

Introduction to Neural Networks

By Vipul Goyal

Why Another Technique?

Linear and Logistics regression are “one-shot”

Give the input, the output comes out “right away”

- In linear regression: output is a simple linear function of the input
- In logistic regression: you apply the logistic function

Why Another Technique?

- But many computations are more complex! Might involve millions of steps to go from input to output.
- Thinking about a program with millions of lines of code (iPhone apps, Zoom software...)
- Think about self driving cars. Car decides whether to apply brakes or not!

Computer Vision: Classification

Training Examples



Cars



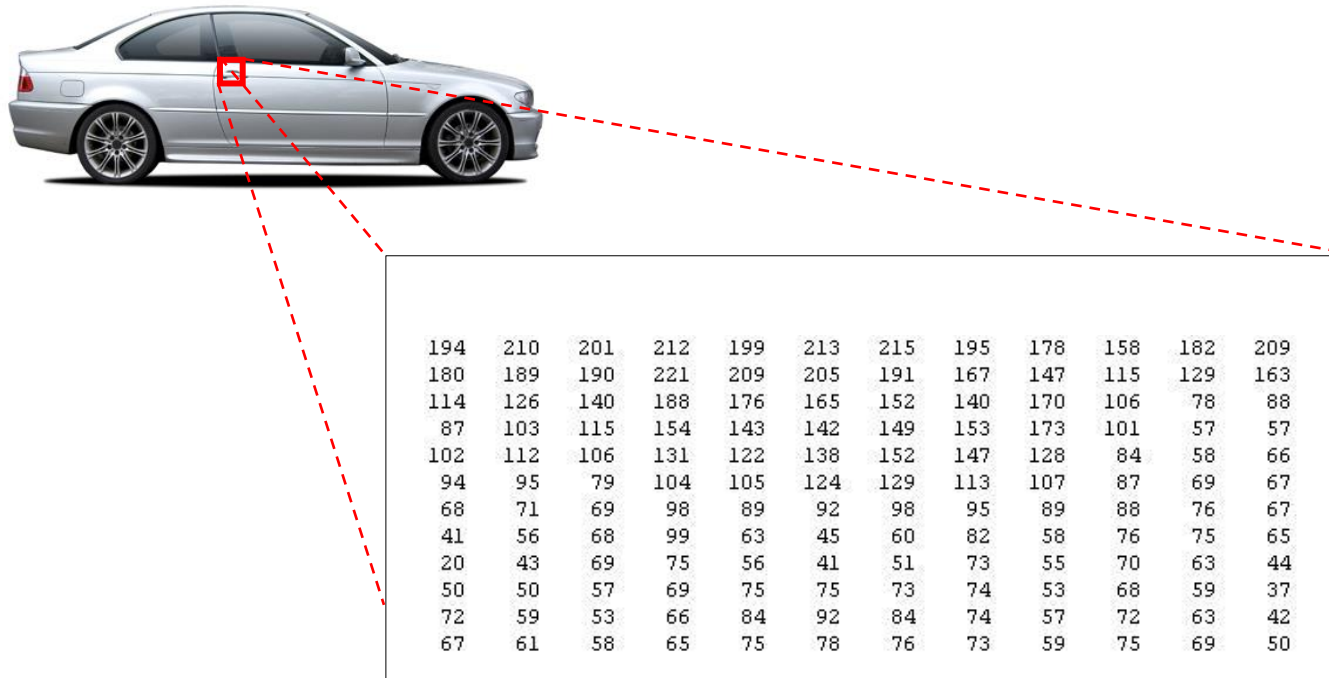
Not a car

Input:



Computer Vision: Classification

We see this:



But the program sees this

Seems unlikely that within a “single shot”, you get the answer from these numbers!

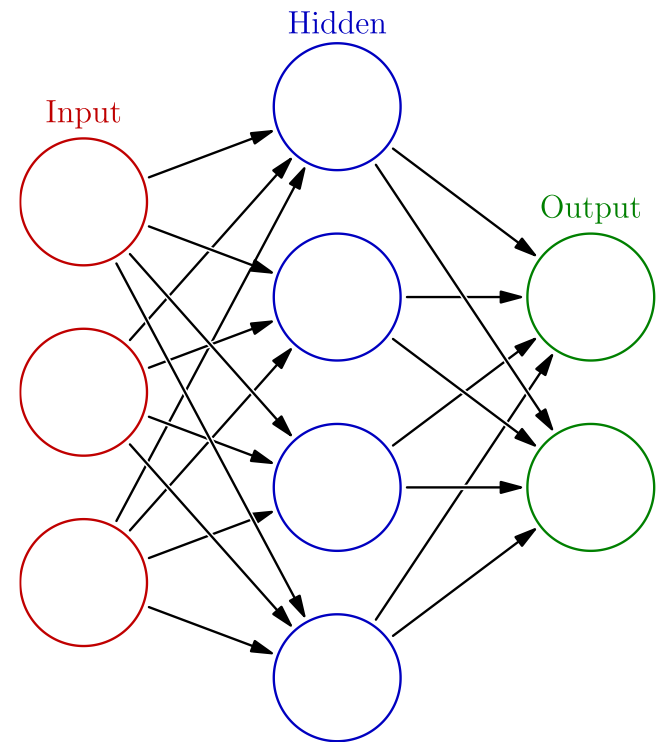
Neural Networks

Short story: several instances of “one-shot” learning algorithms connected with each other.

Example: many logistic regression “gates” arranged like a circuit or a directed acyclic graph.

