CS/ENGR M148 L14:
Introduction to Neural Networks

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Administrative News

This week in discussion section:

In lab this week you'll be learning about PyTorch to apply neural networks to your projects.

No project check-ins this week.

<u>Lecture on 11/25/24 will be via Zoom for the holiday.</u>

Midterm grades posted. Grade distribution on piazza. Regrade requests due by 6 pm 11/20/24.

<u>PS3 due today and quiz Thursday.</u>

<u>Will post final project report guidelines this week also with PS4.</u>

Administrative News

Extra credit Final Exam Review Question Code Bank:

https://forms.gle/XdC97wxwWd8QuTR9A

Questions due by 11:59 pm PT on 11/25/24.

We'll share questions with solutions during week 10 for final exam review.

Join our slido for the week…

https://app.sli.do/event/nCV57u4mC7eUMit9euSBr2

Today's Learning Objectives

Students will be able to:

- Explain how Expectation Maximization (EM) is used for Clustering: Gaussian Mixture Models
- Apply the Forward and Backwards Algorithms to Hidden Markov Models (HMM)
- Describe what a neural network is
- Apply the forward algorithm on the MNIST NN

Expectation Maximization (EM)

- Enables parameter estimation (learning) in probabilistic models with incomplete data.
- Uses Maximum Likelihood Estimation (MLE).
- MLE is a way to assess the quality of a statistical model based on the probability that model assigns to the observed data. The model that has the highest probability of generating the data is the best one.
- EM algorithm is used to find (locally) MLE parameters of a statistical model in cases where the equations cannot be solved directly.

[Shah 2020]

EM Experiment

- We are given 2 biased coins, but we don't know what probability of heads are for each. How can we learn this?

[Shah 2020]

EM Experiment

- What are **maximum likelihood estimates?**

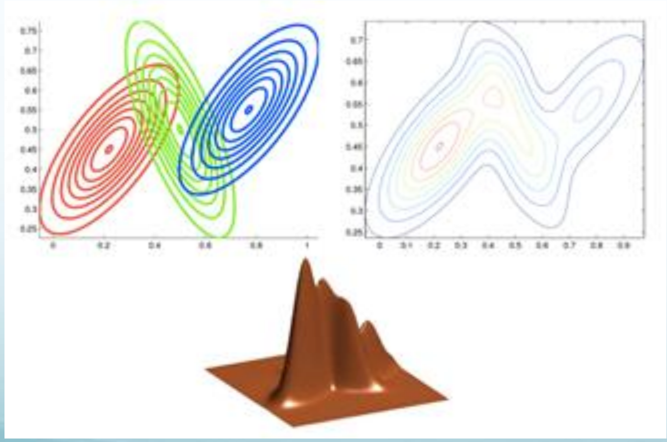
- What if we don't know what coin was tossed?

Gaussian Mixture Models

- A Gaussian mixture model is a family of distributions of the form

$$p(\mathbf{x}) = \sum_{i=1}^{k} \pi_i \mathcal{N}(\mathbf{x}|\mu_i, \Sigma_i).$$

- The π_i are *mixing coefficients* that sum to 1.
- Estimate the mean and covariance matrices from data as parameters for GMM from data
- Each Gaussian distribution represents a cluster.
- This provides a generative model for clustering.



Zemel et al., 2016

Gaussian Mixture Model

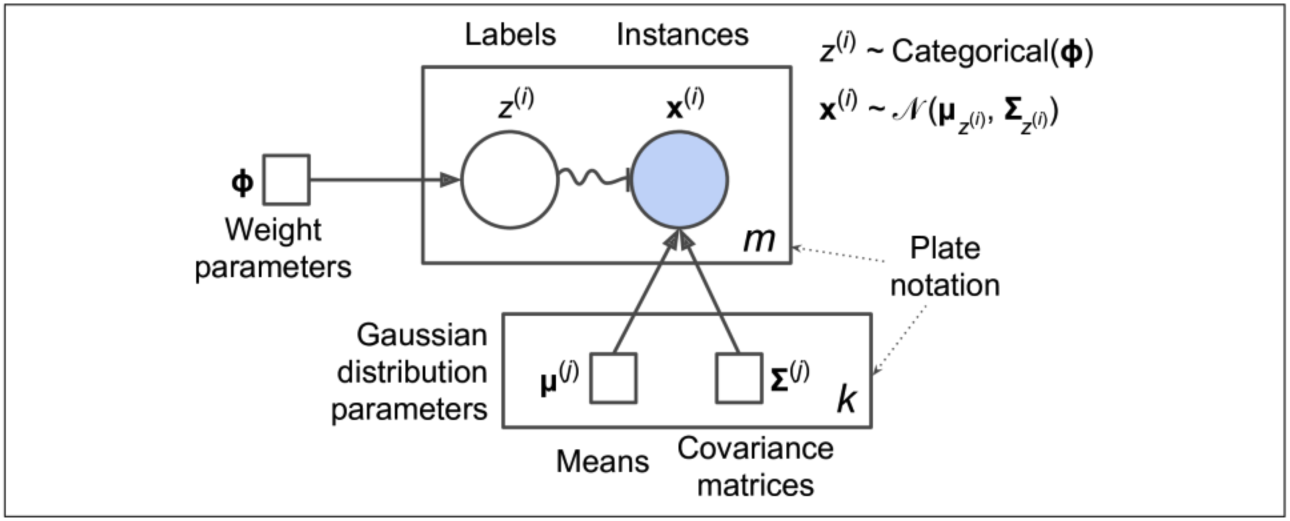


Figure 9-16. Gaussian mixture model

Aurelien Geron. 2019. Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow: Concepts, Tools, and Techniques to Build Intelligent Systems (2nd. ed.). O'Reilly Media, Inc

Maximum likelihood estimation

- The log likelihood function that must be maximized is:

$$\log Pr(x|\pi,\mu,\sigma) = \sum_{j=1}^{n} \log\left(\sum_{i=1}^{k} \pi N(x|\mu_i,\Sigma_i)\right)$$

- Expectation Step: Calculate clusters
- Maximization Step: Update parameters

Shortcoming of EM algorithm for clustering

- How to choose the number of clusters (k)?
- The EM algorithm can get stuck in local maxima; initialization is corncer
- EM algorithm may be slow.
- If data not from a Gaussian mixture process, EM algorithm may converge to a poor solution.

Your turn:
GMM on GPU data

Please get the Jupyter notebook for GPU data:

Go to:

The data file on BruinLearn Week 7 Module:

- `sgemm_product.csv`

Notebook:
https://colab.research.google.com/drive/1iqVnrE7LKQyW_UXExzV3Q06EP10Q2Bvk?usp=sharing

[Shah 2020]

Save a copy to your Google Drive and keep notes there...

