

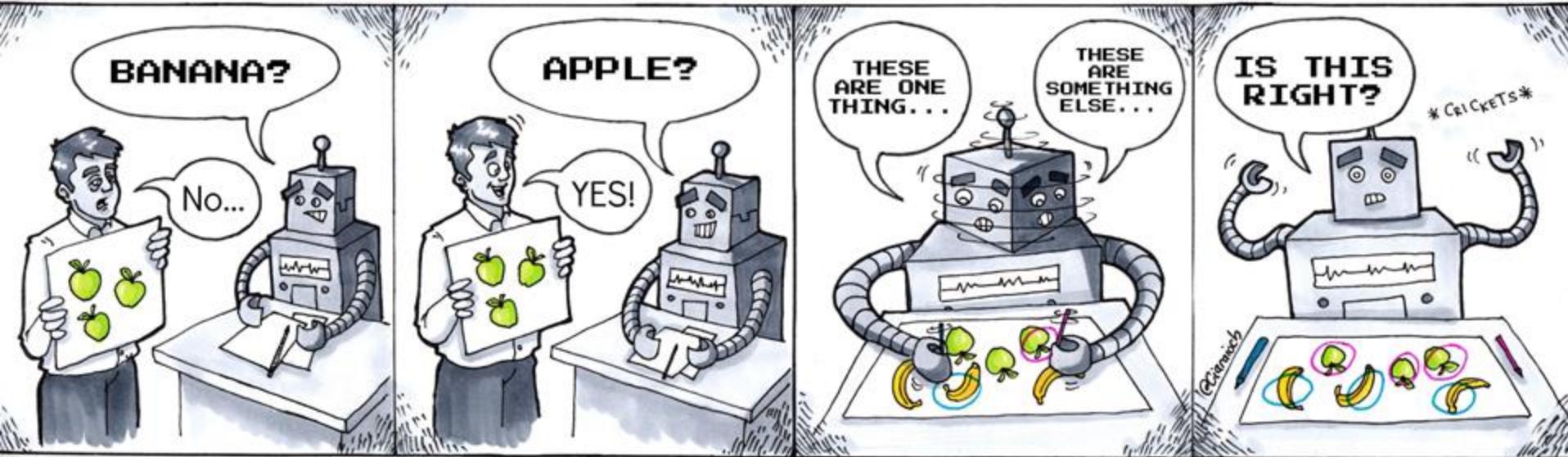


CSC380: Principles of Data Science

Nonlinear Models 2

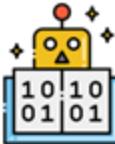
Xinchen Yu

- K-Means
- Neural Networks



Supervised Learning

Unsupervised Learning



Task 1 : Group These Set of Document into 3 Groups based on meaning

Doc1 : Health , Medicine, Doctor

Doc 2 : Machine Learning, Computer

Doc 3 : Environment, Planet

Doc 4 : Pollution, Climate Crisis

Doc 5 : Covid, Health, Doctor



Task 1 : Group These Set of Document into 3 Groups based on meaning

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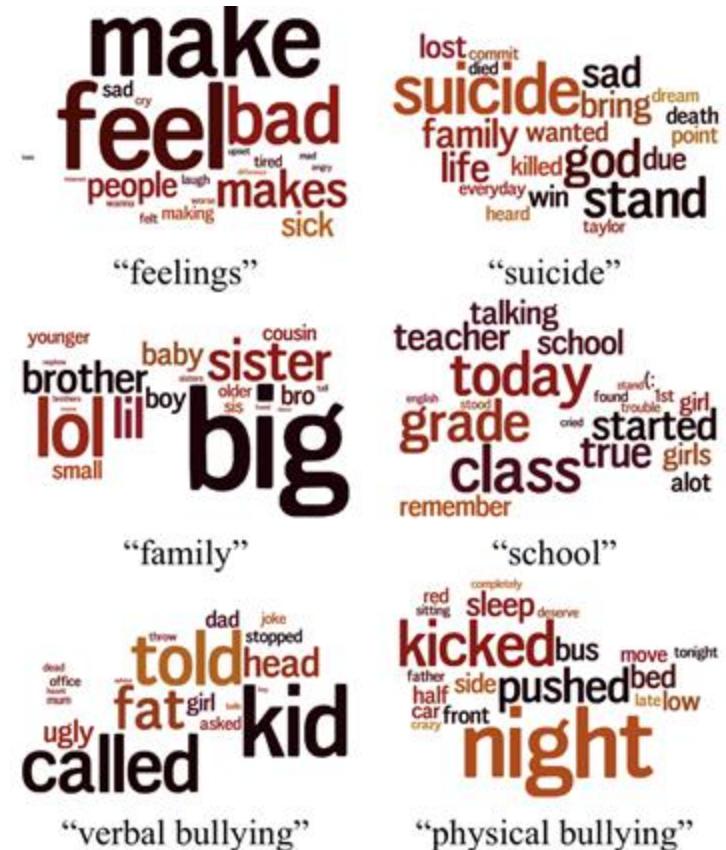
Doc 4 : Pollution, Climate Crisis

Doc 2 : Machine Learning, Computer



Task 2: Topic modeling

- Provides a summary of a corpus.
- Collected n tweets containing the keyword “bullying”, “bullied”, etc.
- Extracts k topics: each topic is a list of words with importance weights.
 - A set of words that co-occurs frequently throughout.



unsupervised learning: learning with unlabeled data

What can we expect to learn?

- **Clustering**: obtain partition of the data that are well-separated. A preliminary classification without predefined class labels.
 - As a summary of the data
 - **Exploratory data analysis**: what are the patterns even without labels?
- **Components**: extract common components, e.g., topic modeling given a set of articles: extract the topics that appear frequently.

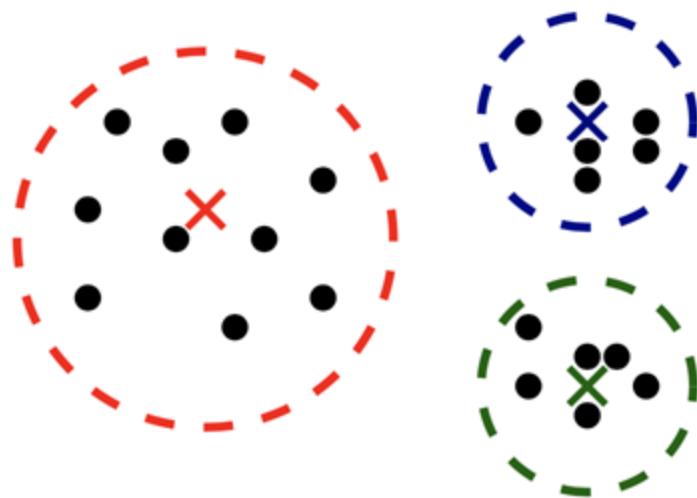
Clustering

- Input: k : the number of clusters (hyperparameter)