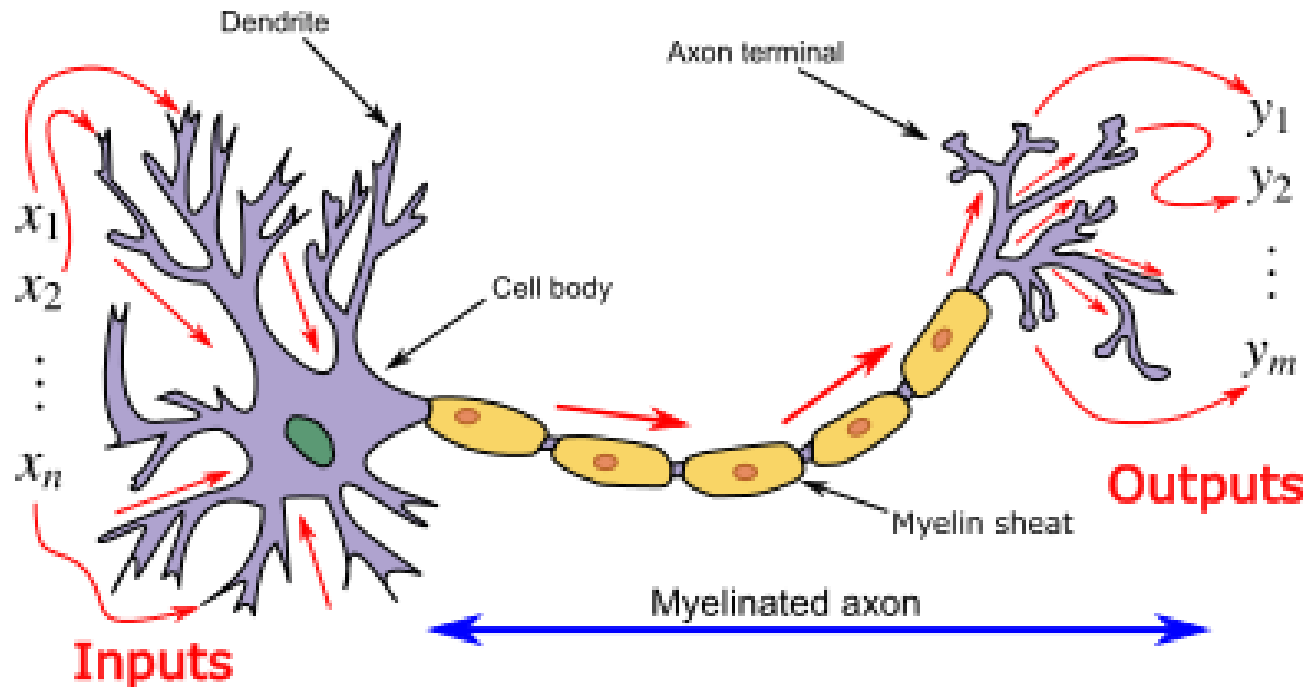
Also called “artificial neural networks”. “Natural” neural networks are inside our brain.

Long story?



“Natural” Neural Networks

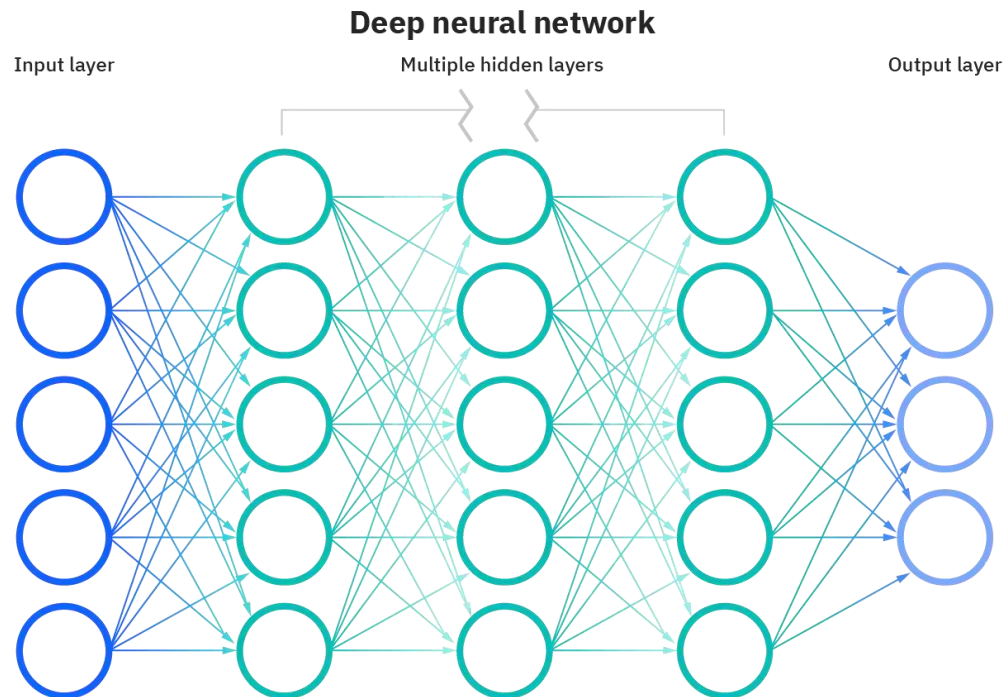
We are all born with neural networks inside our brain



- Dendrites can be seen as input wires. Axon is the output wire. Based on the inputs, a neuron may “fire” or “stay quiet”
- Output of one neuron goes as input to another.

(Artificial) Neural Networks

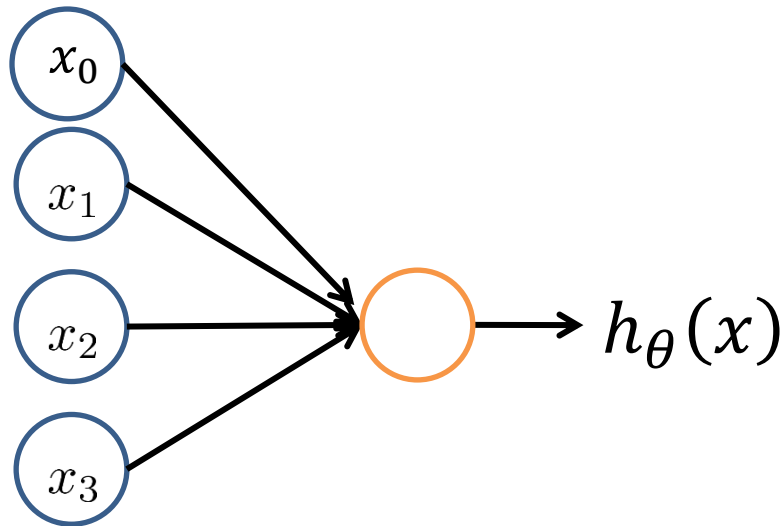
- Composed of (artificial) neurons. Each artificial neuron has inputs and produces a single output which can be sent to multiple other neurons.
- The inputs can be the feature values of a sample of external data, such as images or documents, or they can be the outputs of other neurons.



Neural Networks

- The outputs of the final output neurons of the neural net accomplish the task, such as recognizing an object in an image.
- To find the output of the neuron, first we take the weighted sum of all the inputs, weighted by the weights of the connections from the inputs to the neuron.
- We add a bias term to this sum. Similar to constant θ_0 in linear regression.
- This weighted sum is then passed through a (usually nonlinear) activation function to produce the output.
- The initial inputs are external data, such as images and documents. The ultimate outputs accomplish the task, such as recognizing an object in an image.

