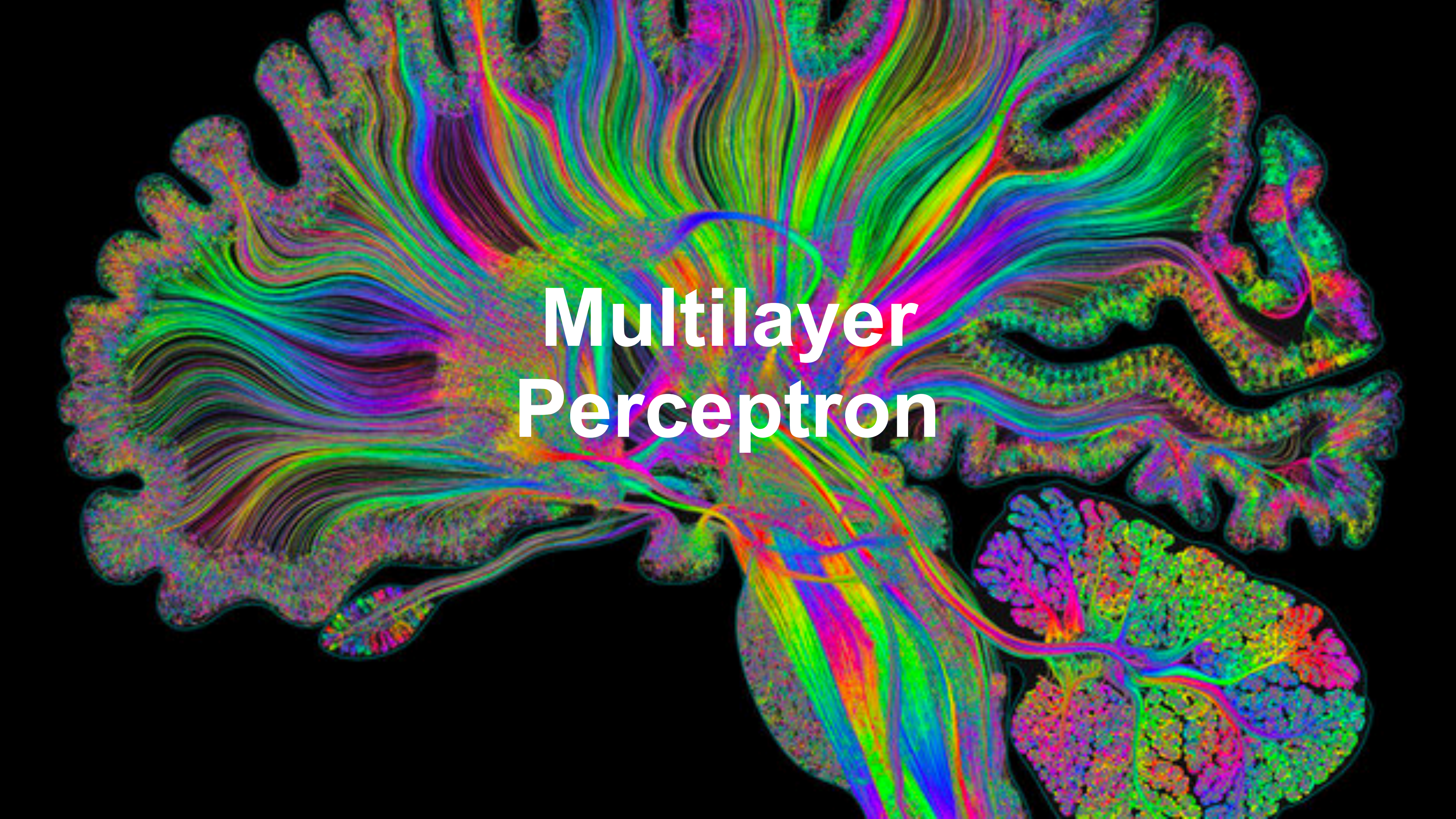


- Single observation is not efficient on GPU

- Sample b examples $i_1, \ldots i_b$ to approximate loss/gradient

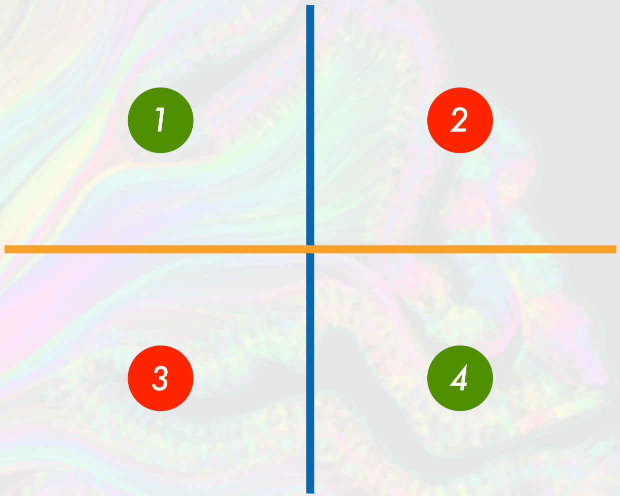
$$\boxed{\frac{1}{b}\sum_{i \in I_b} l(\mathbf{x}_i, y_i, \mathbf{w})} \text{ and } \boxed{\frac{1}{b}\sum_{i \in I_b} \partial_{\mathbf{w}} l(\mathbf{x}_i, y_i, \mathbf{w})}$$

b is the mini-batch size (chosen for GPU efficiency)