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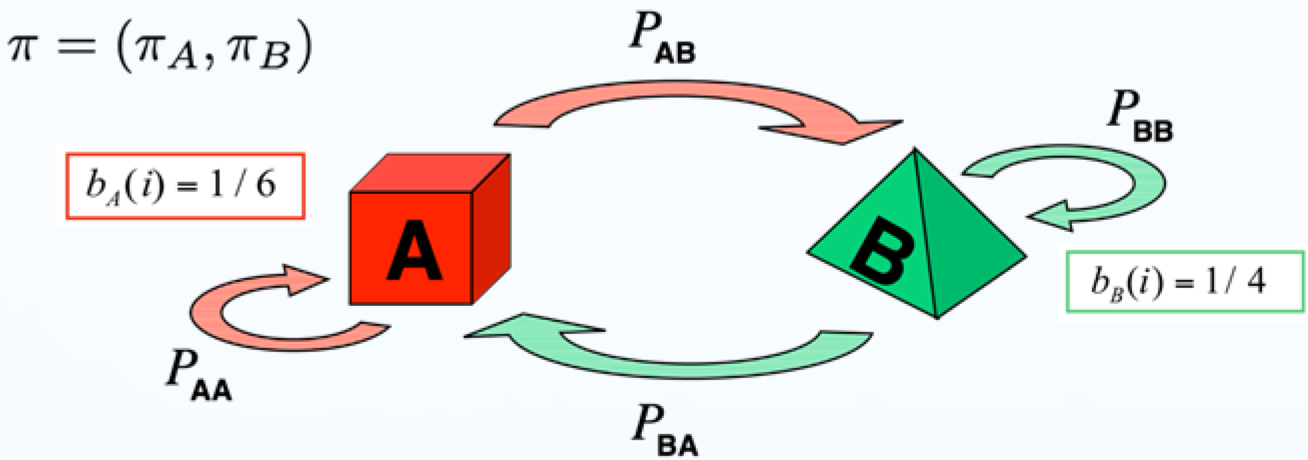
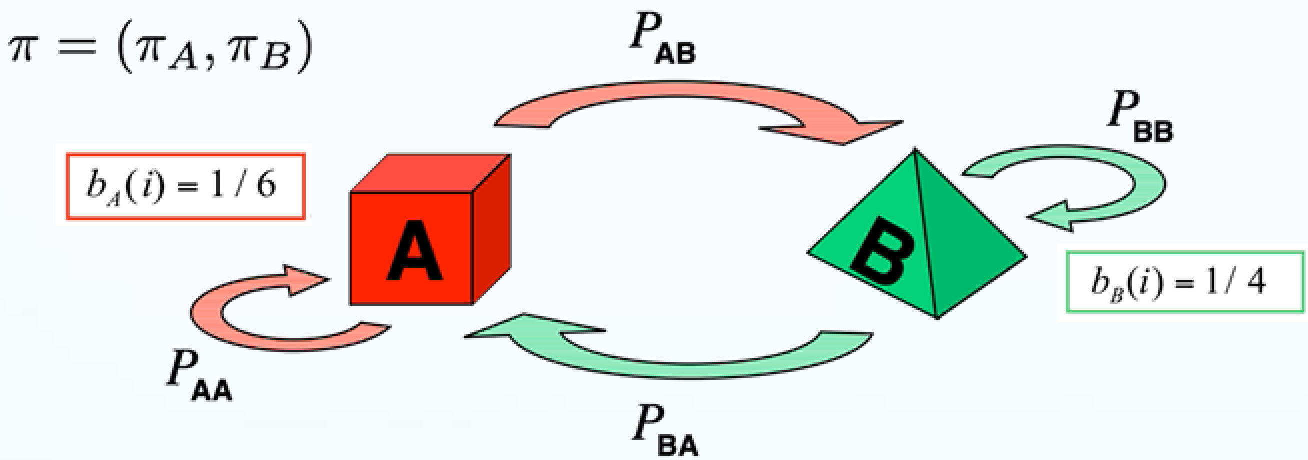
A hidden Markov model



$$\Pr(Y_0 = 1, Y_1 = 4, Y_2 = 3, Y_3 = 6, Y_4 = 6, Y_5 = 4) = ?$$

Solved with the forward algorithm.

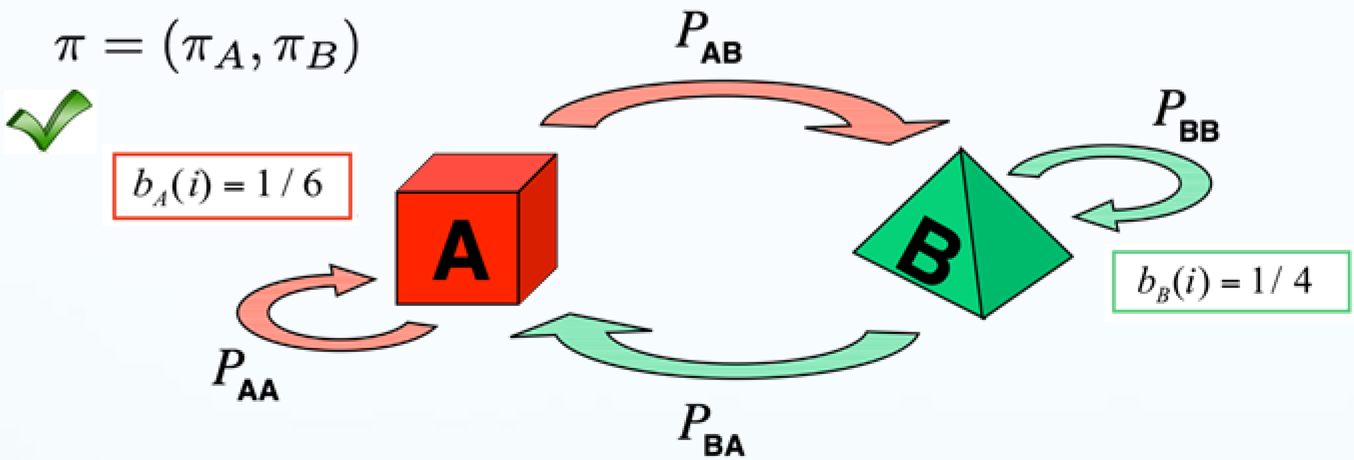
A hidden Markov model



What is the most likely sequence of states of the Markov chain to have resulted in 1,4,3,6,6,4?

Solved with the Viterbi algorithm.

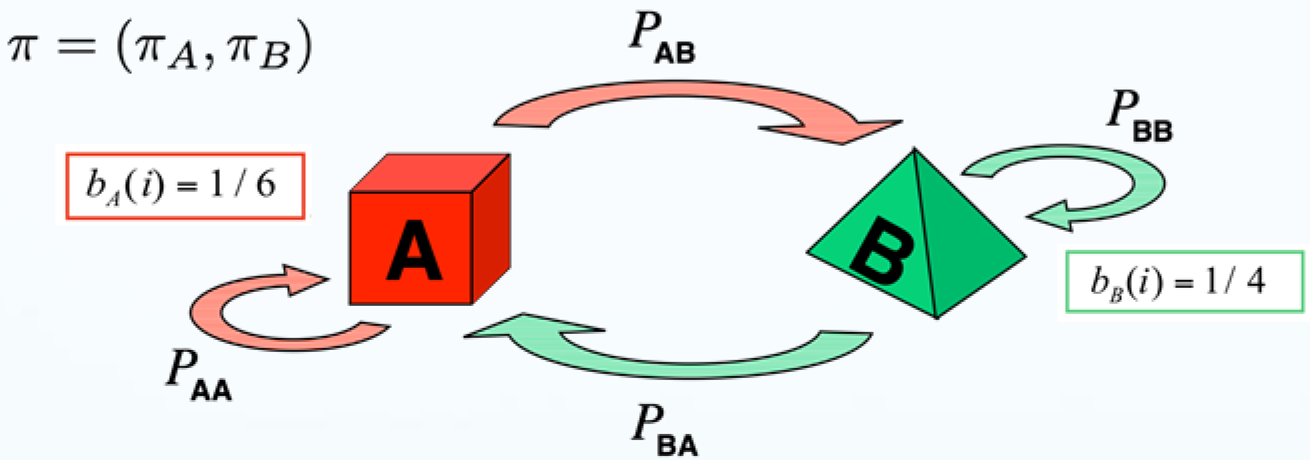
A hidden Markov model



What is the probability that $X_3 = B$ if $Y_0=1, Y_1=4, Y_2=3, Y_3=6, Y_4=6, Y_5=4$?

Solved with the forward-backward algorithm.