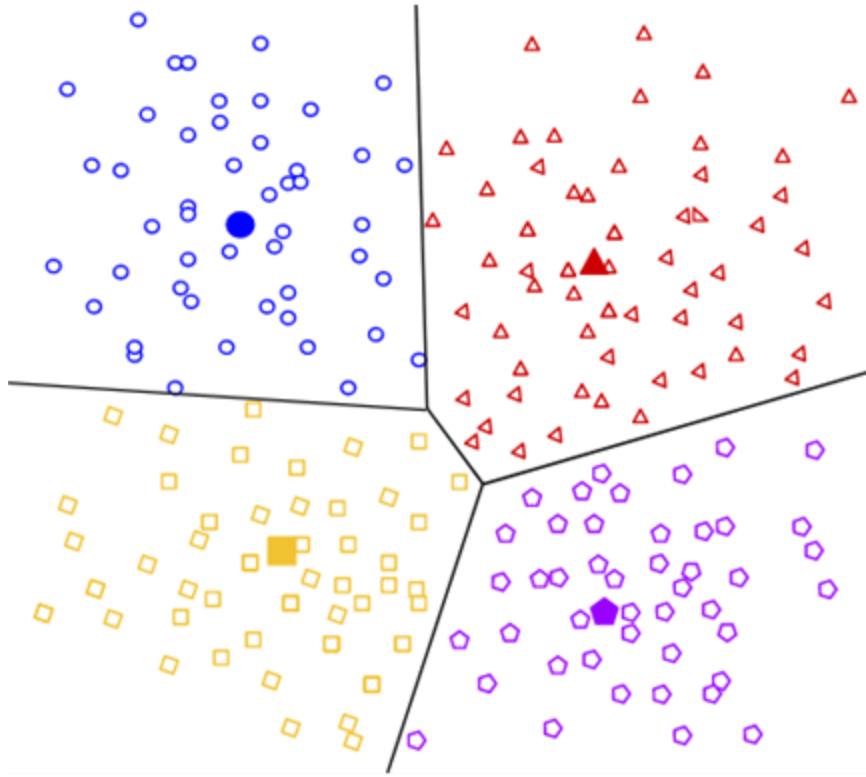
$$S = \{x_1, \dots, x_n\}$$

- Output

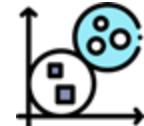
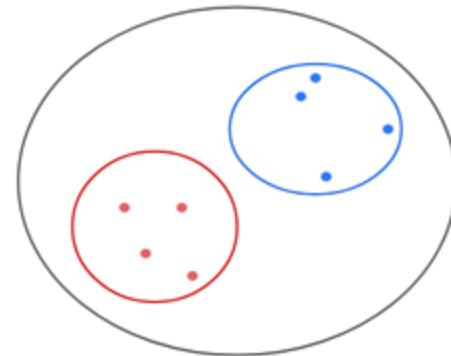
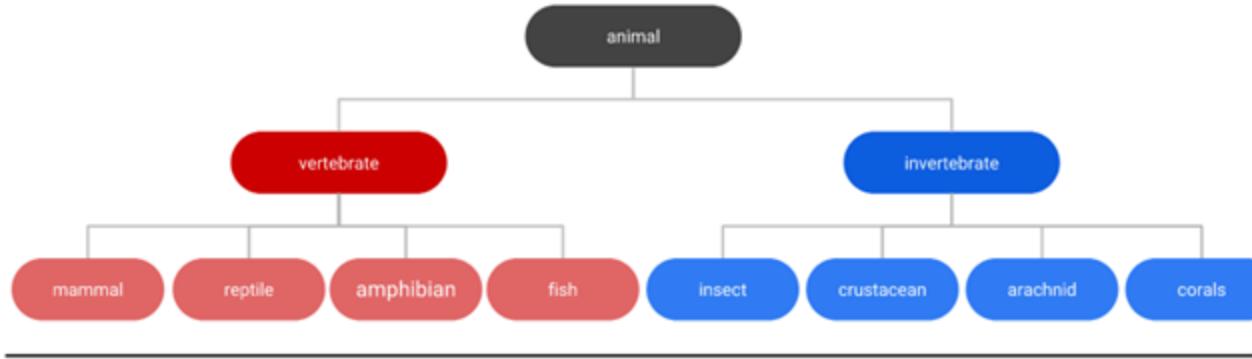
- partition $\{G_i\}_{i=1}^k$ s.t. $S = \bigcup_i G_i$ (disjoint union).
- often, we also obtain 'centroids'



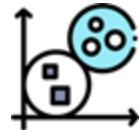
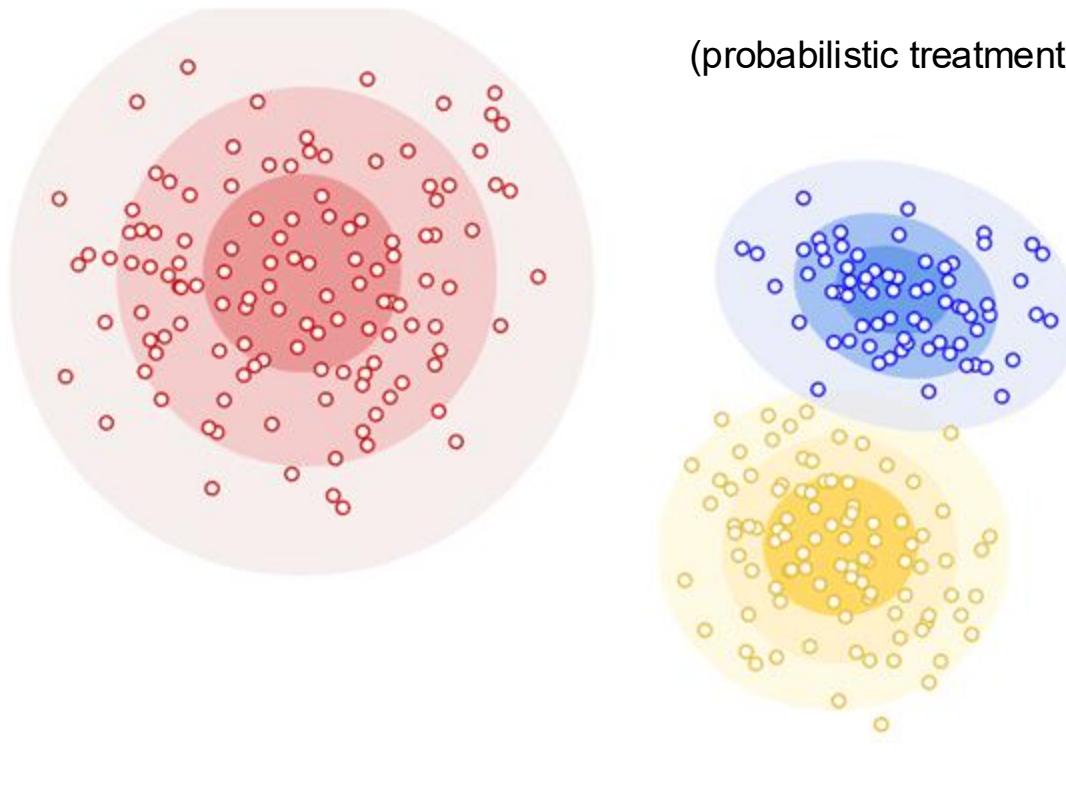
Centroid-based Clustering



Hierarchical Clustering

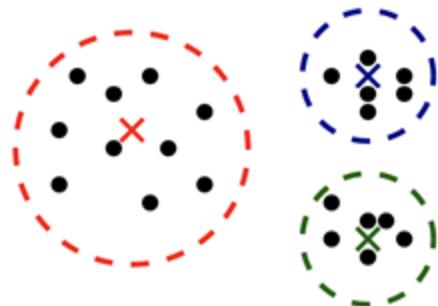


Distribution-based Clustering



k-means: how to define centroids

Lloyd's algorithm: solve it approximately (heuristic)

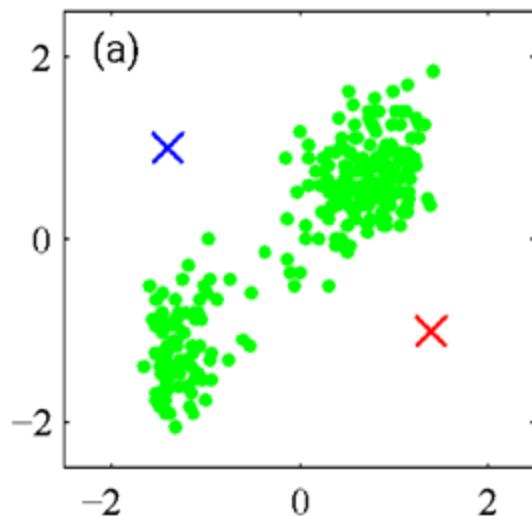


Observation: The chicken-and-egg problem.

- If you knew the **cluster assignments**... just find the **centroids** as the average
- If you knew the **centroids**... make **cluster assignments** by the closest centroid.