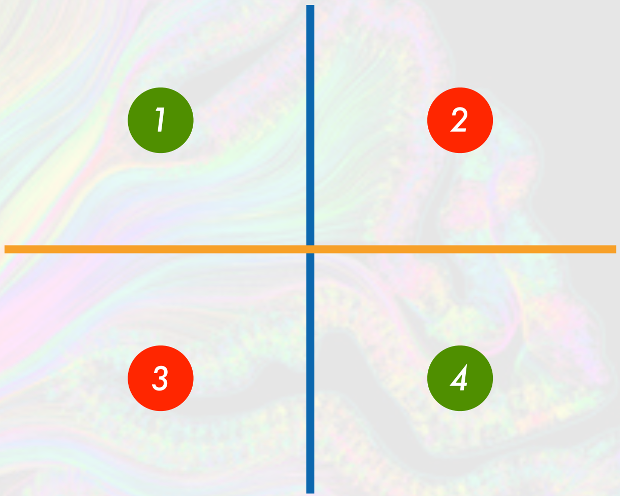
Multilayer Perceptron

Learning XOR



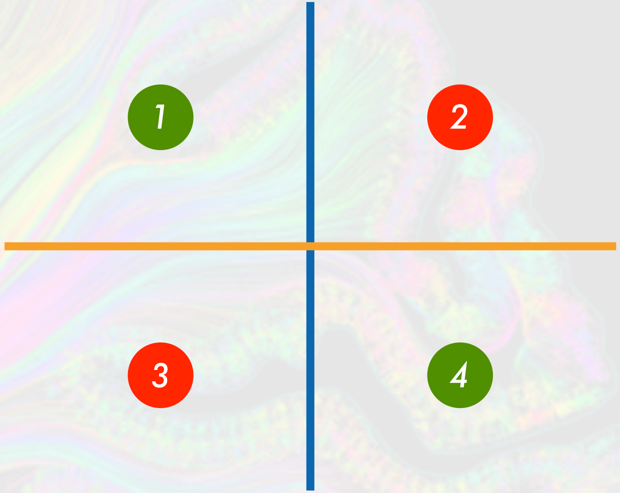
Learning XOR

	1	2	3	4
	+	-	+	-
	+	+	-	-
product	+	-	-	+

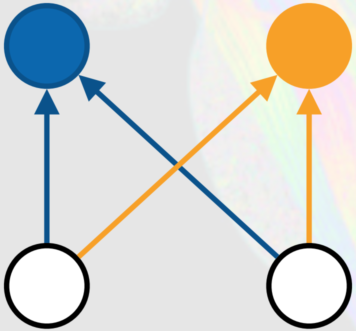


Learning XOR

	1	2	3	4
	+	-	+	-
	+	+	-	-
product	+	-	-	+



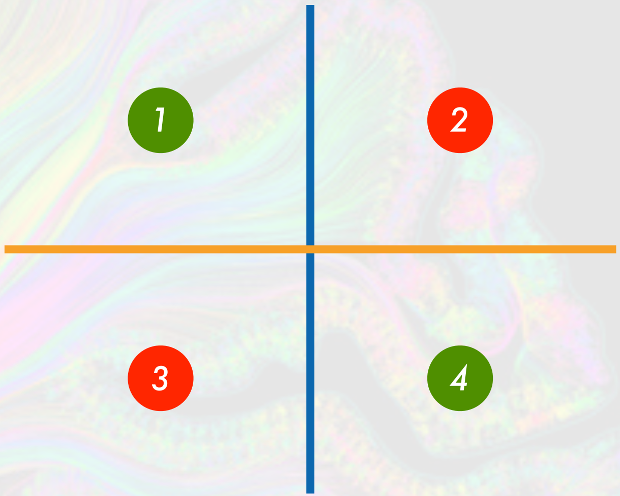