A hidden Markov model



*Given multiple sequences of numbers (observations of **Y**), estimate parameters for the model*

This is expectation-maximization algorithm

The occasionally dishonest casino

A casino uses a fair die most of the time, but occasionally switches to a loaded one

Fair die: Prob(1) = Prob(2) = . . . = Prob(6) = 1/6

Loaded die: Prob(1) = Prob(2) = . . . = Prob(5) = 1/10,

Prob(6) = ½

These are the ***emission*** probabilities

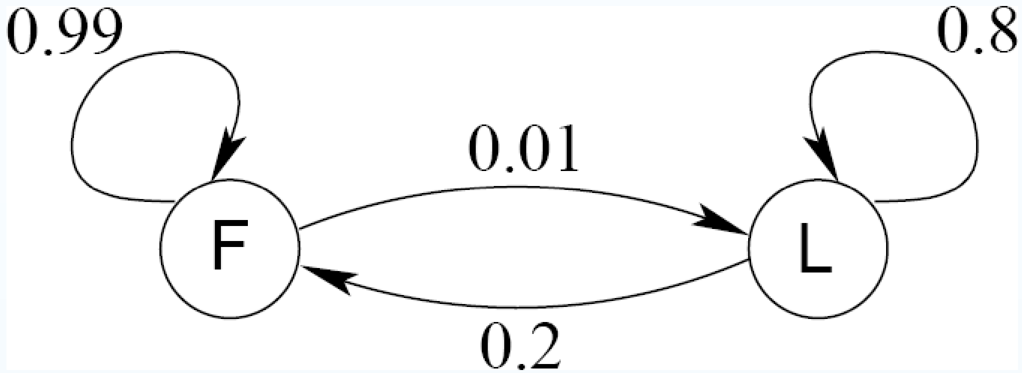
Transition probabilities

Prob(Fair –> Loaded) = 0.01

Prob(Loaded –>Fair) = 0.2

Transitions between states obey a Markov process

An HMM for the occasionally dishonest casino



Notation

- x *is the sequence of symbols emitted by model*
  - x_i *is the symbol emitted at time* i
- *A* ***path****,* π*, is a sequence of states*
  - *The* i*-th state in* π *is* π_i
- a_{kr} *is the probability of making a transition from state* k *to state* r*:*

$$a_{kr} = Pr(\pi_i = r \mid \pi_{i-1} = k)$$

- $e_k(b)$ *is the probability that symbol* b *is emitted when in state* k

$$e_k(b) = Pr(x_i = b \mid \pi_i = k)$$

The most probable path

The most likely path π^* satisfies

$$\pi^* = \underset{\pi}{\arg\max}\, Pr(x, \pi)$$

*To find π^*, consider all possible ways the last symbol of **x** could have been emitted*

Let

$$v_k(i) = \text{Prob. of path } \langle \pi_1, \cdots, \pi_i \rangle \text{ most likely}$$
$$\text{to emit } \langle x_1, \ldots, x_i \rangle \text{ such that } \pi_i = k$$

Then

$$v_k(i) = e_k(x_i) \max_r \left(v_r(i-1) a_{rk} \right)$$

The Viterbi Algorithm

- *Initialization* $(i = 0)$

$$v_0(0) = 1,\ \ v_k(0) = 0 \text{ for } k > 0$$

- *Recursion* $(i = 1, \ldots, L)$: *For each state* k

$$v_k(i) = e_k(x_i)\max_r\left(v_r(i-1)a_{rk}\right)$$

- *Termination:*

$$Pr(x, \pi^*) = \max_k\left(v_k(L)a_{k0}\right)$$

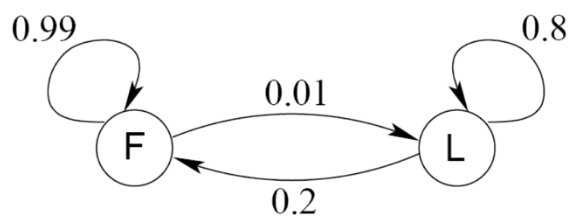
To find π^*, *use trace-back, as in dynamic programming*

Viterbi: Example

x

π	ε	6	2	6
B	**1**	**0**	**0**	**0**
F	**0**	(1/6)×(1/2) = **1/12**	(1/6)×max{(1/12)×0.99, (1/4)×0.2} = **0.01375**	(1/6)×max{0.01375×0.99, 0.02×0.2} = **0.00226875**
L	**0**	(1/2)×(1/2) = **1/4**	(1/10)×max{(1/12)×0.01, (1/4)×0.8} = **0.02**	(1/2)×max{0.01375×0.01, 0.02×0.8} = **0.08**

$$\boxed{v_k(i) = e_k(x_i)\max_r\left(v_r(i-1)a_{rk}\right)}$$



Total probabilty

Many different paths can result in observation x.

The probability that our model will emit x is

$$\Pr(x) = \sum_{\pi} \Pr(x, \pi)$$

Total Probability

If HMM models a family of objects, we want total probability to peak at members of the family. (Training)

Total probability

$\Pr(x)$ can be computed in the same way as probability of most likely path.

Let

$$f_k(i) = \text{Prob. of observing } \langle x_1, \ldots, x_i \rangle$$

$$\text{assuming that } \pi_i = k$$

Then

$$f_k(i) = e_k(x_i) \sum_r f_r(i-1) a_{rk}$$

and

$$\Pr(x) = \sum_k f_k(L) a_{k0}$$

The Forward Algorithm

- *Initialization* ($i = 0$)

$$f_0(0) = 1, \quad f_k(0) = 0 \text{ for } k > 0$$

- *Recursion* ($i = 1, \ldots, L$): *For each state* k

$$f_k(i) = e_k(x_i) \sum_r f_r(i-1) a_{rk}$$

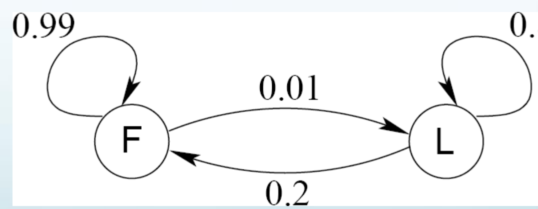
- *Termination:*

$$Pr(x) = \sum_k f_k(L) a_{k0}$$

Forward: Example

		x		

π	ε	6	2	6
B	1	0	0	0
F	0	$(1/6)\times(1/2) = 1/12$		
L	0	$(1/2)\times(1/2) = 1/4$		



The Backward Algorithm

- *Initialization (i = L)*

$$b_k(L) = a_{k0} \text{ for all } k$$

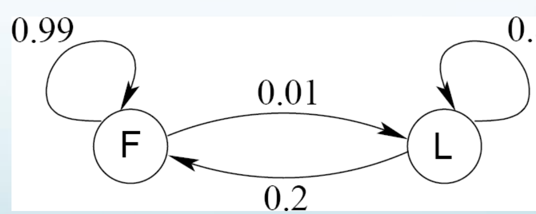
- *Recursion (i = L-1, . . . , 1): For each state k*

$$b_k(i) = \sum_l a_{kl} e_l(x_{i+1}) b_l(i+1)$$

Backward: Example

x

		ε	6	2	6
	B	1	0	0	0
π	F	0			
	L	0			



Backward Algorithm and Posterior Decoding

- *How likely is it that my observation comes from a certain state?*

$$P(x_i \text{ is emitted by state } k \mid \text{whole observation})$$

- *Like the Forward matrix, one can compute a Backward matrix*
- *Multiply Forward and Backward entries*