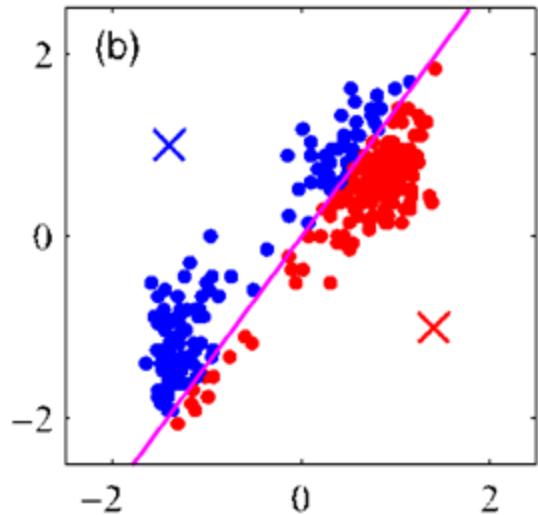
Why not: start from some centroids and then alternate between the two?

Initialization

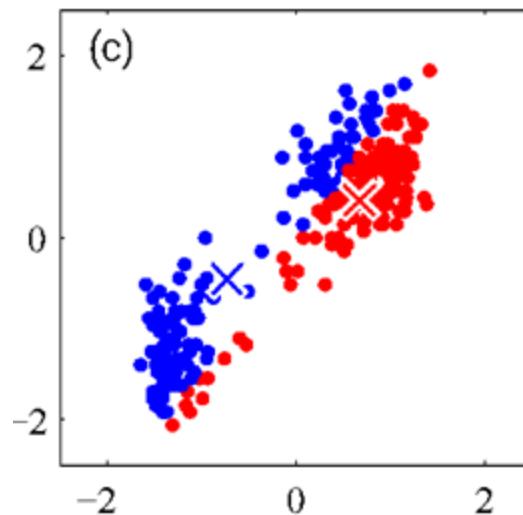


Arbitrary/random initialization of c_1 and c_2

Iteration 1

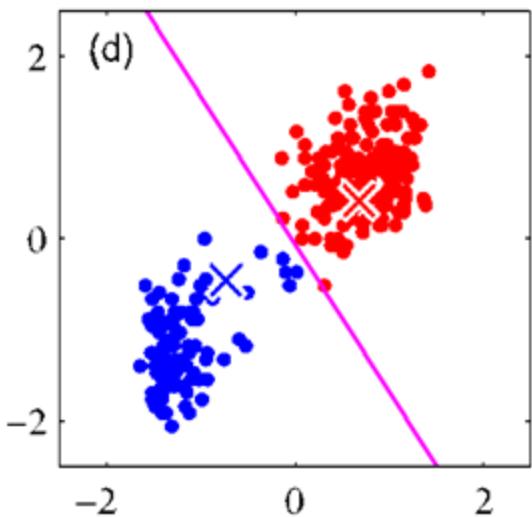


(A) update the cluster assignments.

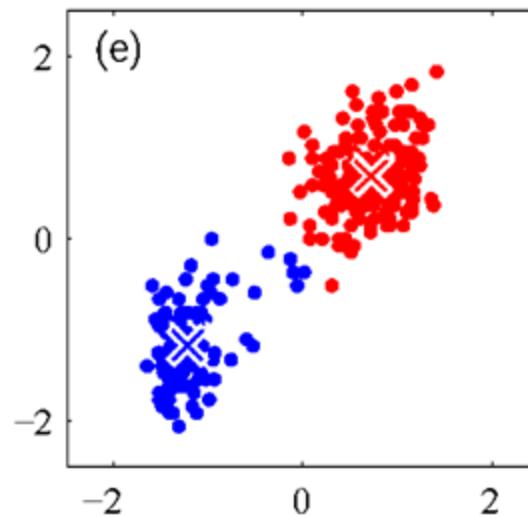


(B) Update the centroids $\{c_j\}$

Iteration 2

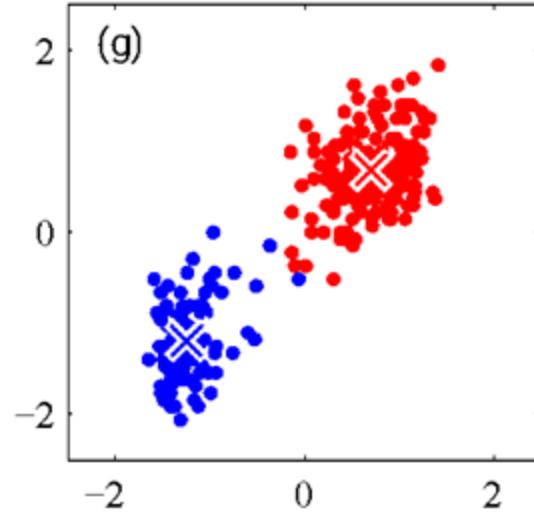
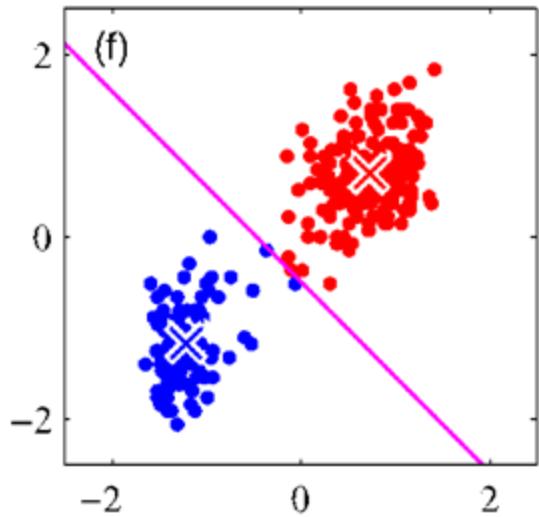


(A) update the cluster assignments.



(B) Update the centroids $\{c_j\}$

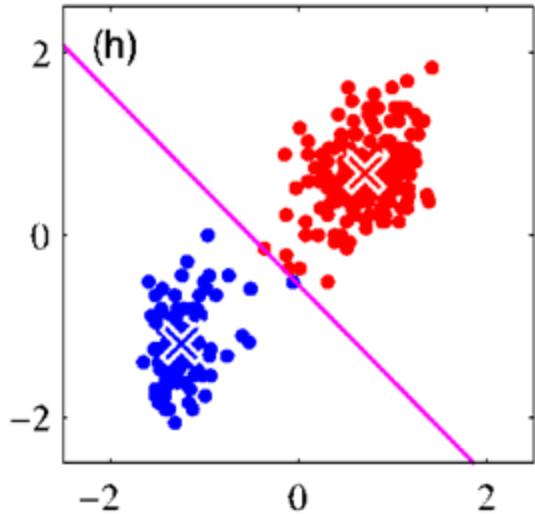
Iteration 3



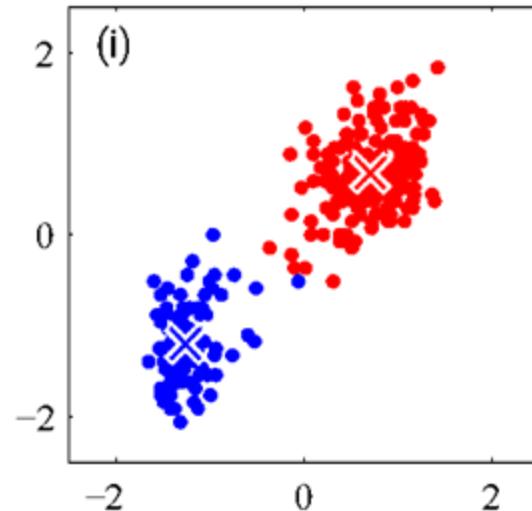
(A) update the cluster assignments.