Using Logistic Unit as Neuron



$$x = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} \quad \theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$$

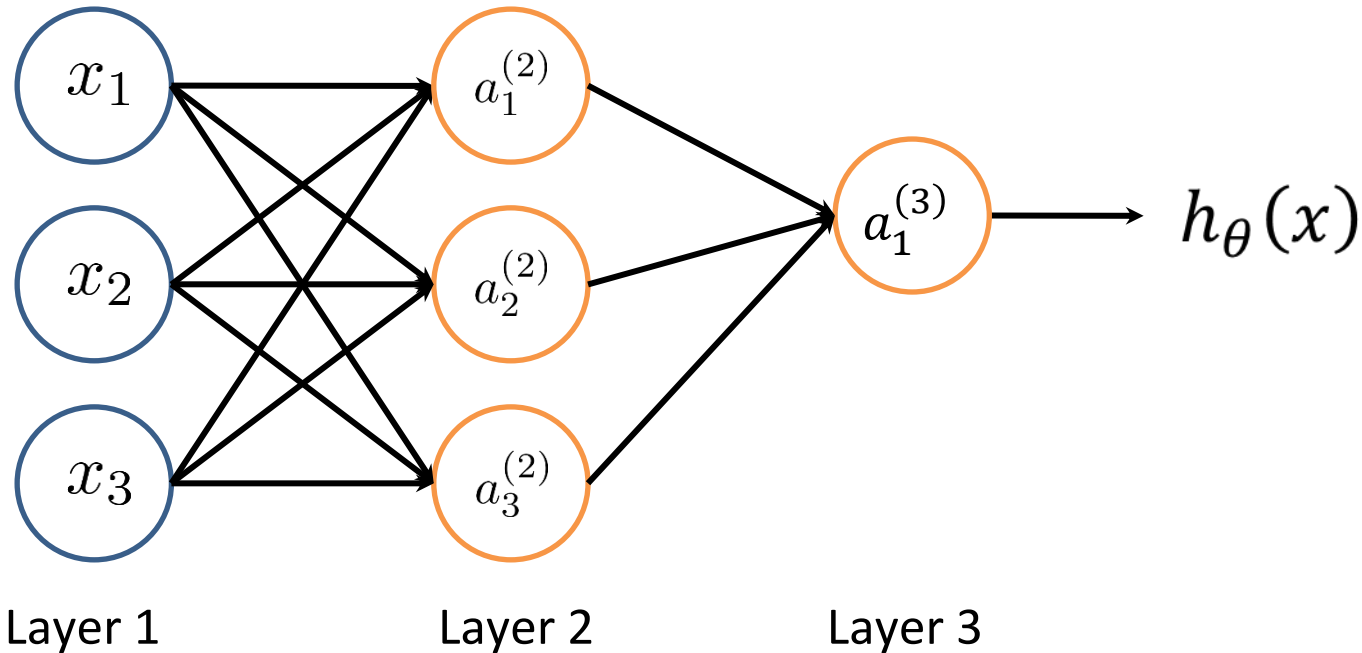
Sigmoid (logistic) activation function.

- x_1, x_2, x_3 are input (features). $x_0=1$ added as bias term.
- $\theta_0, \theta_2 \dots \theta_3$ are the weights.

Step1: compute weighted sum $z = \theta^T x$

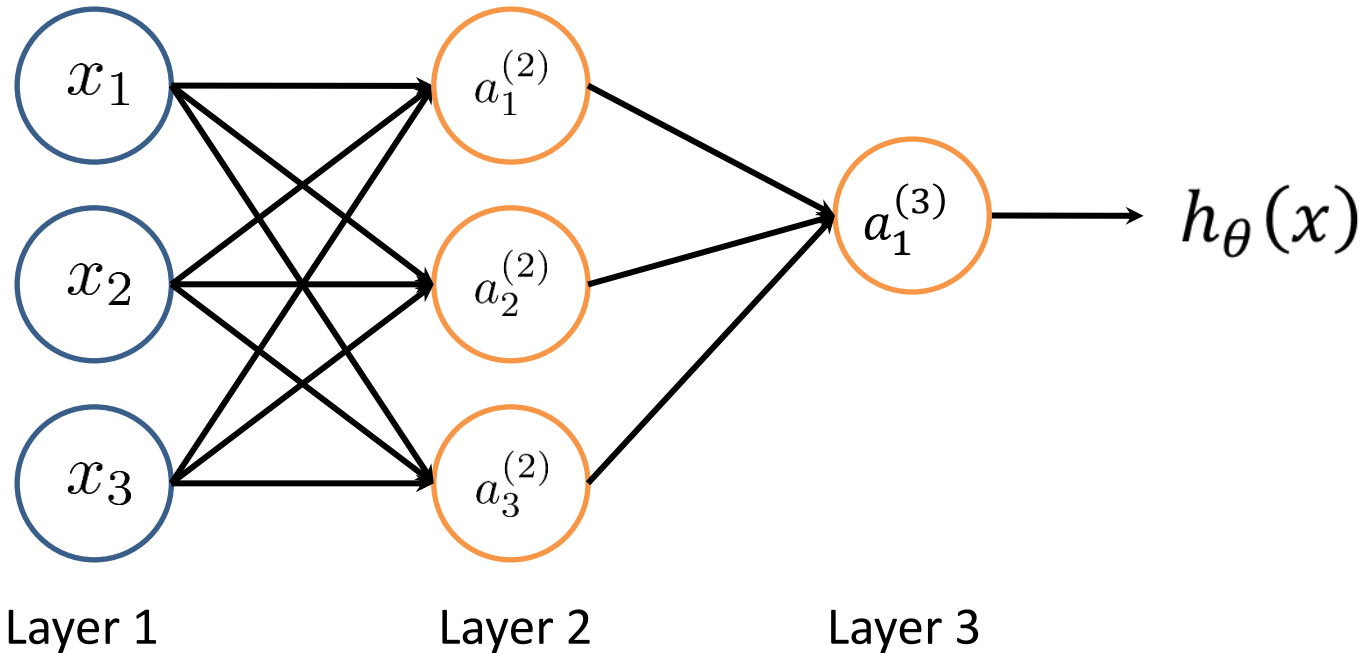
Step2: compute activation function $g(z) = \frac{1}{1+e^{-z}}$ giving us the final output $h_{\theta}(x)$