$$w_{11}x_1 + w_{12}x_2 + b_1$$



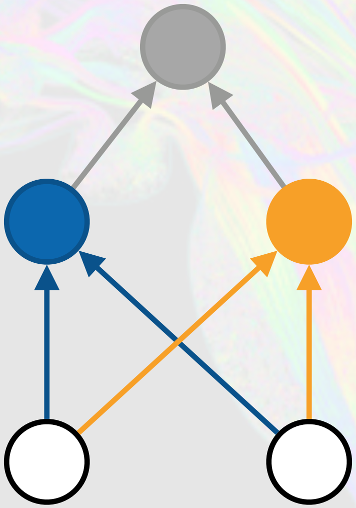
$$w_{21}x_1 + w_{22}x_2 + b_2$$

Learning XOR

	1	2	3	4
	+	-	+	-
	+	+	-	-
product	+	-	-	+

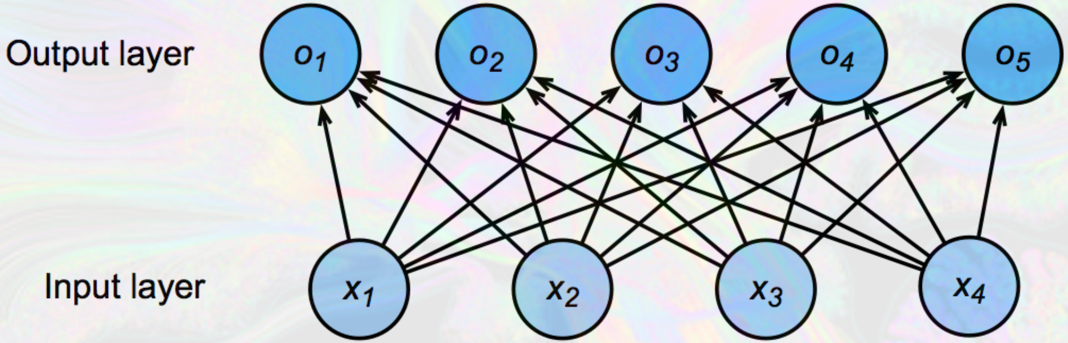


$$w_{11}x_1 + w_{12}x_2 + b_1$$

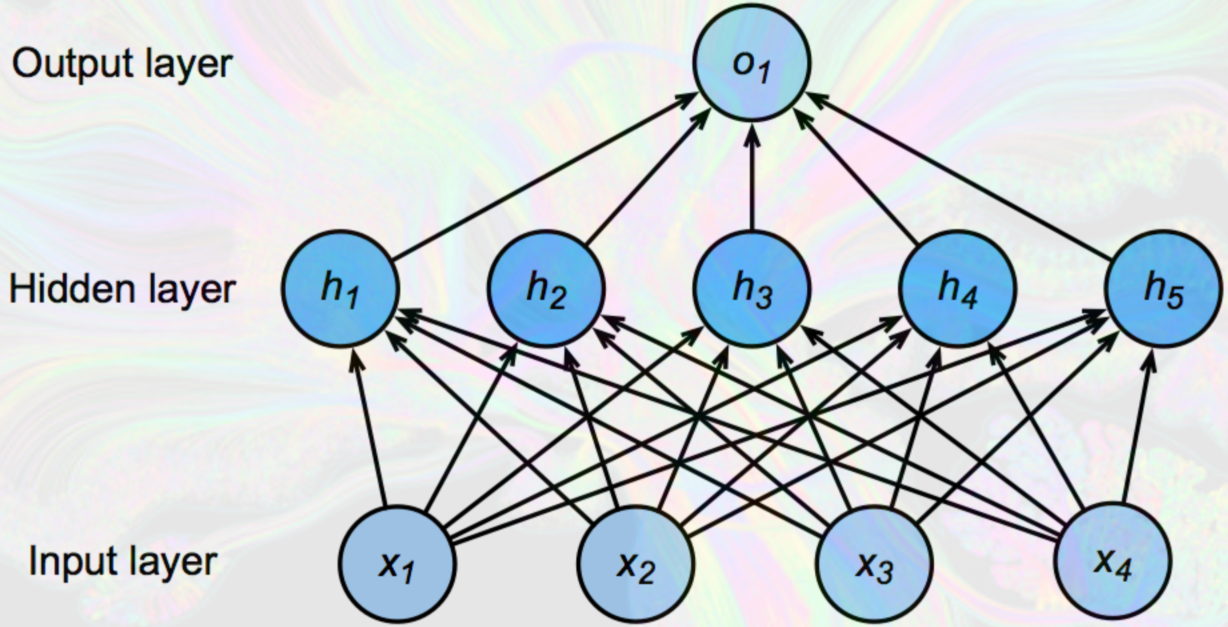