(B) Update the centroids $\{c_j\}$

Iteration 4

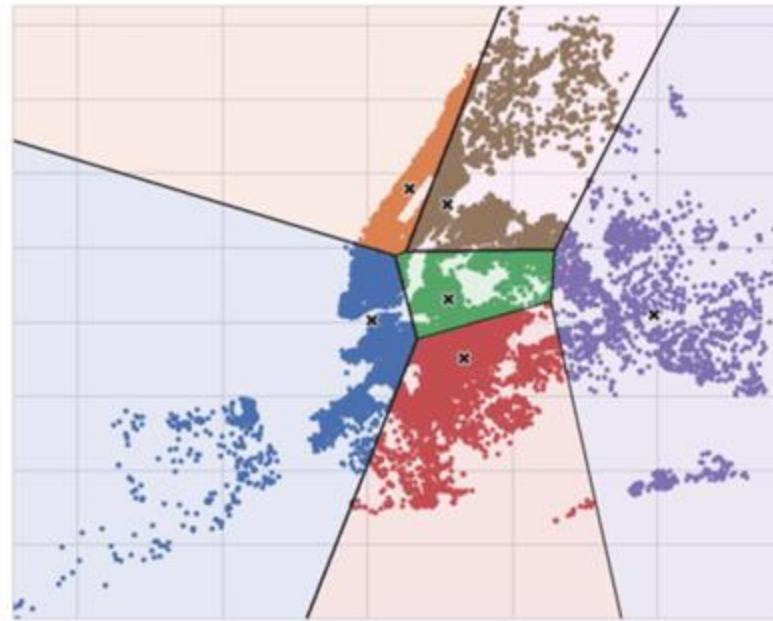


(A) update the cluster assignments.



(B) Update the centroids $\{c_j\}$

Iterating until Convergence



Animation from [Kaggle](#)



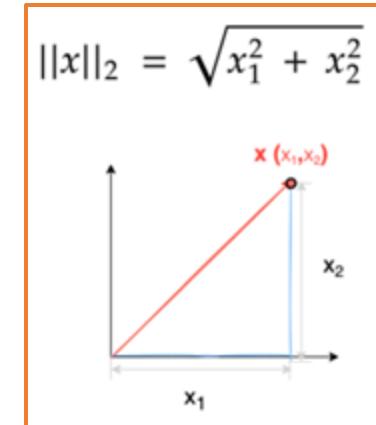
k-means clustering

Input: k : num. of clusters, $S = \{x_1, \dots, x_n\}$

[Initialize] Pick c_1, \dots, c_k as randomly selected points from S (see next slides for alternatives)

For $t=1,2,\dots,\text{max_iter}$

- **[Assignments]** $\forall x \in S, \quad a_t(x) = \arg \min_{j \in [k]} \|x - c_j\|_2^2$
- If $t \neq 1$ AND $a_t(x) = a_{t-1}(x), \forall x \in S$
 - break



k-means clustering

Input: k : num. of clusters, $S = \{x_1, \dots, x_n\}$

[Initialize] Pick c_1, \dots, c_k as randomly selected points from S (see next slides for alternatives)

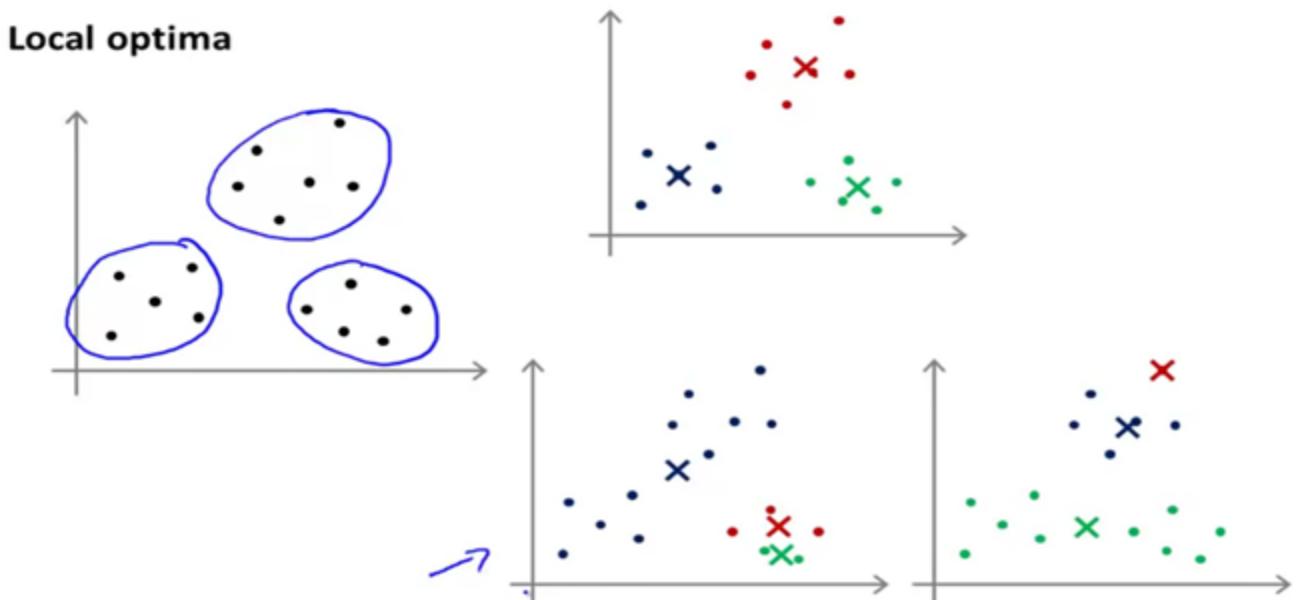
For $t=1,2,\dots,\text{max_iter}$

- **[Assignments]** $\forall x \in S, a_t(x) = \arg \min_{j \in [k]} \|x - c_j\|_2^2$
- If $t \neq 1$ AND $a_t(x) = a_{t-1}(x), \forall x \in S$
 - break
- **[Centroids]** $\forall j \in [k], c_j \leftarrow \text{average}(\{x \in S : a_t(x) = j\})$

Output: c_1, \dots, c_k and $\{a_t(x_i)\}_{i \in [n]}$

Issue: Unreliable solution

It may converge to a local rather than global minimum.



Andrew Ng

Issue: Unreliable solution

- You usually get suboptimal solutions
- You usually get different solutions every time you run.
- **Standard practice:** Run it 50 times and take the one that achieves the smallest objective function

- Recall:
$$\min_{c_1, \dots, c_k} \sum_{i=1}^n \min_{j \in [k]} \|x_i - c_j\|_2^2$$
 Each run of algorithm outputs c_1, \dots, c_k .
Compute this to evaluate the quality!

- K-means
- Neural Networks

Neural Networks

Forms of NNs are used all over the place nowadays...



FB Auto Tagging



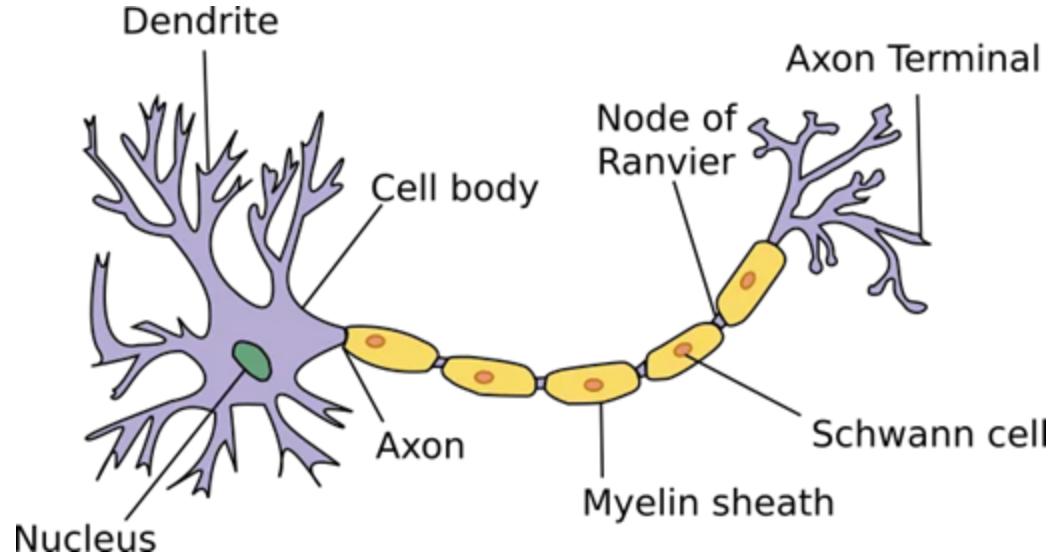
Self-Driving Cars



Creepy Robots

A screenshot of a machine translation tool. At the top, it says "Text" and "Documents". Below that, it shows "DETECT LANGUAGE" set to "ENGLISH" and "SPANISH", "FRENCH", and "ARABIC". The main area shows the English input "Hello world!" and its Spanish translation "¡Hola Mundo!". There are also audio icons and a "Send feedback" button at the bottom right.