$$P(\pi_i = k \mid x) = \frac{f_k(i) \cdot b_k(i)}{P(x)}$$

  - *P(x) is the total probability computed by, e.g., forward algorithm*

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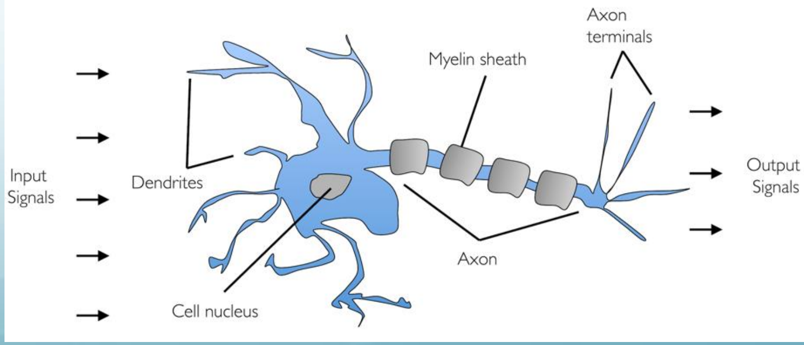
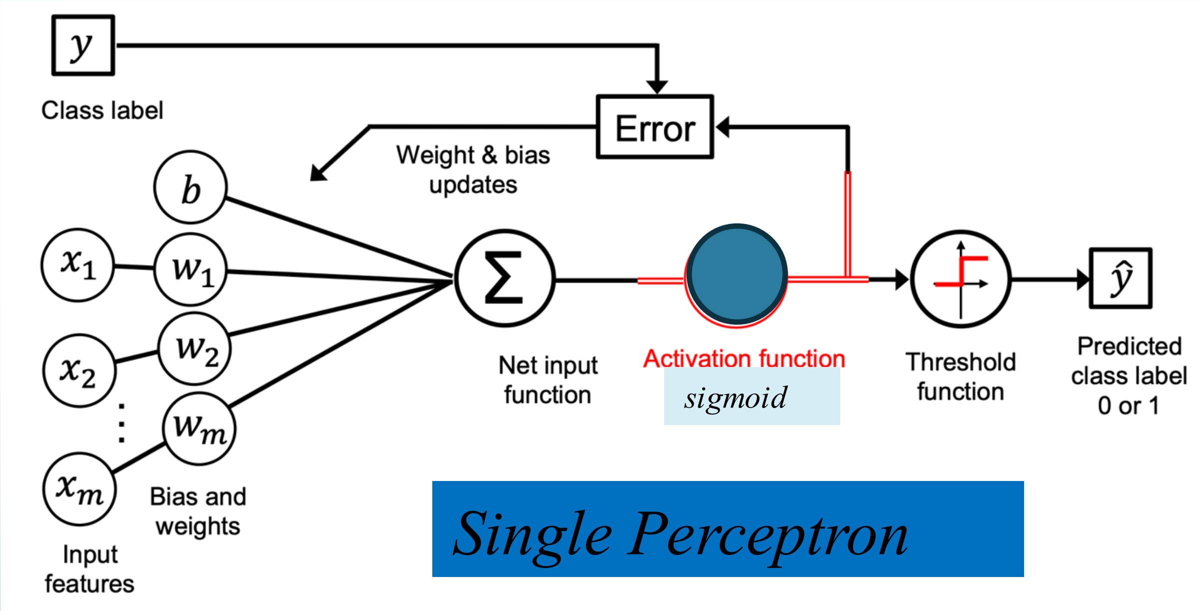
Neural Networks (NN)

- *Based on models for how brain works using artificial neurons*
- *Many varied successful applications such as mood recognition in pictures, modeling virus mutations, and predicting needed medical resources*
- *Used to model complex, nonlinear models*
- *We'll focus on using them for **classification**.*



What is a neural network?

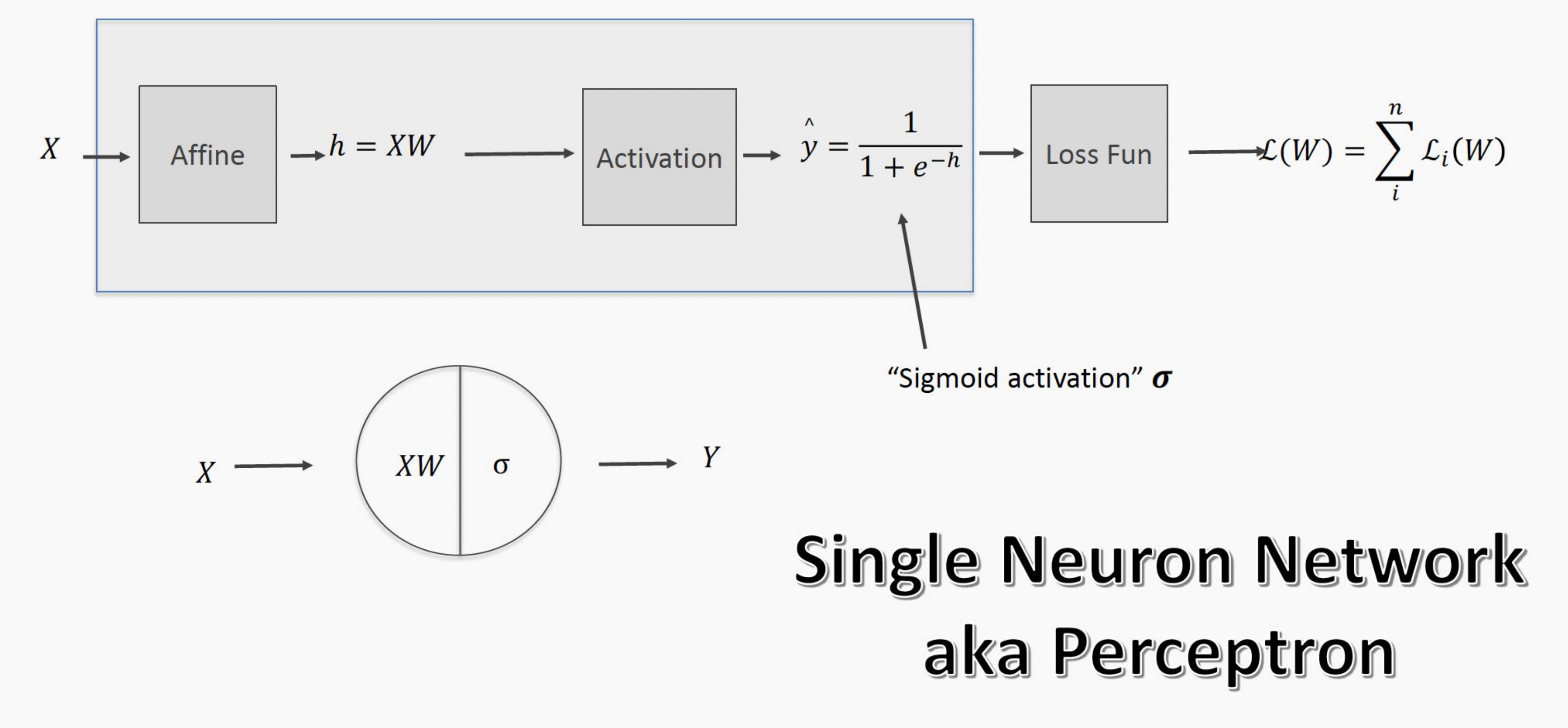
- *A **neural network** consists of layers of nodes or **artificial neurons***