$$w_{21}x_1 + w_{22}x_2 + b_2$$

Single Hidden Layer



Single Hidden Layer



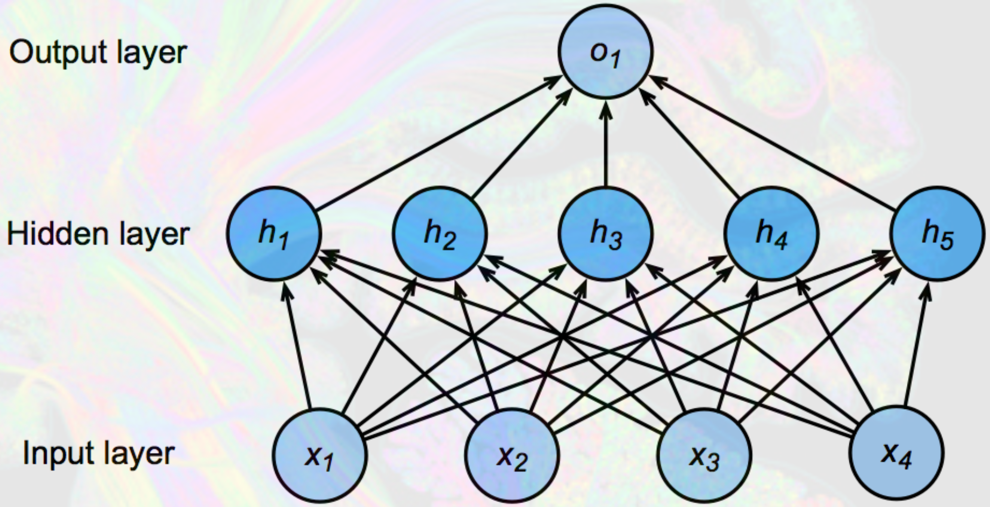
Single Hidden Layer

- Input $\mathbf{x} \in \mathbb{R}^n$
- Hidden $\mathbf{W}_1 \in \mathbb{R}^{m \times n}, \mathbf{b}_1 \in \mathbb{R}^m$
- Output $\mathbf{w}_2 \in \mathbb{R}^m, b_2 \in \mathbb{R}$