Biological Neuron



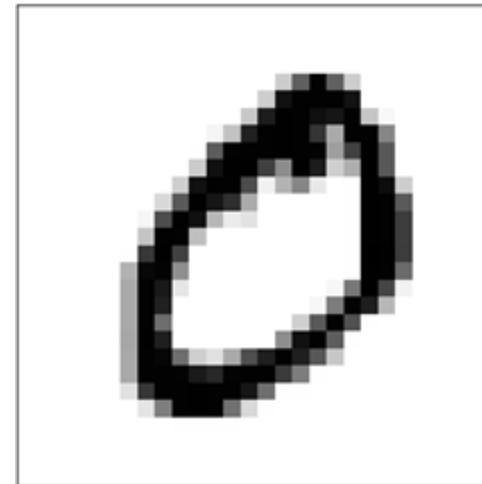
1. It takes inputs from its dendrites;
2. A weighted sum of inputs is passed on to the axon hillock;
3. If weighted sum is larger than threshold limit, the neuron will fire. Otherwise, it stays at rest.
4. The state of our neuron (on or off) then propagates through its axon and is passed on to the other connected neurons via its synapses.

Handwritten Digit Classification

Classifying handwritten digits is the “Hello World” of NNs



Each character is centered
in a $28 \times 28 = 784$ pixel
grayscale image

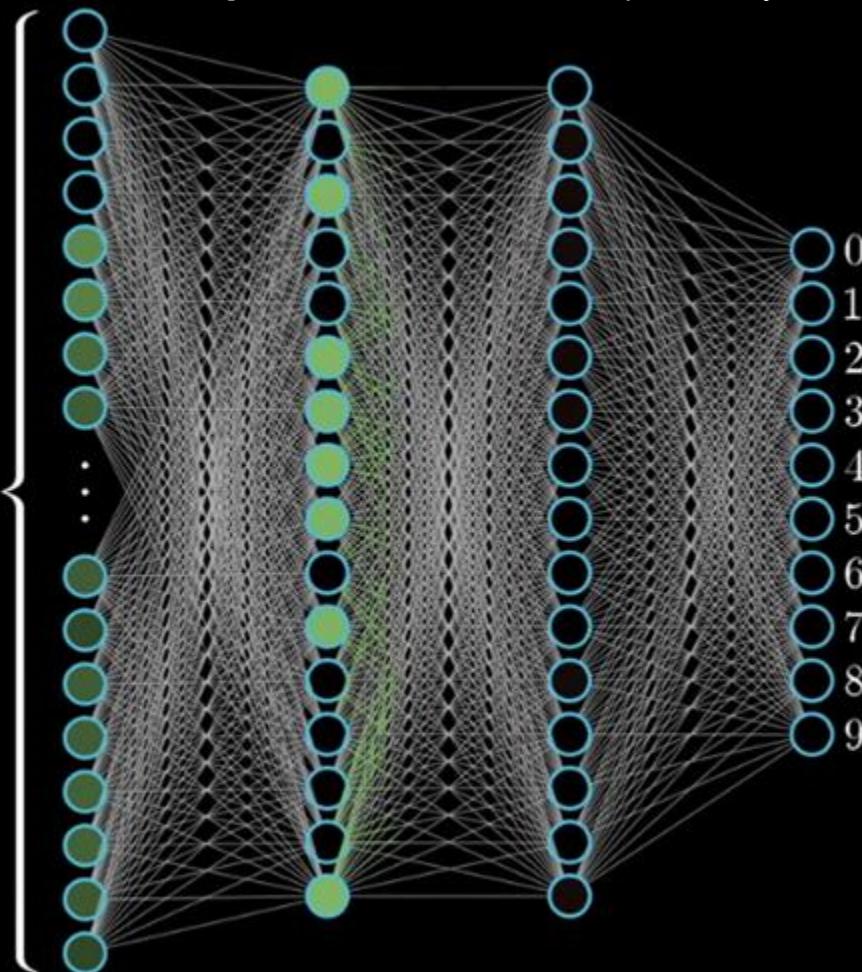


Modified National Institute of
Standards and Technology
(MNIST) database contains 60k
training and 10k test images