Neural Networks



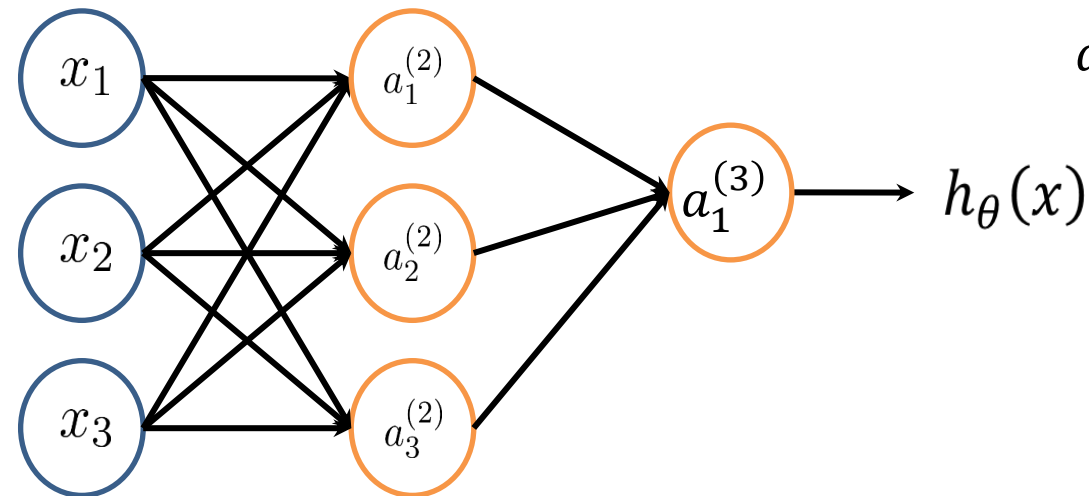
- Logistic units are in orange color. **No computation in initial layer.**
- Input layer, hidden layer(s), output layer
- Need to add x_0 as the bias term to all logistic units.

Neural Networks



- Each $a_i^{(j)}$ unit has its own weights $(\theta_{i1}^{(j)}, \theta_{i2}^{(j)}, \dots)$
- $a_i^{(2)}$ units take x_i 's as input (plus bias term)
- $a_1^{(3)}$ unit takes $a_i^{(2)}$'s as input (output of the previous layer)

Running the Neural Network



$a_i^{(j)}$ = “activation” of unit i in layer j

$\theta^{(j)}$ = matrix of weights
controlling function mapping
from layer j to layer $j+1$

$$a_1^{(2)} = g(\theta_{10}^{(1)}x_0 + \theta_{11}^{(1)}x_1 + \theta_{12}^{(1)}x_2 + \theta_{13}^{(1)}x_3)$$

$$a_2^{(2)} = g(\theta_{20}^{(1)}x_0 + \theta_{21}^{(1)}x_1 + \theta_{22}^{(1)}x_2 + \theta_{23}^{(1)}x_3)$$

$$a_3^{(2)} = g(\theta_{30}^{(1)}x_0 + \theta_{31}^{(1)}x_1 + \theta_{32}^{(1)}x_2 + \theta_{33}^{(1)}x_3)$$

$$h_{\theta}(x) = a_1^{(3)} = g(\theta_{10}^{(2)}a_0^{(2)} + \theta_{11}^{(2)}a_1^{(2)} + \theta_{12}^{(2)}a_2^{(2)} + \theta_{13}^{(2)}a_3^{(2)})$$

Question: how do we compute θ 's? Training the neural network.

More General Neural Networks



Pedestrian



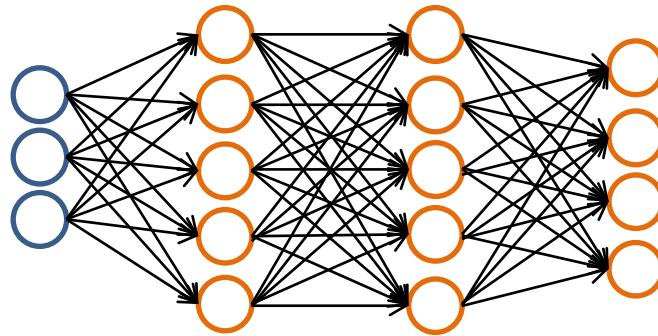
Car



Motorcycle



Truck

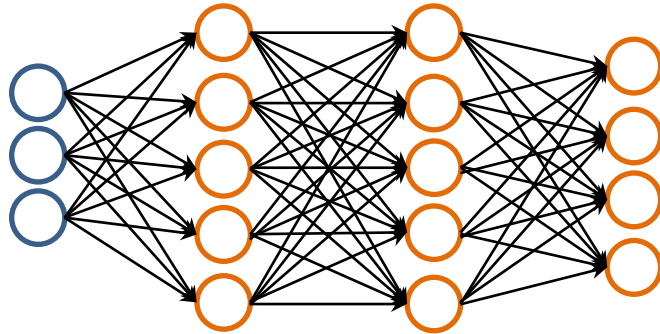


$$h_{\theta}(x) \in R^4$$

Want $h_{\theta}(x) \approx \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$, $h_{\theta}(x) \approx \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$, $h_{\theta}(x) \approx \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$ etc.

Pedestrian, car, motorcycle

More General Neural Networks



$$h_{\theta}(x) \in R^4$$

Want $h_{\theta}(x) \approx \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, h_{\theta}(x) \approx \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, h_{\theta}(x) \approx \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \text{ etc.}$

when pedestrian, when car, when motorcycle, etc.

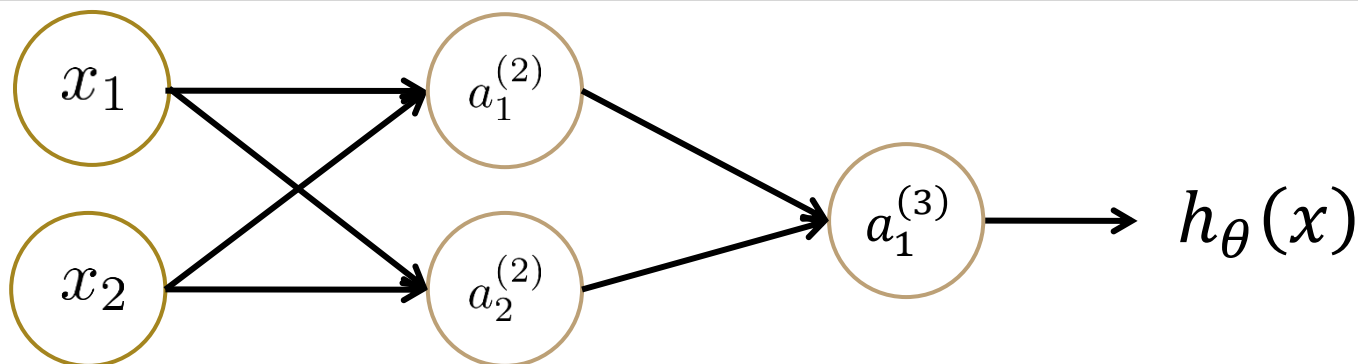
Training set: $(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \dots, (x^{(m)}, y^{(m)})$

$y^{(i)}$ is one of $\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$
Pedestrian, car, motorcycle, truck

Why Non-Linear Activation?

- Can the neurons be linear regression units?
- Turns out that in this case, even arbitrarily deep neural networks are (roughly) **equivalent to a *single* linear regression unit**
- This is because composition of many linear functions is still a linear function. Why?