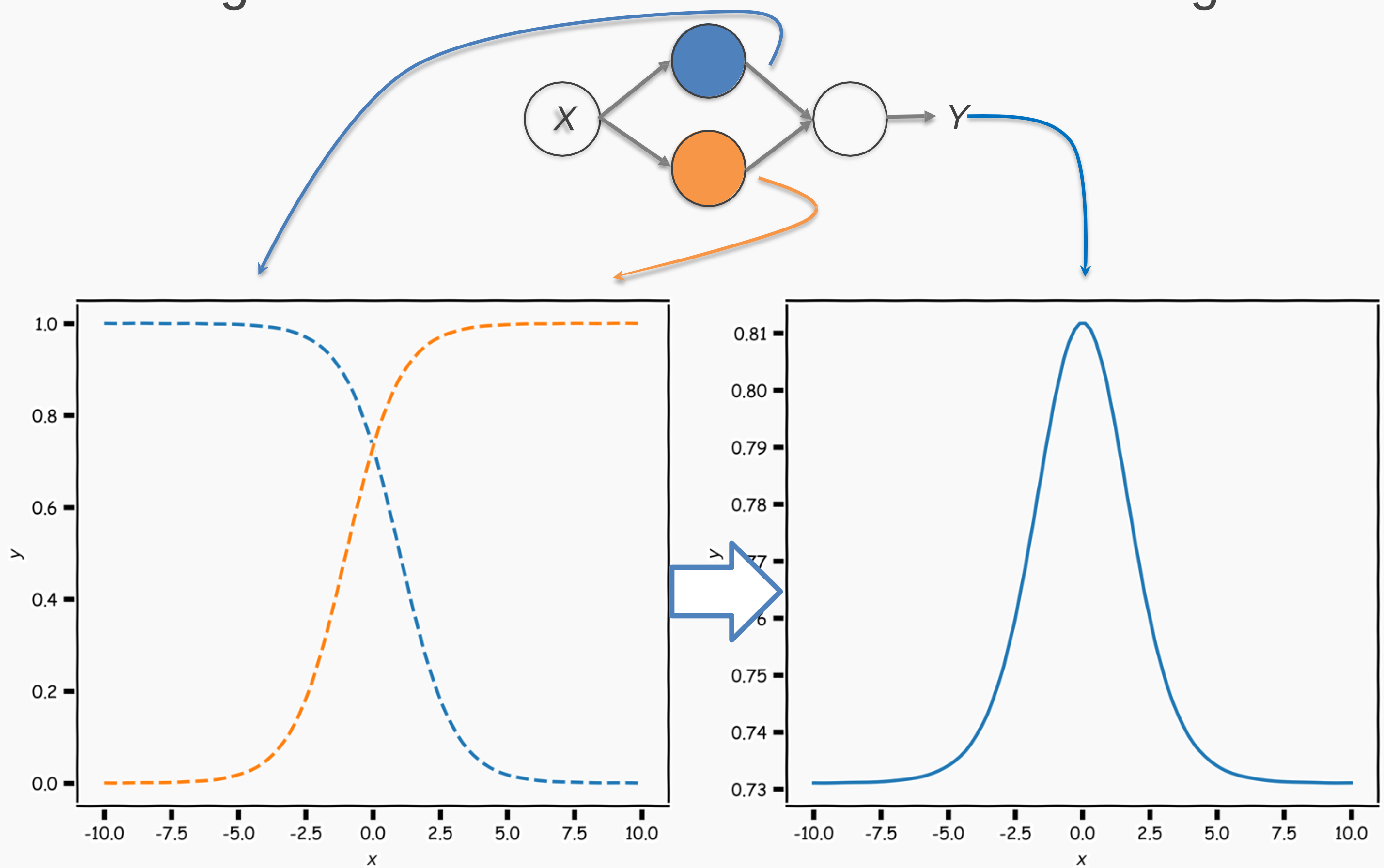
A single neuron can be a logistic regression or linear unit or other activation functions.

What is a neural network?

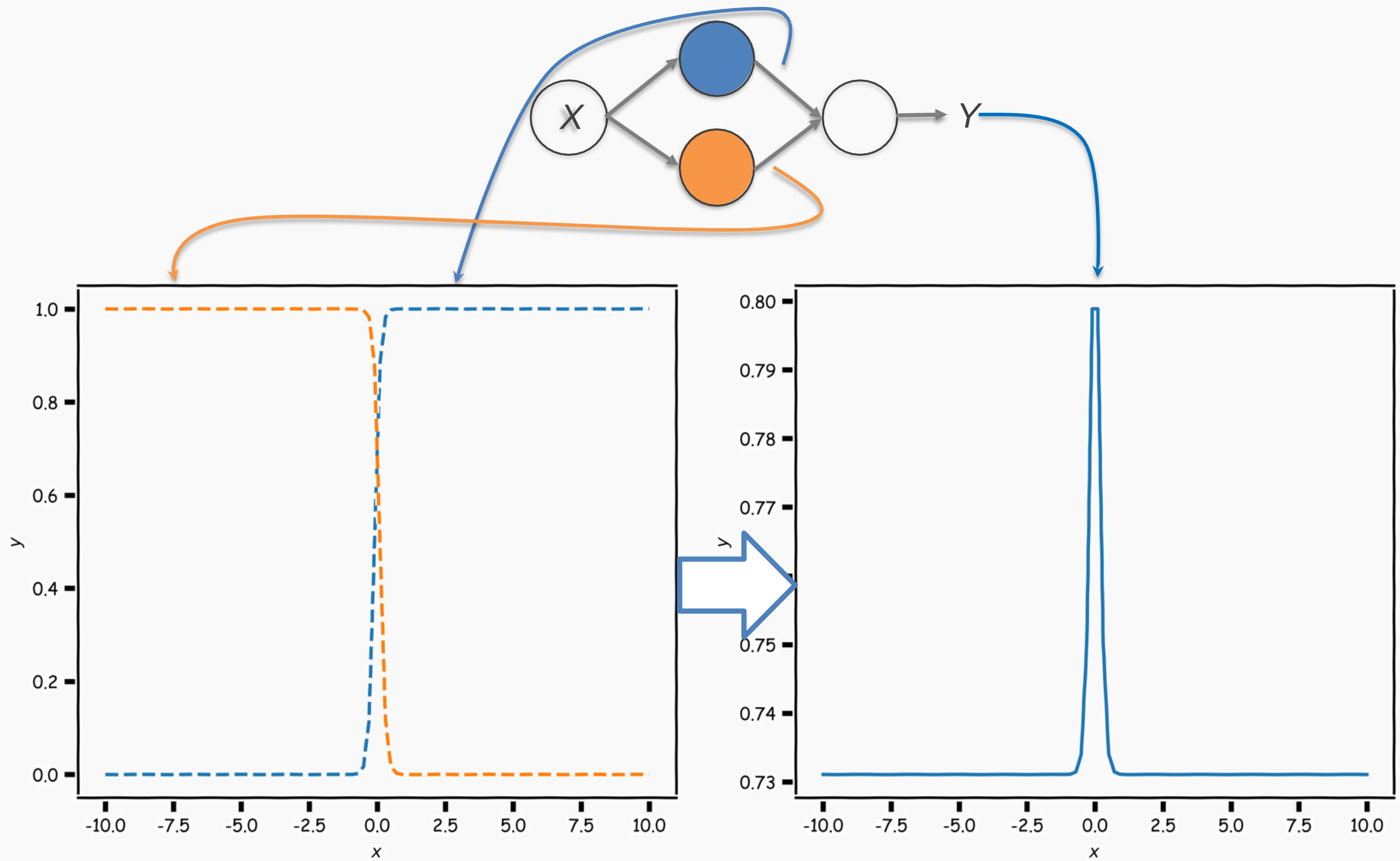
- *A **neural network** consists of layers of nodes or **artificial neurons***



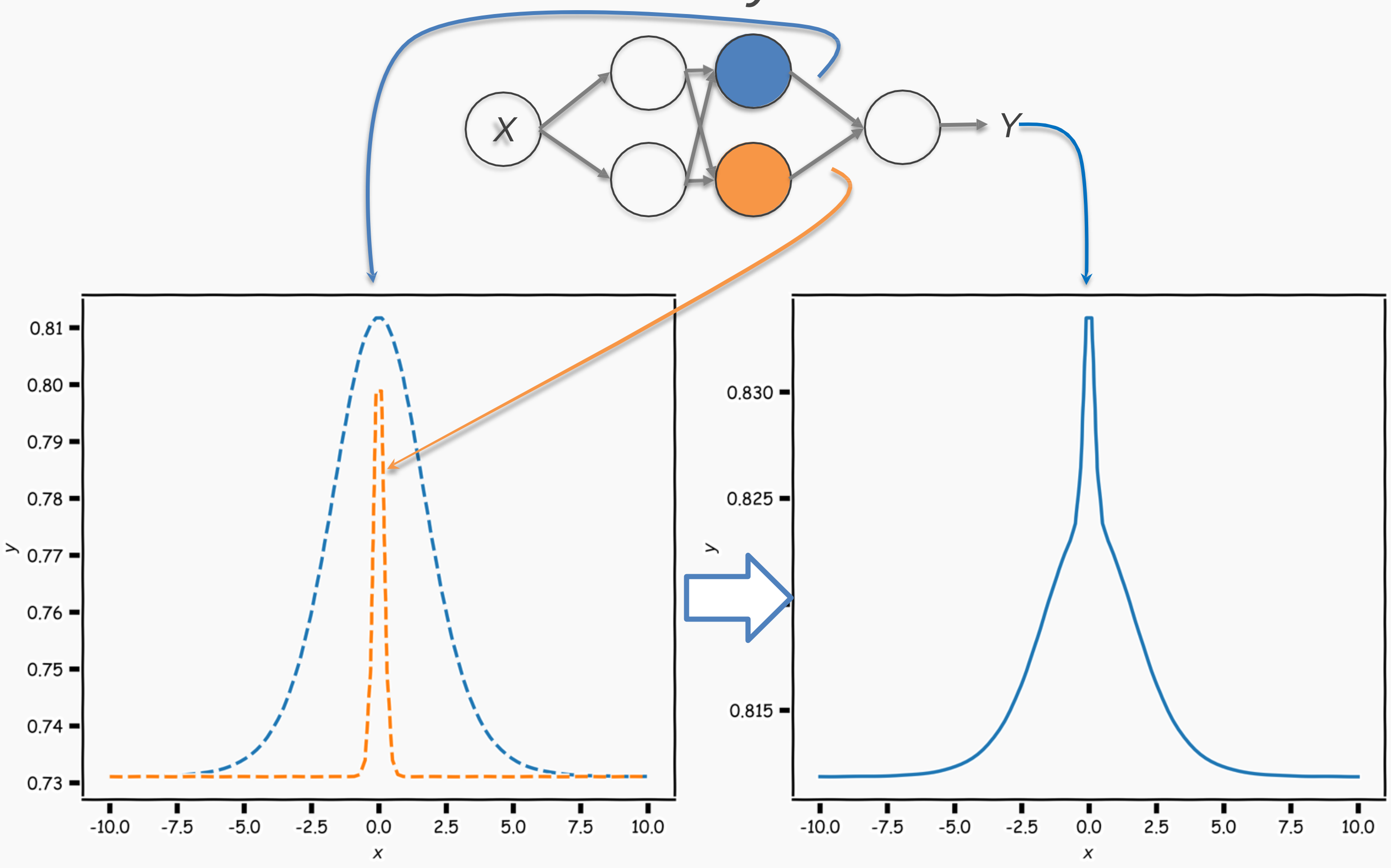
Combining neurons allows us to model interesting functions