$$\mathbf{h} = \sigma(\mathbf{W}_1 \mathbf{x} + \mathbf{b}_1)$$

$$\mathbf{o} = \mathbf{w}_2^T \mathbf{h} + b_2$$

σ is an element-wise activation function



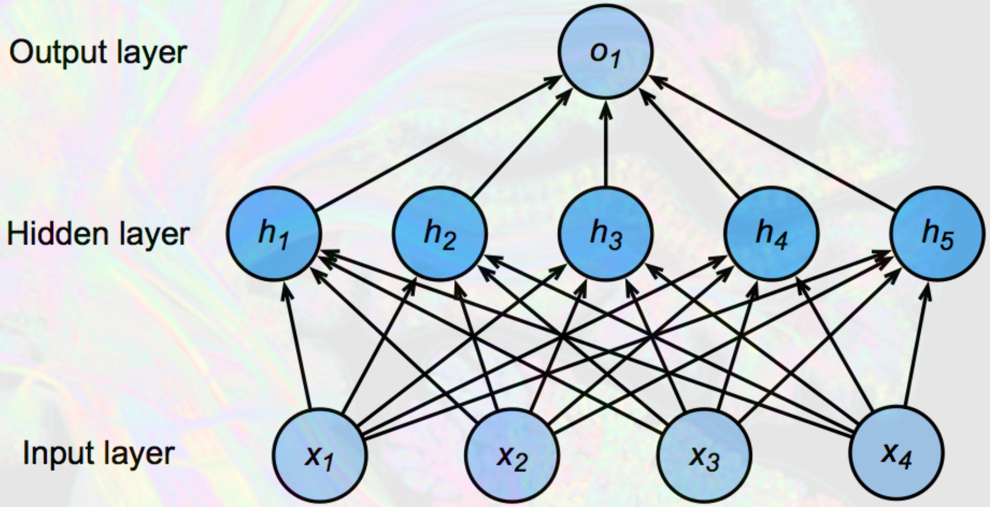
Single Hidden Layer

Why do we need an a nonlinear activation?

$$\mathbf{h} = \sigma(\mathbf{W}_1\mathbf{x} + \mathbf{b}_1)$$

$$\mathbf{o} = \mathbf{w}_2^T\mathbf{h} + b_2$$

σ is an element-wise activation function



Single Hidden Layer

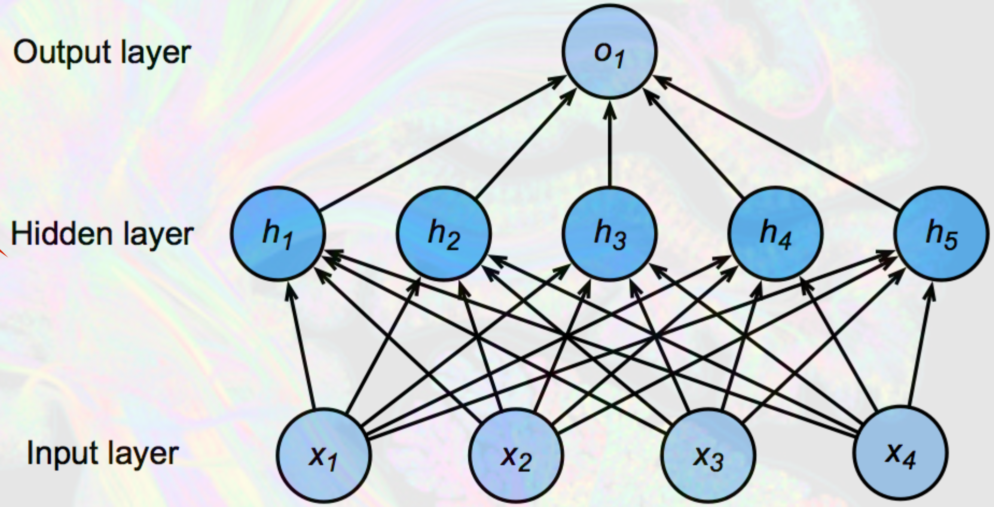
Why do we need an a nonlinear activation?