Why Non-Linear Activation?



$$a_1^{(2)} = \theta_{11}^{(1)} x_1 + \theta_{12}^{(1)} x_2$$

$$a_2^{(2)} = \theta_{21}^{(1)} x_1 + \theta_{22}^{(1)} x_2$$

$$a_1^{(3)} = \theta_{11}^{(2)} a_1^{(2)} + \theta_{12}^{(2)} a_2^{(2)}$$

$$= \theta_{11}^{(2)} \left(\theta_{11}^{(1)} x_1 + \theta_{12}^{(1)} x_2 \right) + \theta_{12}^{(2)} \left(\theta_{21}^{(1)} x_1 + \theta_{22}^{(1)} x_2 \right)$$

$$= \left(\theta_{11}^{(2)} \theta_{11}^{(1)} + \theta_{12}^{(2)} \theta_{21}^{(1)} \right) x_1 + \left(\theta_{11}^{(2)} \theta_{12}^{(1)} + \theta_{12}^{(2)} \theta_{22}^{(1)} \right) x_2$$

$$= \theta'_1 x_1 + \theta'_2 x_2$$

Training the Neural Network

A Million (Trillion?) Dollar Question

We have learnt how to evaluate a neural network

Question: how does one compute the weights $\theta_{ij}^{(k)}$?

- First step: define a cost function
- Second step: select $\theta_{ij}^{(k)}$ carefully to minimize the cost function

Cost Function for Neural Network*

Logistics regression:

$$J(\theta) = -\frac{1}{m} \left[\sum_{i=1}^m y^{(i)} \log h_{\theta}(x^{(i)}) + (1 - y^{(i)}) \log(1 - h_{\theta}(x^{(i)})) \right]$$

Neural Networks

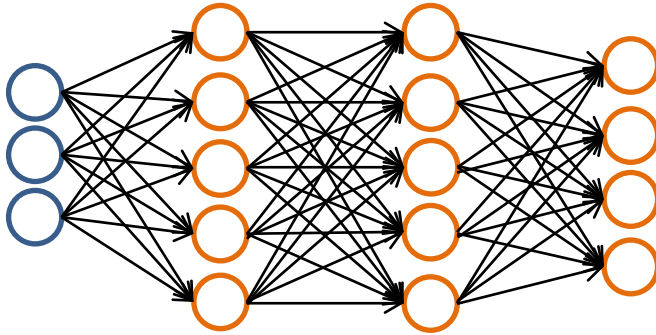
$$h_{\theta}(x) \in R^K$$

$$(h_{\theta}(x))_i = i^{\text{th}} \text{ output}$$

$$J(\theta) = -\frac{1}{m} \left[\sum_{i=1}^m \sum_{k=1}^K y_k^{(i)} \log \left(h_{\theta}(x^{(i)}) \right)_k + \left(1 - y_k^{(i)} \right) \log(1 - \left(h_{\theta}(x^{(i)}) \right)_k) \right]$$

*somewhat oversimplified, ignores bias terms

Intuition



$$h_{\theta}(x) \in R^K$$

$$(h_{\theta}(x))_i = i^{\text{th}} \text{ output}$$

$$J(\theta) = -\frac{1}{m} \left[\sum_{i=1}^m \sum_{k=1}^K y_k^{(i)} \log \left(h_{\theta}(x^{(i)}) \right)_k + \left(1 - y_k^{(i)} \right) \log \left(1 - \left(h_{\theta}(x^{(i)}) \right)_k \right) \right]$$

Our cost function is just the sum of the cost function for each individual logistic unit in the output.

Optimizing the Cost

$$J(\theta) = -\frac{1}{m} \left[\sum_{i=1}^m \sum_{k=1}^K y_k^{(i)} \log \left(h_{\theta}(x^{(i)}) \right)_k + \left(1 - y_k^{(i)} \right) \log(1 - \left(h_{\theta}(x^{(i)}) \right)_k) \right]$$

- To minimize the cost function, we need to make sure **partial derivatives w.r.t. EACH $\theta_{ij}^{(k)}$ is close to 0**
- Thus, we need to be able to compute the cost function and all the partial derivatives
- Afterwards: run gradient descent

Computing the Partial Derivatives

- Partial derivatives can be computed using what is known as the **backpropagation algorithm**
- **Idea: compute an error term for each node in the network**
- For output nodes: error term computed using the training examples. For hidden layer nodes: computed by going backwards from output layer by utilizing some known as chain rule and dynamic programming
- Exact math: messy and involved

Gradient Descent for NN

Want $\min_{\theta} J(\theta)$:

Repeat {

$$\theta_{ij}^{(k)} := \theta_{ij}^{(k)} - \alpha \frac{\partial}{\partial \theta_{ij}^{(k)}} J(\theta)$$

}

(simultaneously update all $\theta_{ij}^{(k)}$)

- Keep in mind: it's important for all $\theta_{ij}^{(k)}$ to be initialized at random for symmetry breaking
- If initialized to the same value: all nodes within a given layer become identical and may remain identical

Flavors of Gradient Descent

- **Batch gradient descent**: all available data is injected at once.
- **Stochastic gradient descent (SGD)**: a single random sample is introduced on each iteration.
- **(Stochastic) Mini-batch gradient descent**: instead of feeding the network with single samples, N random items are introduced on each iteration.

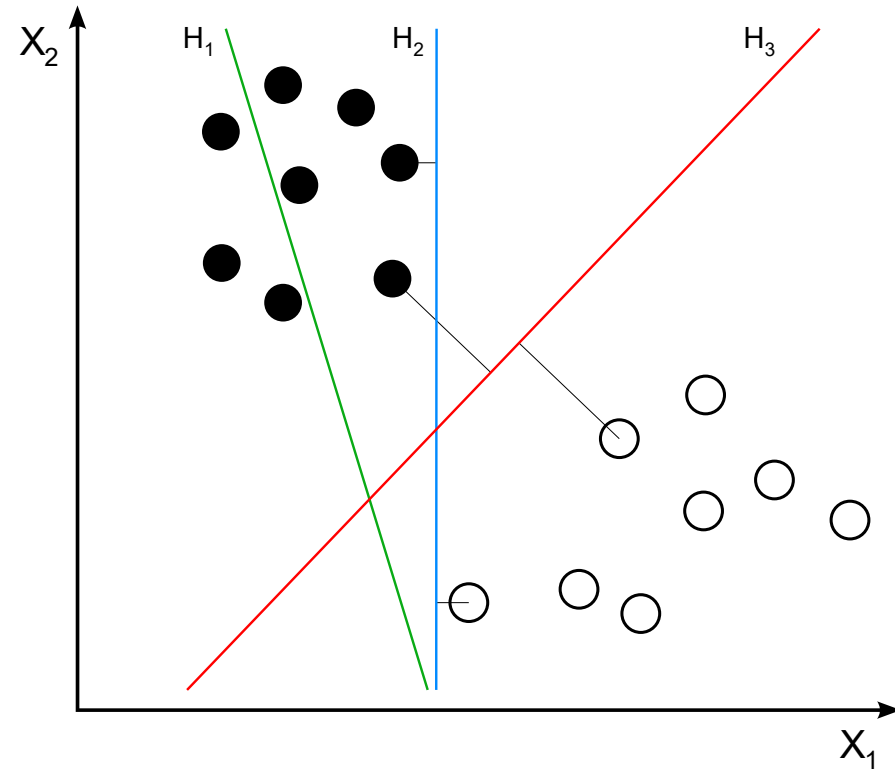
Support Vector Machines

Support Vector Machine (SVM)

Classification: black=0, white=1

Linear classifiers: H_1 , H_2 and H_3

Which one is the best?