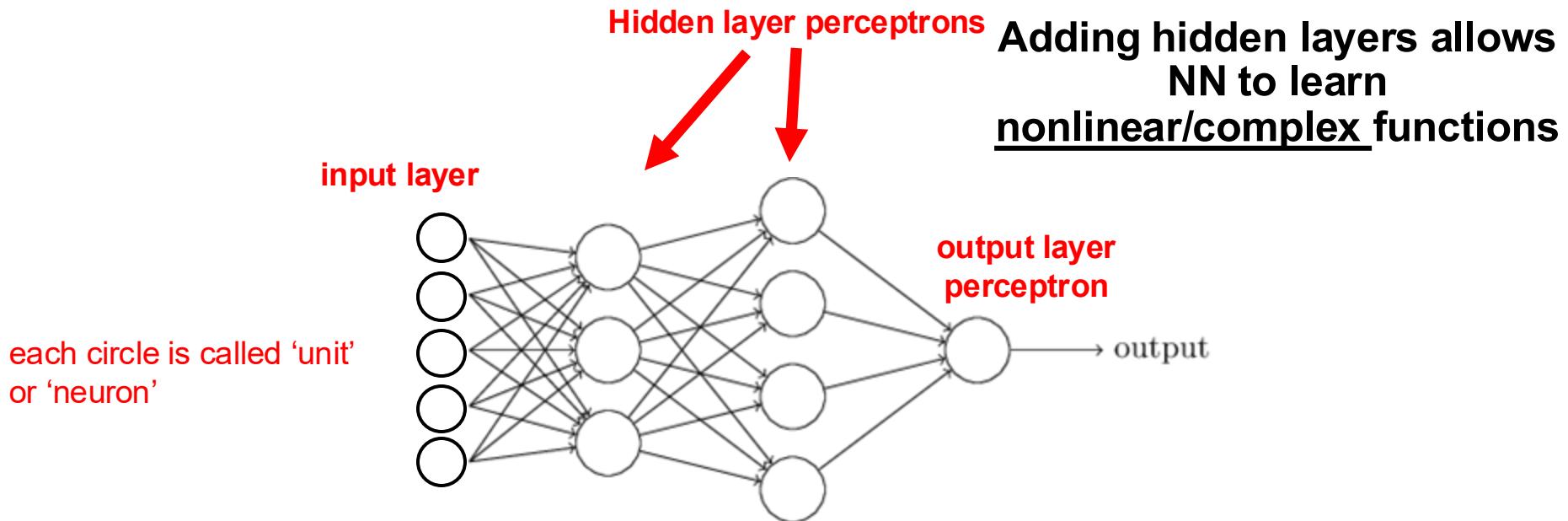


784

Each image pixel is a number in $[0, 1]$ indicated by highlighted color



Multilayer Perceptron

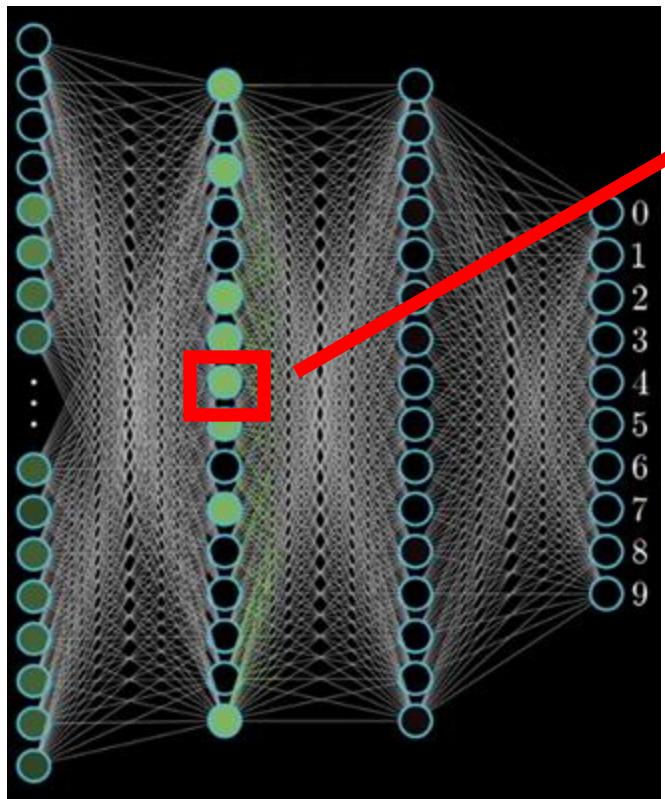


This is the quintessential (*Artificial*) Neural Network...

... the image above is a special case called *Feed Forward Neural Net*

feed forward: no backward connection

Feedforward Procedure



Each node computes a *weighted combination* of nodes at the previous layer...

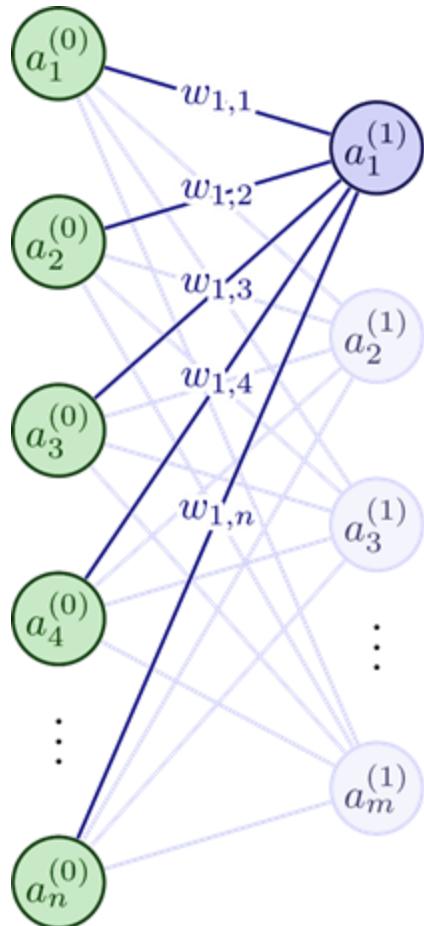
$$w_1x_1 + w_2x_2 + \dots + w_nx_n$$

Then applies a *nonlinear function* to the result

$$\sigma(w_1x_1 + w_2x_2 + \dots + w_nx_n + b)$$

Usually, we also introduce a constant *bias* parameter
(usually hidden when we visualize the network)

Feedforward Procedure

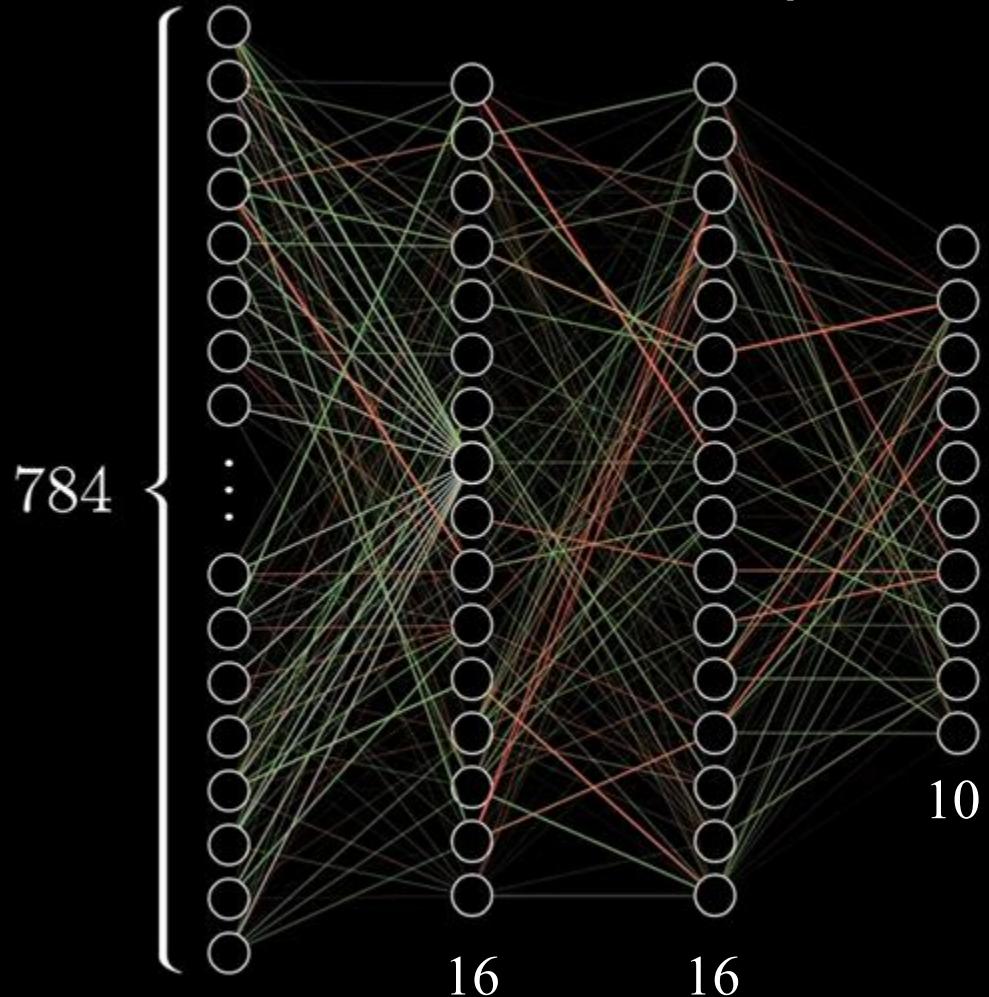


$$\begin{aligned}
 a_1^{(1)} &= \sigma \left(w_{1,0}a_0^{(0)} + w_{1,1}a_1^{(0)} + \dots + w_{1,n}a_n^{(0)} + b_1^{(0)} \right) \\
 a_2^{(1)} &= \sigma \left(\sum_{i=1}^n w_{1,i}a_i^{(0)} + b_1^{(0)} \right)
 \end{aligned}$$

$$\begin{pmatrix} a_1^{(1)} \\ a_2^{(1)} \\ \vdots \\ a_m^{(1)} \end{pmatrix} = \sigma \left[\begin{pmatrix} w_{1,0} & w_{1,1} & \dots & w_{1,n} \\ w_{2,0} & w_{2,1} & \dots & w_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ w_{m,0} & w_{m,1} & \dots & w_{m,n} \end{pmatrix} \begin{pmatrix} a_1^{(0)} \\ a_2^{(0)} \\ \vdots \\ a_n^{(0)} \end{pmatrix} + \begin{pmatrix} b_1^{(0)} \\ b_2^{(0)} \\ \vdots \\ b_m^{(0)} \end{pmatrix} \right]$$

$$a^{(1)} = \sigma (\mathbf{W}^{(0)} a^{(0)} + \mathbf{b}^{(0)})$$

Number of parameters in this example: $m \times n + m$



$$784 \times 16 + 16 \times 16 + 16 \times 10$$

weights

$$16 + 16 + 10$$

biases

13,002

Each parameter has some impact
on the output...need to train all
these parameters simultaneously
to have a good prediction
accuracy