$$\mathbf{h} = \mathbf{W}_1\mathbf{x} + \mathbf{b}_1$$

$$\mathbf{o} = \mathbf{w}_2^T\mathbf{h} + b_2$$

hence $o = \mathbf{w}_2^\top \mathbf{W}_1 \mathbf{x} + b'$

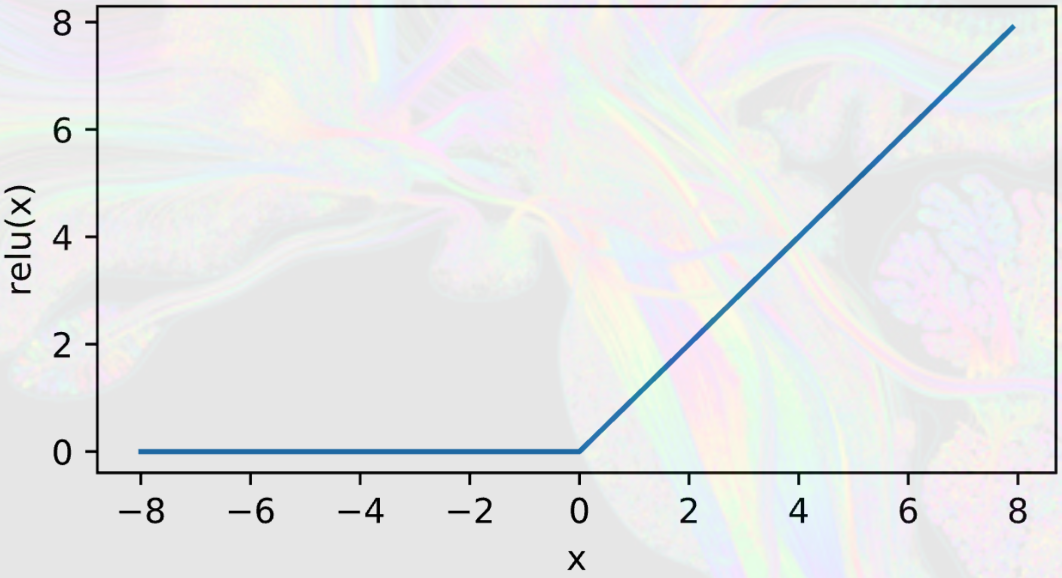
Linear ...