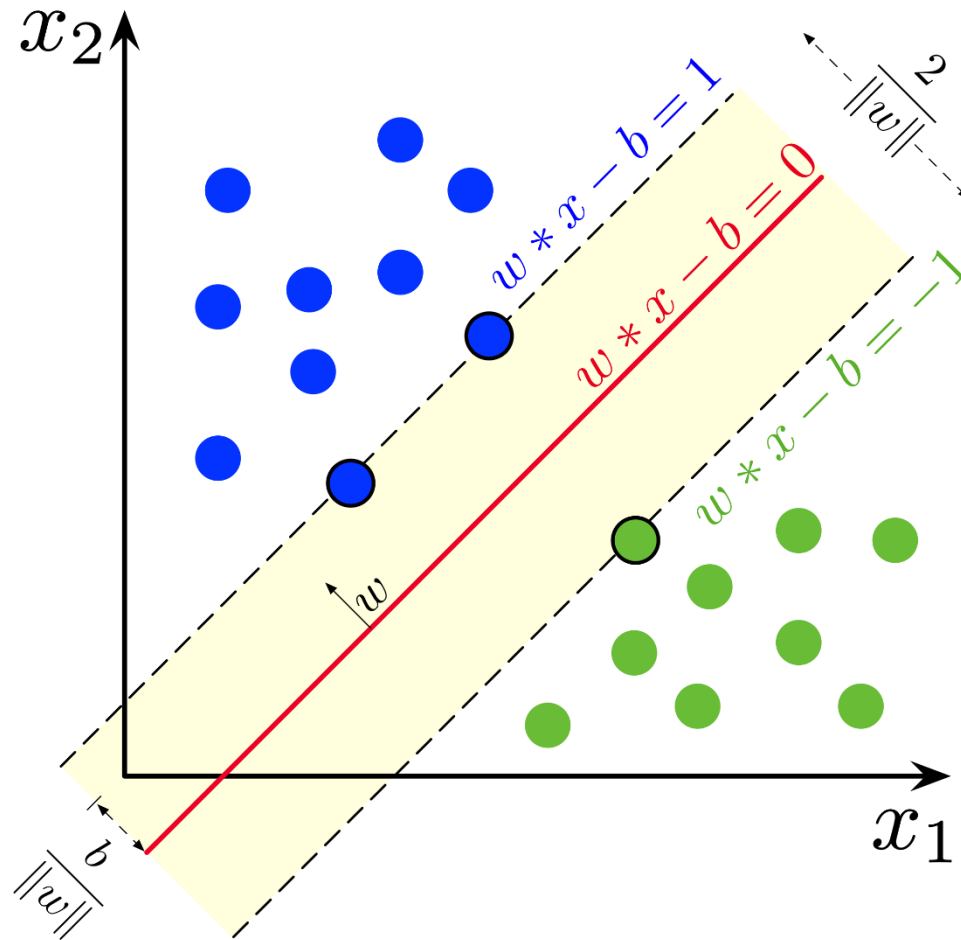


Are H_2 and H_3 equally good?
Probably Not.

Maximum-Margin Hyperplane

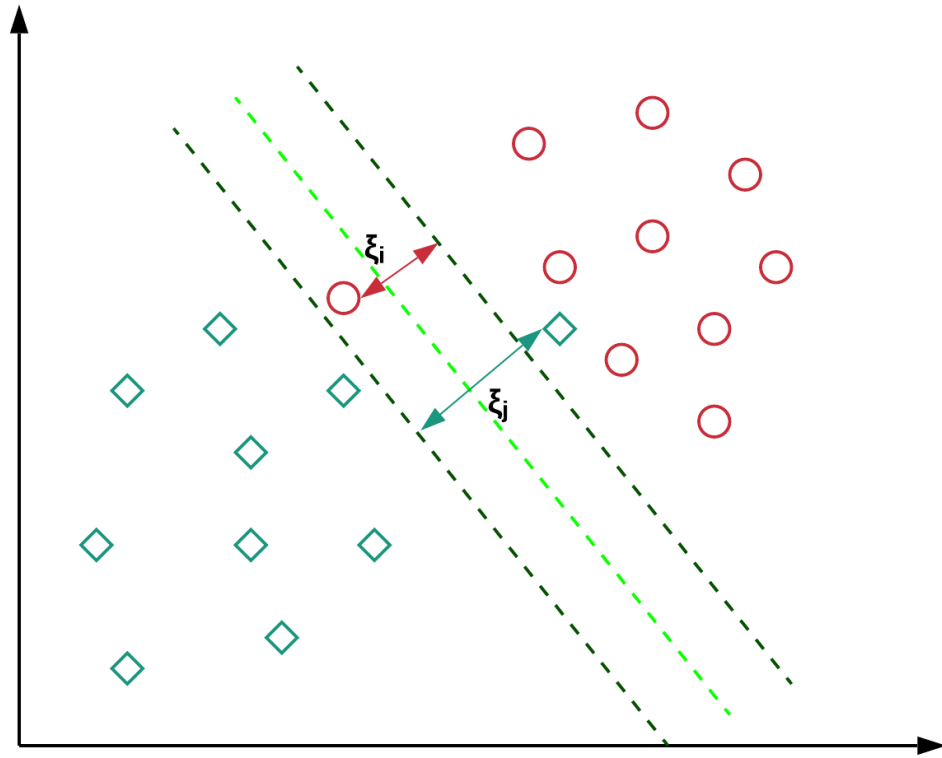
- Hyperplane: equivalent of line in higher dimensions (many features)
- A reasonable choice as the best hyperplane: the one that represents the largest separation, or margin, between the two classes. It is known as the maximum-margin hyperplane
- The linear classifier it defines is known as a maximum-margin classifier
- To compute such a hyperplane: define a cost function which increases if the hyperplane is “close” to any data point