Activation functions

We call this an *activation function* and typically write it in vector form,

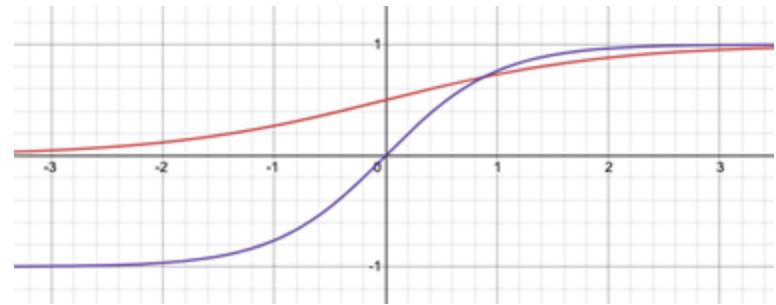
$$\sigma(w_1x_1 + w_2x_2 + \dots + w_nx_n + b) = \sigma(w^T x + b)$$

An early choice was the *logistic function*,

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

Later, people found that a scaled version called **tanh** trains faster (=converges faster)

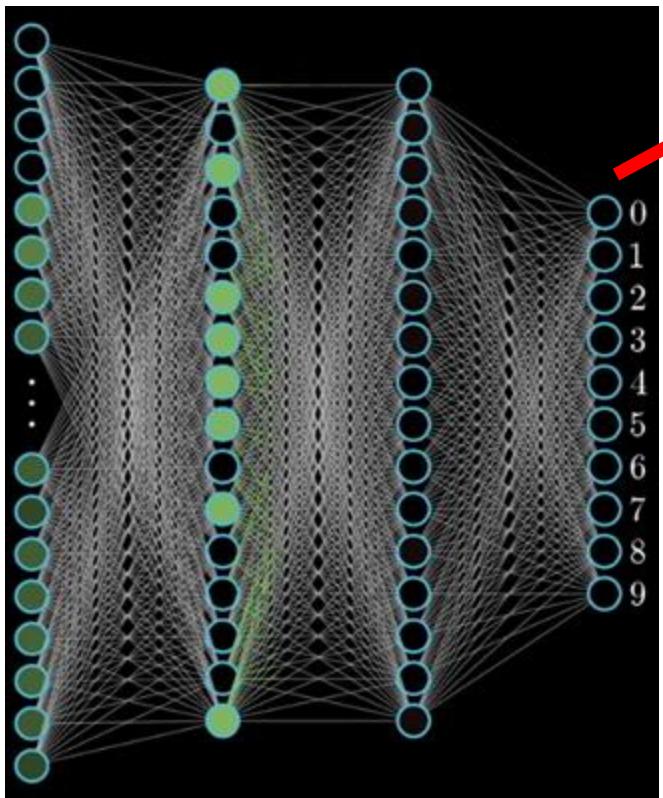
$$\tanh(z) = 2\sigma(2z) - 1$$



| | |
|--|-------|
| $\frac{1}{(1 + e^{-x})} = \sigma(x)$ | <hr/> |
| $\frac{(e^x - e^{-x})}{e^x + e^{-x}} = \tanh(x)$ | |

Multilayer Perceptron

33



Final layer is a linear model...

for classification this is a logistic regression

$$\sigma(w^T x + b) = \frac{1}{1 + e^{-(w^T x + b)}}$$

Vector of activations from
previous layer

Training Multilayer Perceptron

Our cost function for i^{th} input is error in terms of weights / biases...

$$\text{Cost}_i(w_1, \dots, w_n, b_1, \dots, b_n)$$

13,002 Parameters in this network

...minimize cost over all training data...

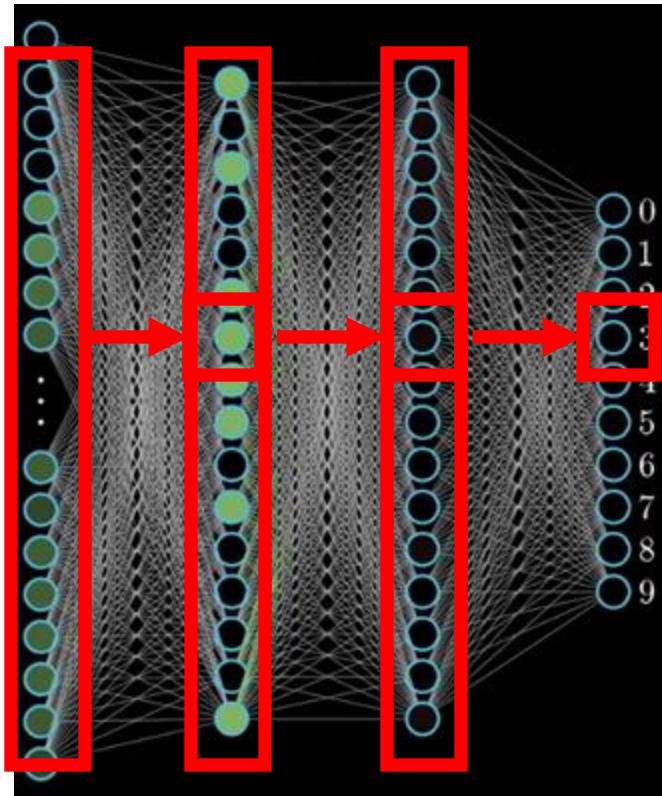
$$\min_{w,b} \mathcal{L}(w, b) = \sum_i \text{Cost}_i(w_1, \dots, w_n, b_1, \dots, b_n)$$

This is a super high-dimensional optimization (13,002 dimensions in this example)...how do we solve it?

Gradient descent!

Backpropagation

[Source : 3Blue1Brown : <https://www.youtube.com/watch?v=aircAruvnKk>]



Randomly initialize $\{w^{(u)}\}_{u \in \text{units in neural net}}$

For $i \in \{1, \dots, n_{\text{epochs}}\}$

- For (x, y) in train set:
 - Forward pass:
 - evaluate the neural net output
 - measure the loss
 - Backward pass: compute the gradients.
 - Take the gradient step to update the weights $\{w^{(u)}\}$

Dependencies between layers.

No dependencies between units at the same layer.
⇒ Many GPU supported libraries available.

Backpropagation: an example

$$\begin{cases} z_1^{(1)} = w_{11}^{(1)}x_1 + w_{21}^{(1)}x_2 + b_1^{(1)} \\ z_2^{(1)} = w_{12}^{(1)}x_1 + w_{22}^{(1)}x_2 + b_2^{(1)} \end{cases}$$

$$\begin{pmatrix} h_1 = \sigma(z_1^{(1)}) \\ h_2 = \sigma(z_2^{(1)}) \end{pmatrix}$$