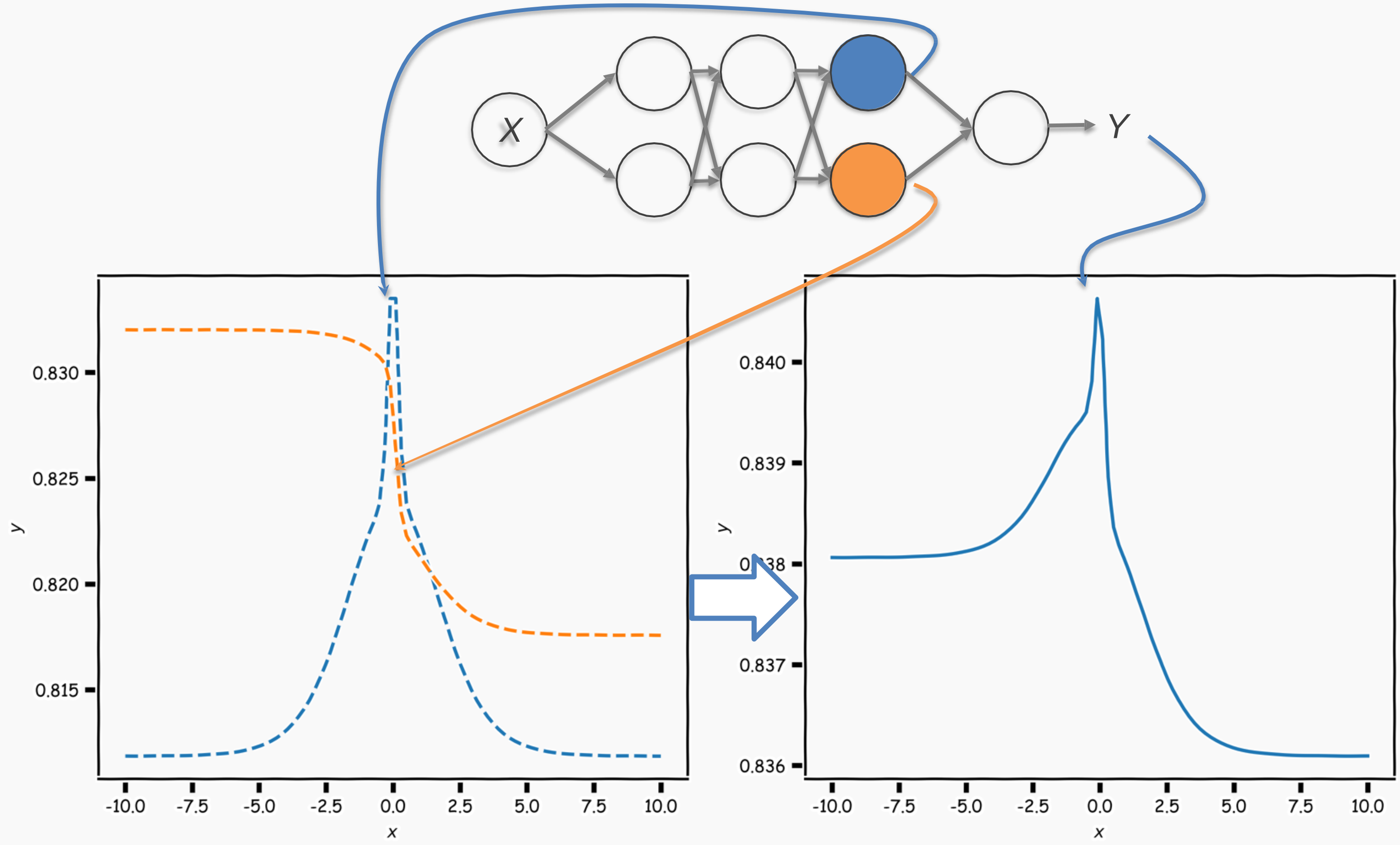
Different weights change the shape and position



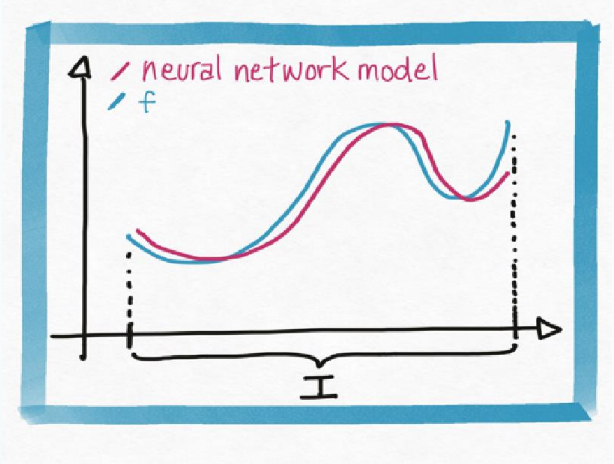
Neural networks can model *any* reasonable function



Adding layers allows us to model increasingly complex functions



Neural Networks as Universal Approximators



Theorem:

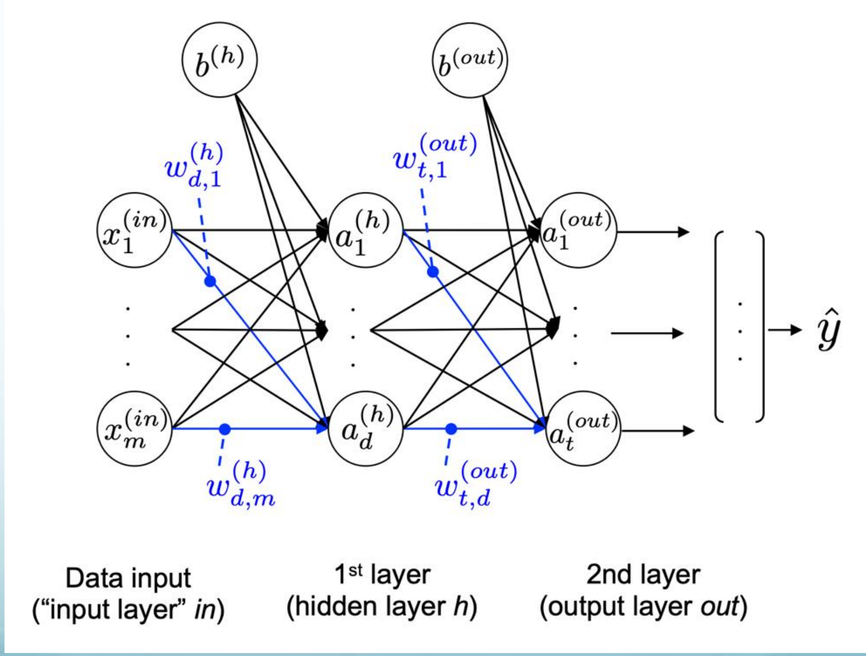
For any continuous function f defined on a bounded domain, we can find a neural network that approximates f with an arbitrary degree of accuracy.