ReLU Activation

ReLU: rectified linear unit

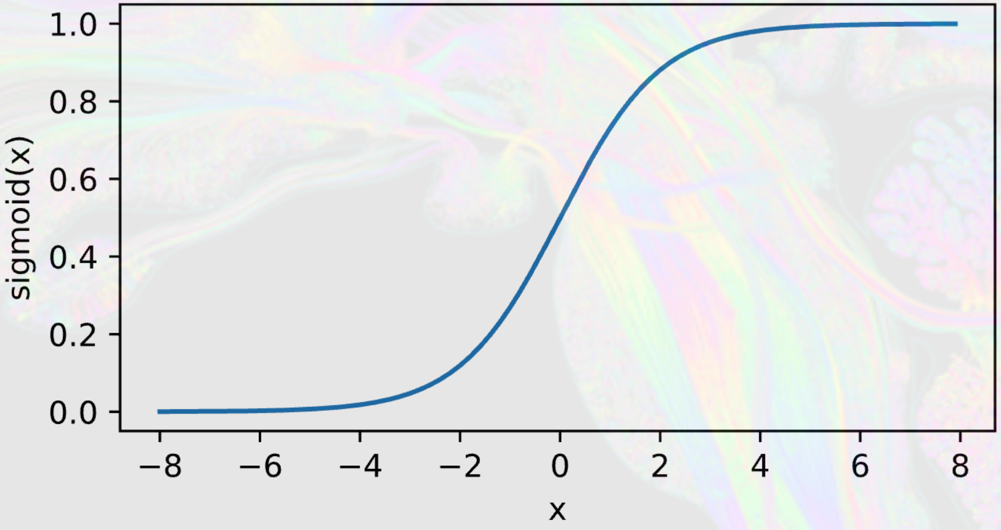
$$\mathrm{ReLU}(x) = \max(x, 0)$$



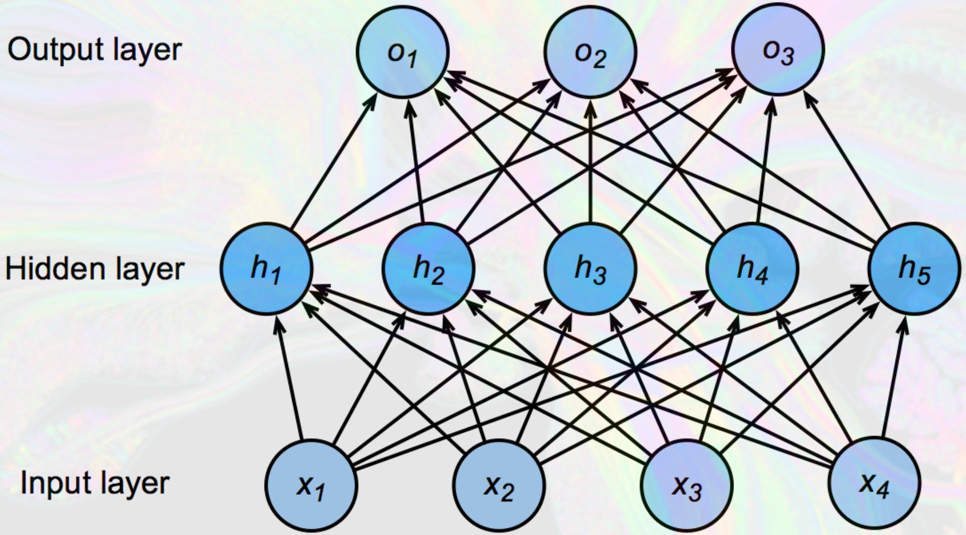
Sigmoid Activation

Map input into (0, 1), a soft version of $\sigma(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{otherwise} \end{cases}$