Maximum-Margin Hyperplane



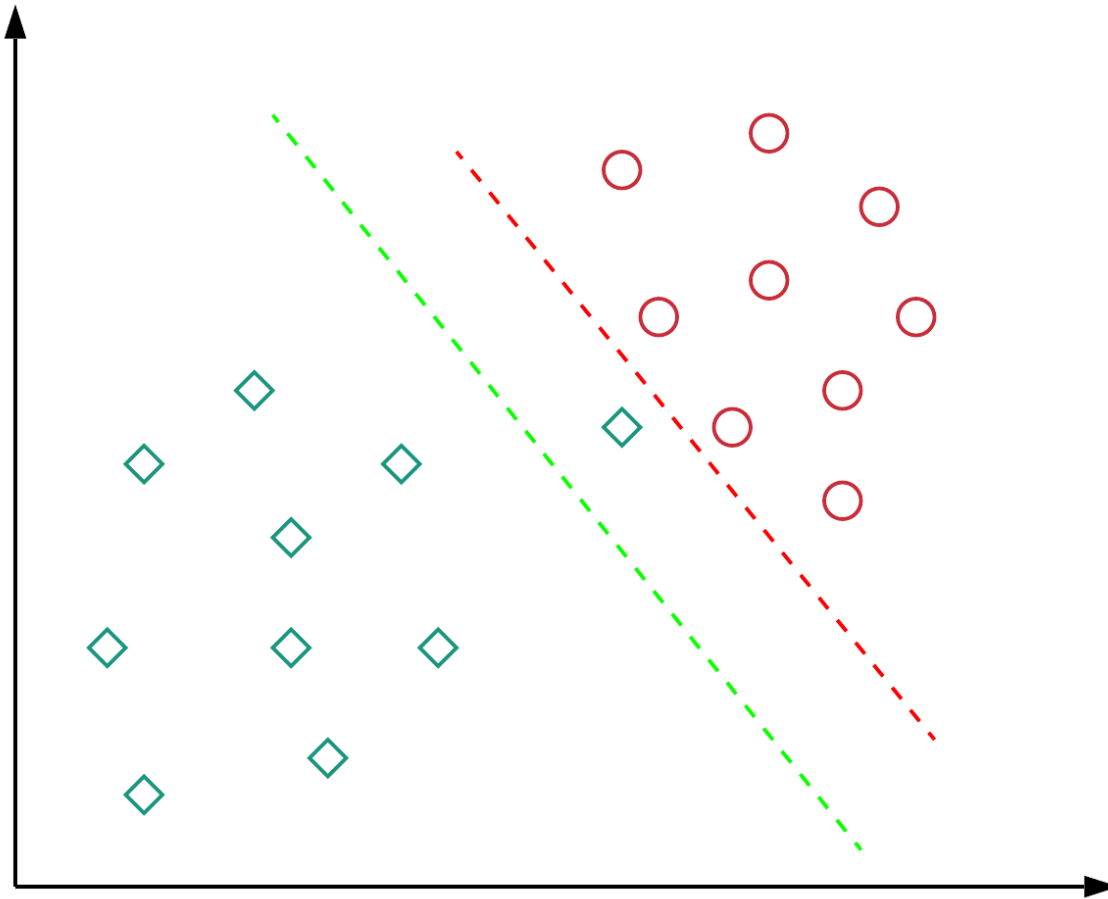
Soft-Margin SVMs

- Sometimes data may not be linearly separable
- Data points on the wrong side are known as outliers



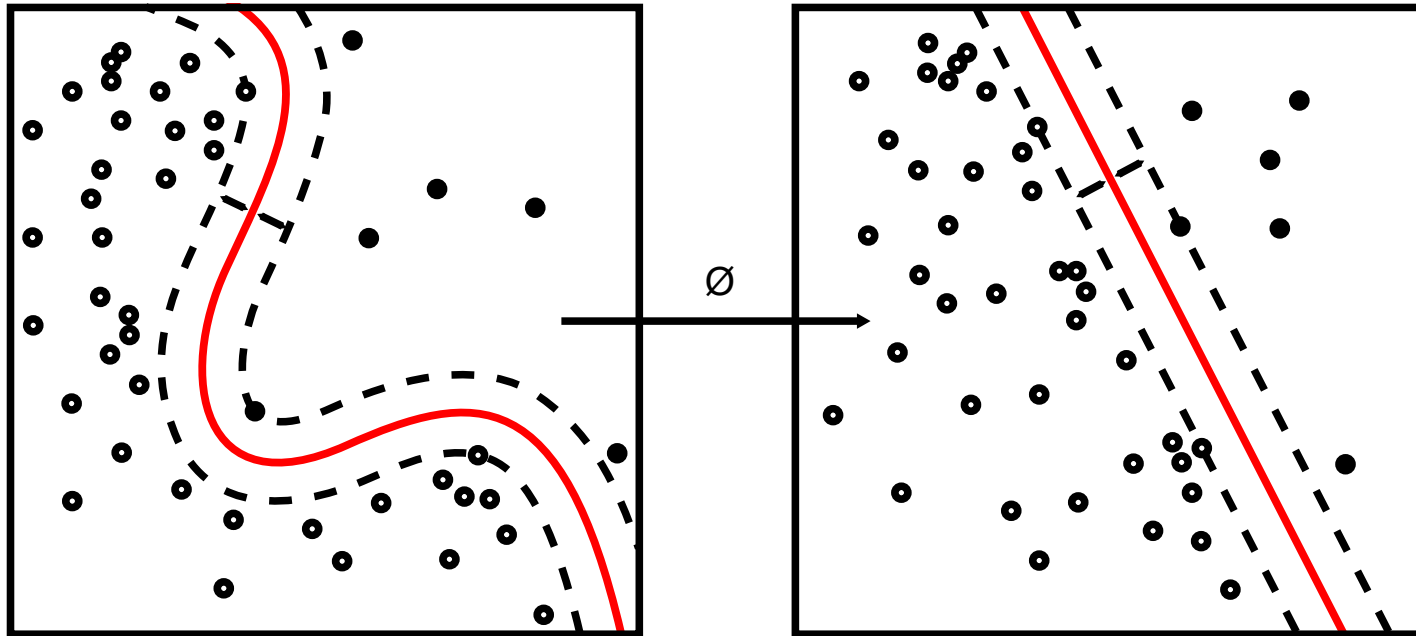
- To compute SVMs in such cases: we define a hinge loss function. Cost increases if the hyperplane: (a) doesn't separate the two classes, (b) is "close" to any data point

Outliers Maybe Acceptable



Green line maybe preferred over red since it has a higher margin (even though it results in 1 outlier) !!!

Nonlinear Classification



SVMs can be used for non-linear classification as well using so called “kernel functions”. These functions transform space which can change its shape.