One hidden layer is enough to represent an approximation of any function to an arbitrary degree of accuracy.

A neural network can approximate non-linear functions either for regression or classification.

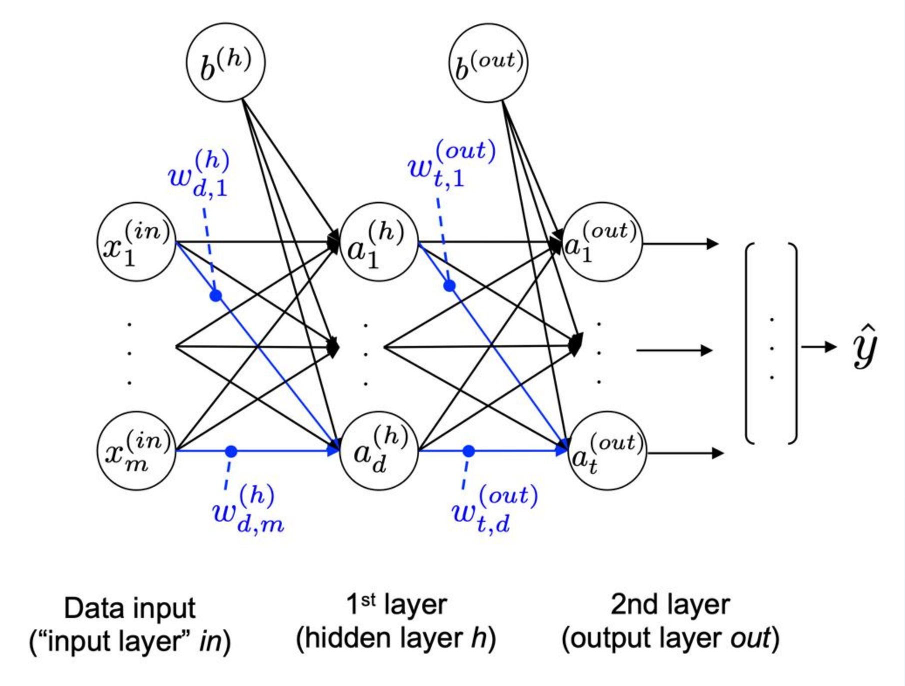
Multilayer Perceptron

- *A neural network is a combination of neurons such as logistic regression (or other types) units.*
- *A **multilayer perceptron (MLP)** is a fully connected network of neurons.*
- *An MLP is a multilayer **feedforward** NN because each layer is input to the next.*
- *A network with more than one hidden layer is a **deep NN.***

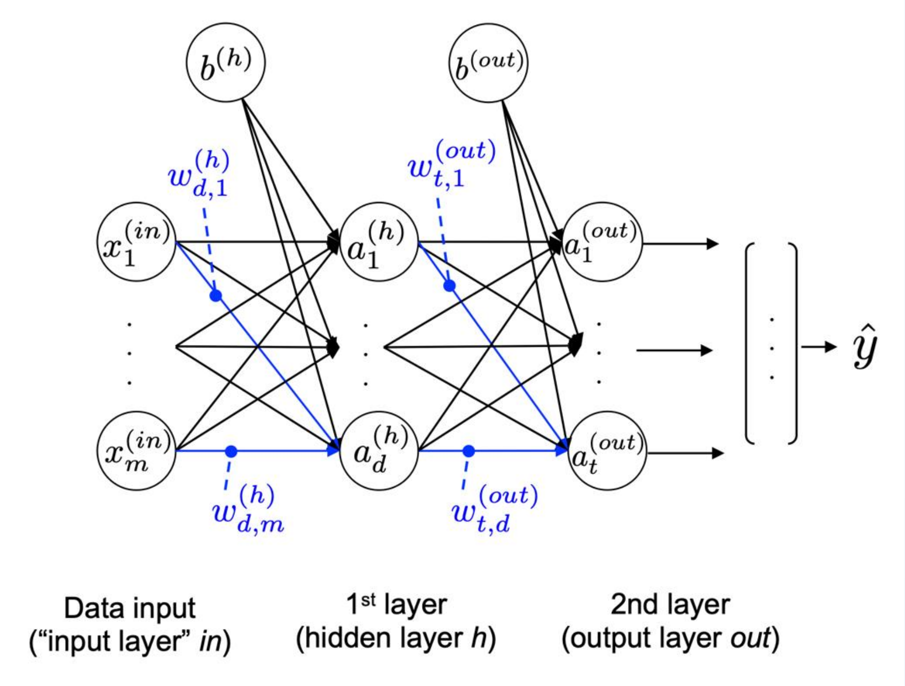


[Raschka et al 2022]