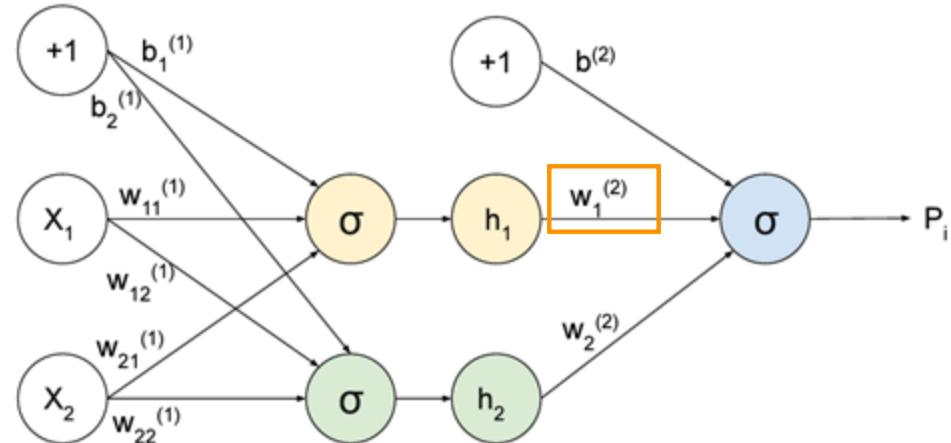
$$(z^{(2)} = w_1^{(2)}h_1 + w_2^{(2)}h_2 + b^{(2)})$$

$$\left(p_i = \sigma(z^{(2)}) \right)$$

Useful to know:

$$If \ p = \sigma(x) = \frac{1}{1 + e^{-x}}$$

$$Then \ \frac{dp}{dx} = (1 + e^{-x})^{-2} e^{-x} = \frac{1}{1 + e^{-x}} \times \frac{e^{-x}}{1 + e^{-x}} = p(1 - p)$$



$$Error: L = \frac{1}{2} \|p - y\|^2 = \sum_i \frac{1}{2} (p_i - y_i)^2$$

$$Compute: \frac{\partial L}{\partial w_1^{(2)}}$$

Backpropagation: an example

$$\begin{cases} z_1^{(1)} = w_{11}^{(1)}x_1 + w_{21}^{(1)}x_2 + b_1^{(1)} \\ z_2^{(1)} = w_{12}^{(1)}x_1 + w_{22}^{(1)}x_2 + b_2^{(1)} \end{cases}$$

$$\begin{pmatrix} h_1 = \sigma(z_1^{(1)}) \\ h_2 = \sigma(z_2^{(1)}) \end{pmatrix}$$

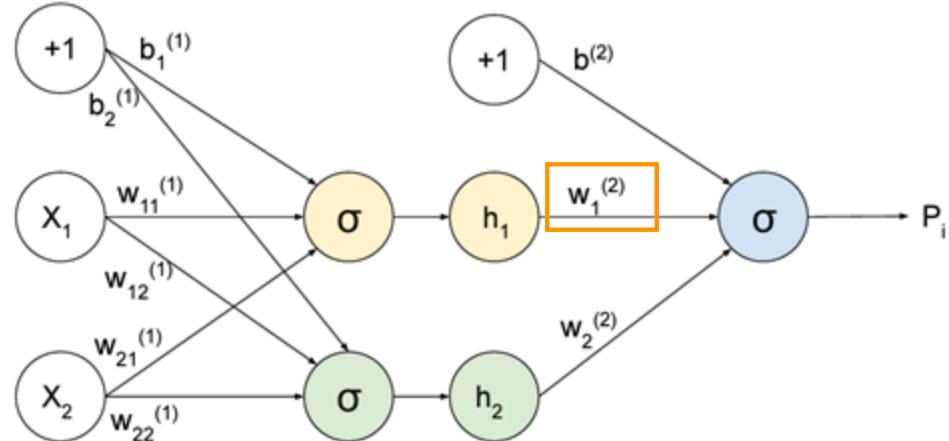
$$(z^{(2)} = w_1^{(2)}h_1 + w_2^{(2)}h_2 + b^{(2)})$$

$$\left(p_i = \sigma(z^{(2)}) \right)$$

$$\frac{\partial L}{\partial w_1^{(2)}} = \sum_i \frac{\partial L_i}{\partial w_1^{(2)}}$$

$$\frac{\partial L_i}{\partial w_1^{(2)}} = \frac{\partial z^{(2)}}{\partial w_1^{(2)}} \times \frac{\partial p_i}{\partial z^{(2)}} \times \frac{\partial L_i}{\partial p_i} = h_1 \times p_i(1 - p_i) \times (p_i - y)$$

Chain rule



$$Error: L = \frac{1}{2} \|p - y\|^2 = \sum_i \frac{1}{2} (p_i - y_i)^2$$

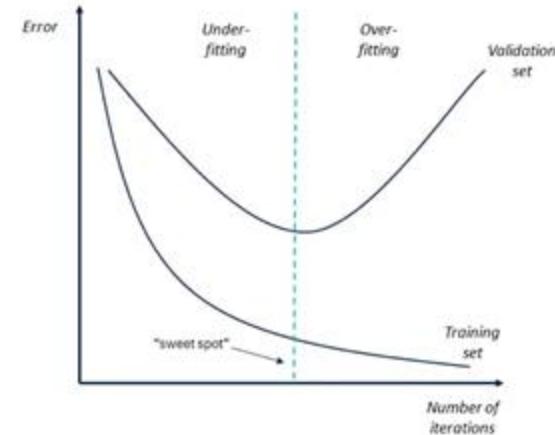
$$Compute: \frac{\partial L}{\partial w_1^{(2)}}$$

With four parameters I can fit an elephant. With five I can make him wiggle his trunk. - John von Neumann

$$w = \arg \min_w \text{Cost}(w) + \alpha \cdot \text{Regularizer}(\text{Model})$$

Our example model has 13,002 parameters...that's a lot of elephants!
Regularization is critical to avoid overfitting...

...numerous regularization schemes are used in training neural networks.
but the standard is of course, $\sum_i w_i^2$



sklearn.neural_network.MLPClassifier

hidden_layer_sizes : tuple, length = n_layers - 2, default=(100,)

The ith element represents the number of neurons in the ith hidden layer.

activation : {'identity', 'logistic', 'tanh', 'relu'}, default='relu'

Activation function for the hidden layer.

solver : {'lbfgs', 'sgd', 'adam'}, default='adam'

The solver for weight optimization.

alpha : float, default=0.0001

L2 penalty (regularization term) parameter.

learning_rate : {'constant', 'invscaling', 'adaptive'}, default='constant'

Learning rate schedule for weight updates.

early_stopping : bool, default=False

Whether to use early stopping to terminate training when validation score is not improving. If set to true,

Fetch MNIST data from www.openml.org :

```
X, y = fetch_openml("mnist_784", version=1, return_X_y=True)
X = X / 255.0
```

Train test split (60k / 10k),

```
X_train, X_test = X[:60000], X[60000:]
y_train, y_test = y[:60000], y[60000:]
```

Create MLP classifier instance,

- Single hidden layer (50 nodes)
- Use stochastic gradient descent
- Maximum of 10 learning iterations
- Small L2 regularization alpha=1e-4

```
mlp = MLPClassifier(
    hidden_layer_sizes=(50,),
    max_iter=10,
    alpha=1e-4,
    solver="sgd",
    verbose=10,
    random_state=1,
    learning_rate_init=0.1,
)
```

Scikit-Learn : Multilayer Perceptron

41

Fit the MLP and print stuff...

```
mlp.fit(X_train, y_train)  
  
print("Training set score: %f" % mlp.score(X_train, y_train))  
print("Test set score: %f" % mlp.score(X_test, y_test))
```

```
Iteration 1, loss = 0.32009978  
Iteration 2, loss = 0.15347534  
Iteration 3, loss = 0.11544755  
Iteration 4, loss = 0.09279764  
Iteration 5, loss = 0.07889367  
Iteration 6, loss = 0.07170497  
Iteration 7, loss = 0.06282111  
Iteration 8, loss = 0.05530788  
Iteration 9, loss = 0.04960484  
Iteration 10, loss = 0.04645355  
Training set score: 0.986800  
Test set score: 0.970000
```

Visualize the weights for each node...

coefs_[i]: n_input x n_output matrix of weights for layer i

```
vmin, vmax = mlp.coefs_[0].min(), mlp.coefs_[0].max()  
for coef, ax in zip(mlp.coefs_[0].T, axes.ravel()):  
    ax.matshow(coef.reshape(28, 28), cmap=plt.cm.gray,  
              vmin=0.5 * vmin, vmax=0.5 * vmax)  
    ax.set_xticks(())  
    ax.set_yticks(())
```

...magnitude of weights indicates which input features are important in prediction