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

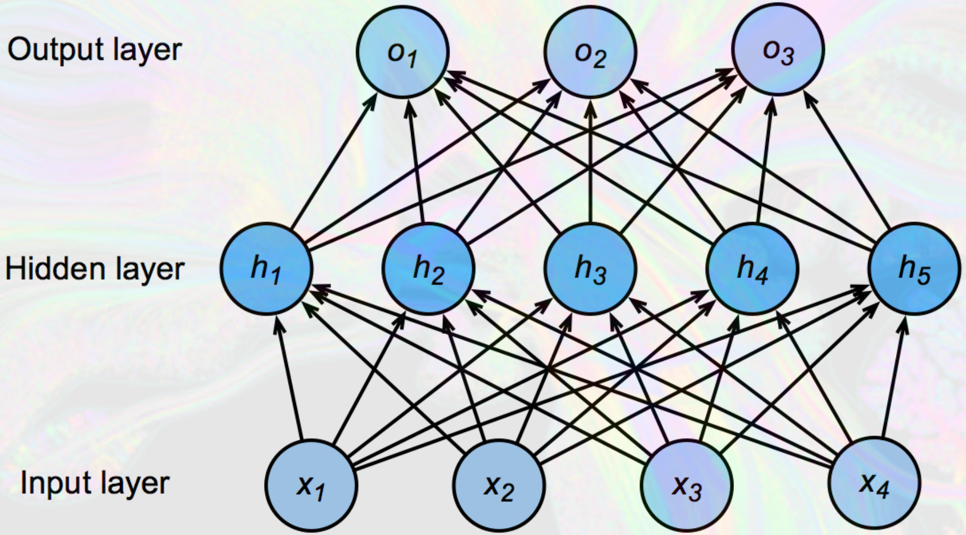


Multiclass Classification



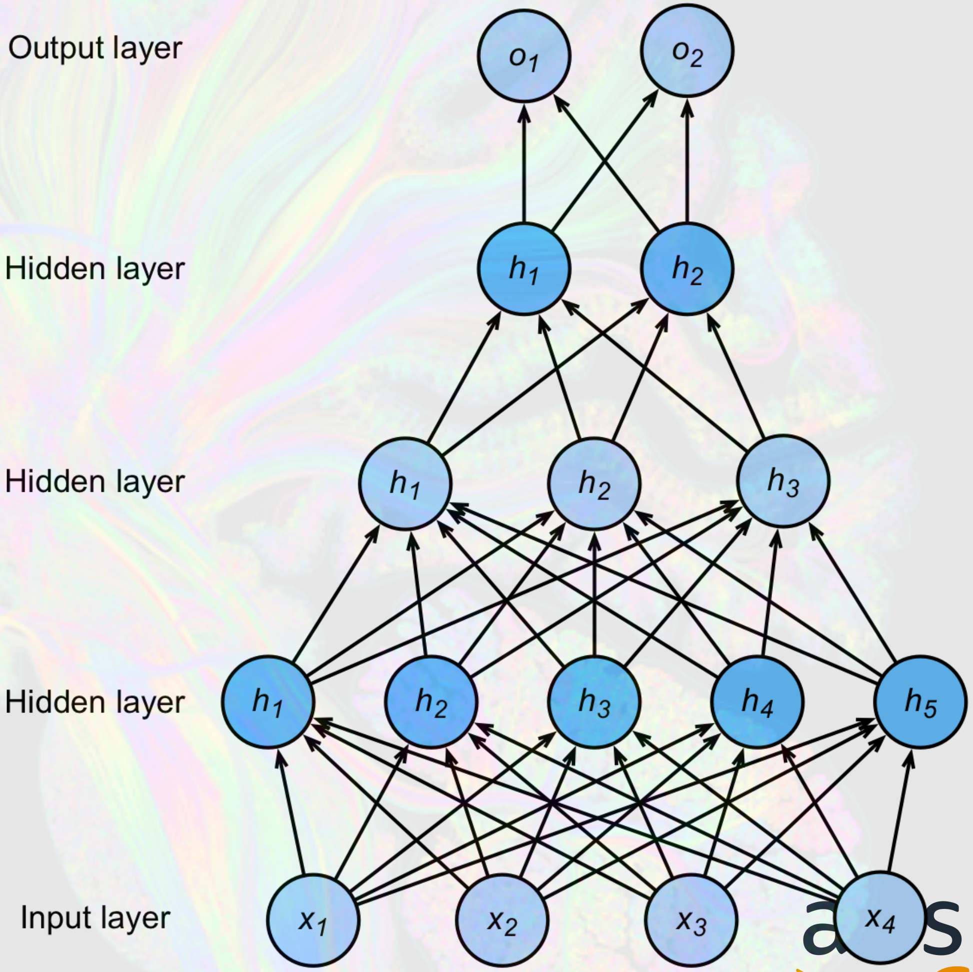
Multiclass Classification

$$y_1, y_2, \ldots, y_k = \text{softmax}(o_1, o_2, \ldots, o_k)$$



Multiple Hidden Layers

$$\mathbf{h}_1 = \sigma(\mathbf{W}_1\mathbf{x} + \mathbf{b}_1)$$
$$\mathbf{h}_2 = \sigma(\mathbf{W}_2\mathbf{h}_1 + \mathbf{b}_2)$$
$$\mathbf{h}_3 = \sigma(\mathbf{W}_3\mathbf{h}_2 + \mathbf{b}_3)$$
$$\mathbf{o} = \mathbf{W}_4\mathbf{h}_3 + \mathbf{b}_4$$



Hyper-parameters
- # of hidden layers
- Hidden size for each layer

MLP Notebook

Summary

- Installation
- Linear Algebra and Deep Numpy
- Autograd
- Softmax Classification
- Optimization
- Multilayer Perceptron