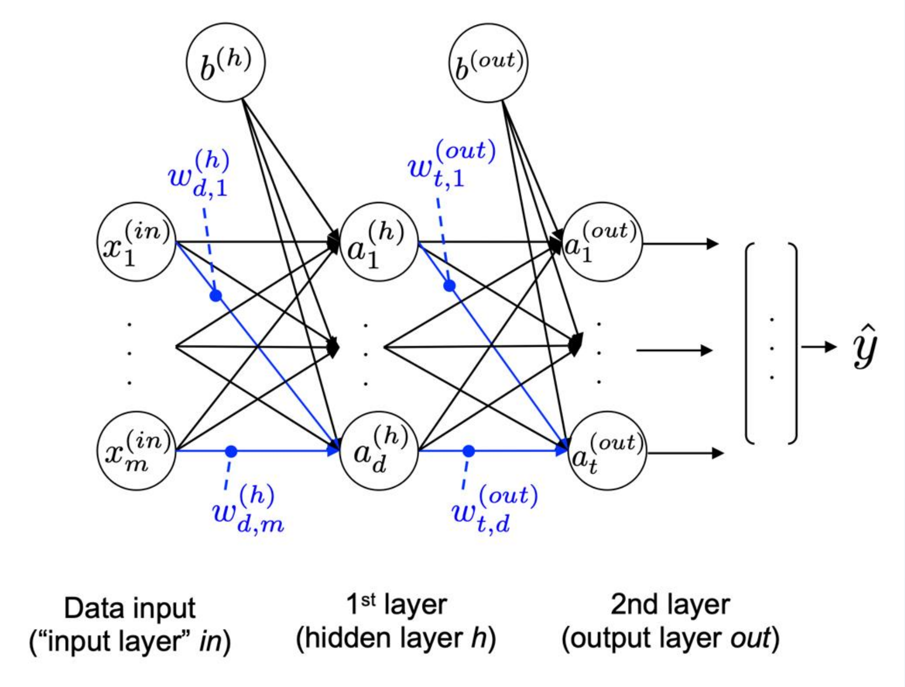
Multilayer Perceptron



Multilayer Perceptron



Multilayer Perceptron



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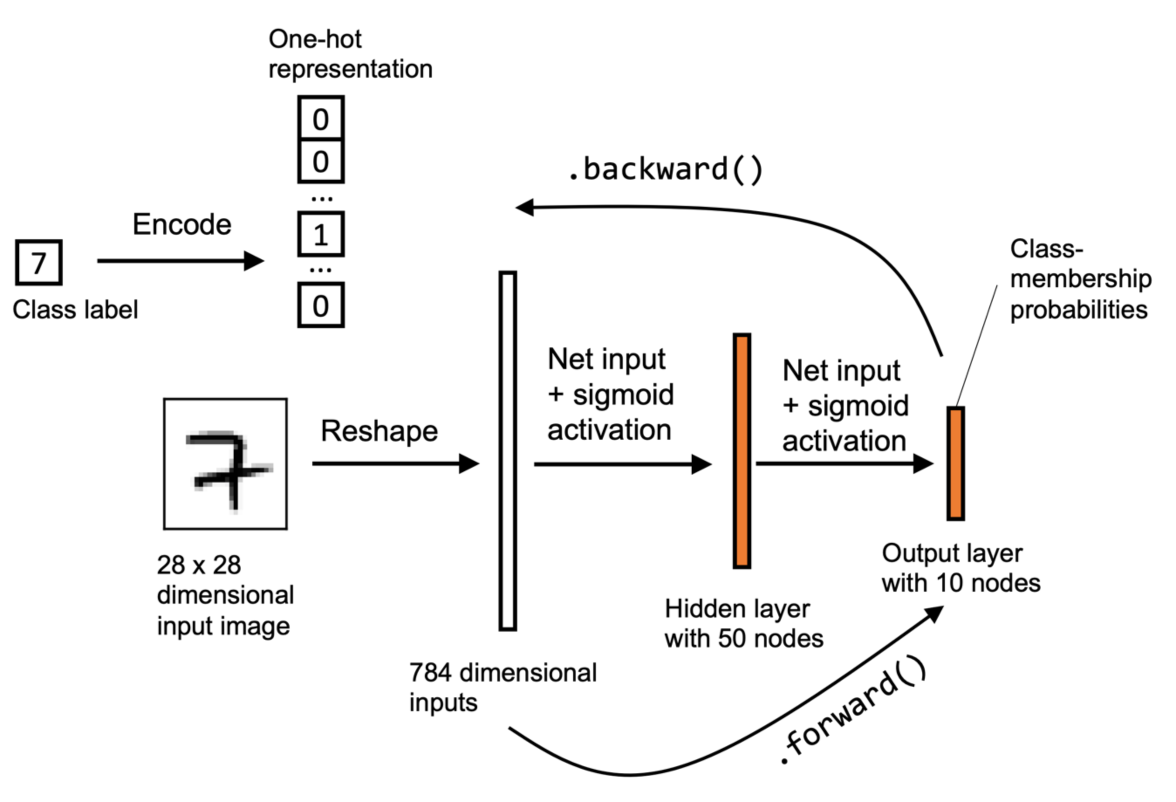
Modified National Institute of Standards and Technology (MNIST) Classification NN from Scratch

Hand-written digit recognition: MNIST data

MNIST NN

Today we'll work on forward algorithm..
Next lecture backpropagation, gradient descent, training, and evaluating network performance



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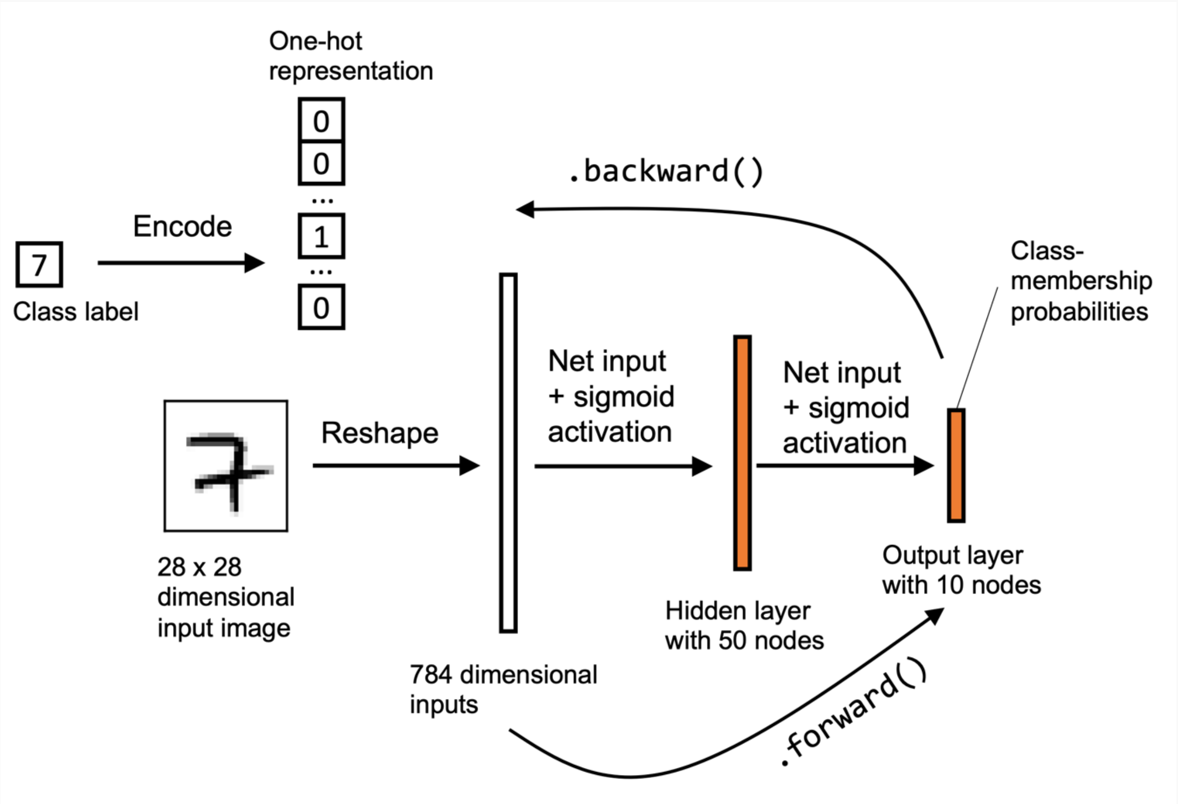

[Raschka et al 2022]

MNIST NN utility code

How would the following sample labels be one-hot encoded: [1, 0,2] ?

```
def sigmoid(z):
    return 1. / (1. + np.exp(-z))


def int_to_onehot(y, num_labels):

    ary = np.zeros((y.shape[0], num_labels))
    for i, val in enumerate(y):
        ary[i, val] = 1

    return ary
```


[Raschka et al 2022]

MNIST NN initialization

```
class NeuralNetMLP:

    def __init__(self, num_features, num_hidden, num_classes, random_seed=123):
        super().__init__()

        self.num_classes = num_classes

        # hidden
        rng = np.random.RandomState(random_seed)

        self.weight_h = rng.normal(
            loc=0.0, scale=0.1, size=(num_hidden, num_features))
        self.bias_h = np.zeros(num_hidden)

        # output
        self.weight_out = rng.normal(
            loc=0.0, scale=0.1, size=(num_classes, num_hidden))
        self.bias_out = np.zeros(num_classes)
```

[Raschka et al 2022]

MNIST NN Forward

How do we use the output for prediction?

```
def forward(self, x):
    # Hidden layer
    # input dim: [n_examples, n_features] dot [n_hidden, n_features].T
    # output dim: [n_examples, n_hidden]
    z_h = np.dot(x, self.weight_h.T) + self.bias_h
    a_h = sigmoid(z_h)

    # Output layer
    # input dim: [n_examples, n_hidden] dot [n_classes, n_hidden].T
    # output dim: [n_examples, n_classes]
    z_out = np.dot(a_h, self.weight_out.T) + self.bias_out
    a_out = sigmoid(z_out)
    return a_h, a_out
```


[Raschka et al 2022]

Backpropagation Algorithm

We'll start here next time, but a question to consider….

How was the backward forward algorithm we already considered for the casino an example of this?

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Citations:.

Shah. C. (2020) A hands-on introduction to data science. Cambridge University Press.

Sebastian **Raschka**, Yuxi (Hayden) **Liu**, and Vahid Mirjalili. **Machine Learning** with PyTorch and Scikit-Learn. Packt Publishing, **2022**.

Baharan Mirzasoleiman, UCLA CS M148 Winter 2024 Lecture 13 Notes

Some slides from https://www.molgen.mpg.de/3379148/Hidden_Markov_Models_vin.pdf

Thank You