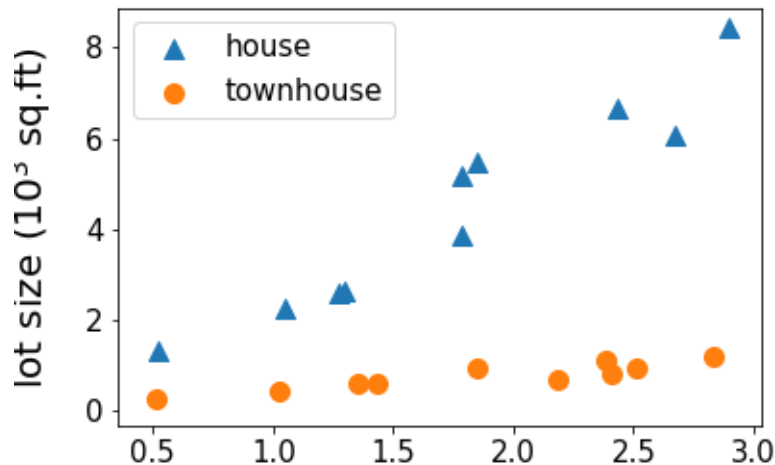
Uses: higher dimensional linear algebra, inner products, vector spaces....

Unsupervised Learning (Clustering)

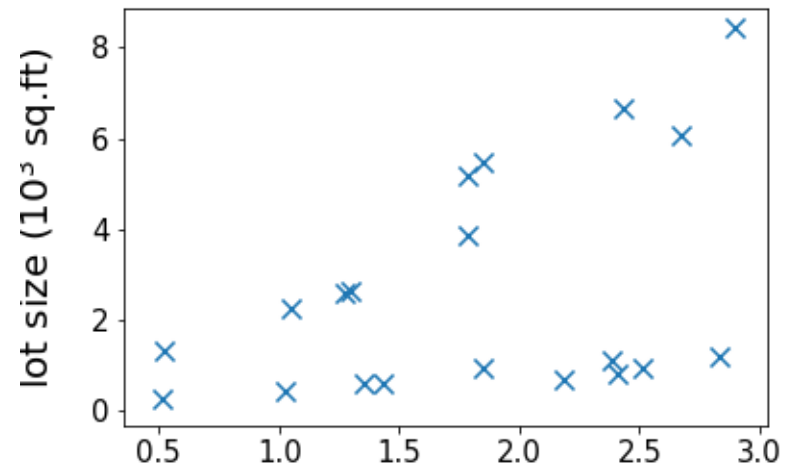
Unsupervised Learning

- Dataset contains **no labels**: $x^{(1)}, \dots, x^{(m)}$
- **Goal** (vaguely-posed): to find interesting structures in the data

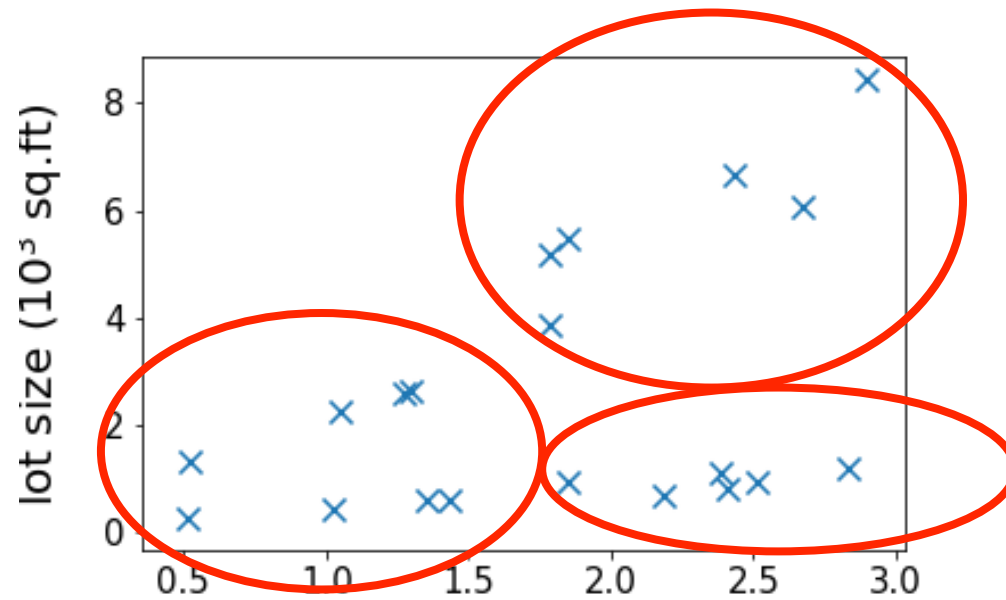
supervised



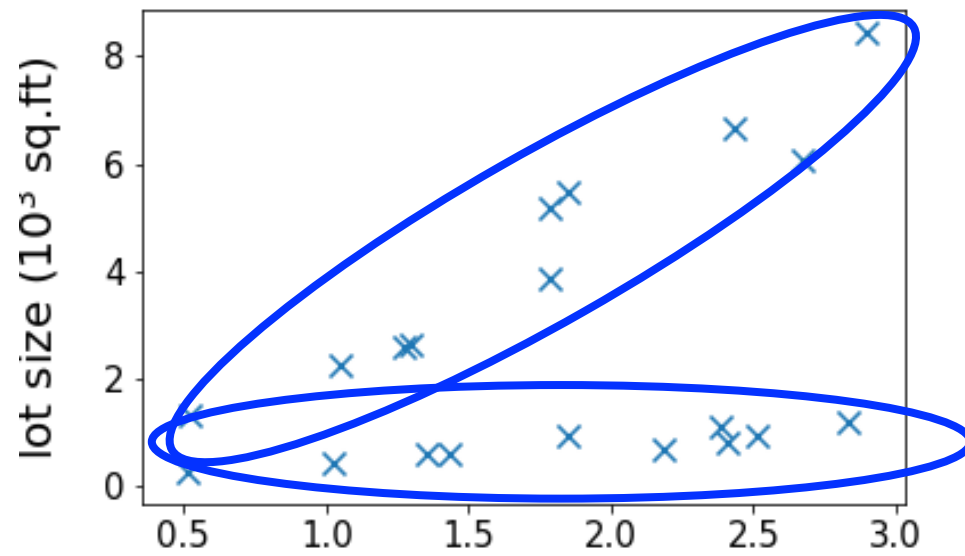
unsupervised



Clustering



Clustering



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Jacksonville



Rain
55°F



Today



57°F
47°F

Sun



61°F
45°F

Mon



62°F
47°F

Tue



67°F
53°F

Wed



72°F
56°F

C | F | K

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Fact check

[Did Kyrsten Sinema Bring Cake to the Senate and Vote Against Raising Minimum Wage?](#)

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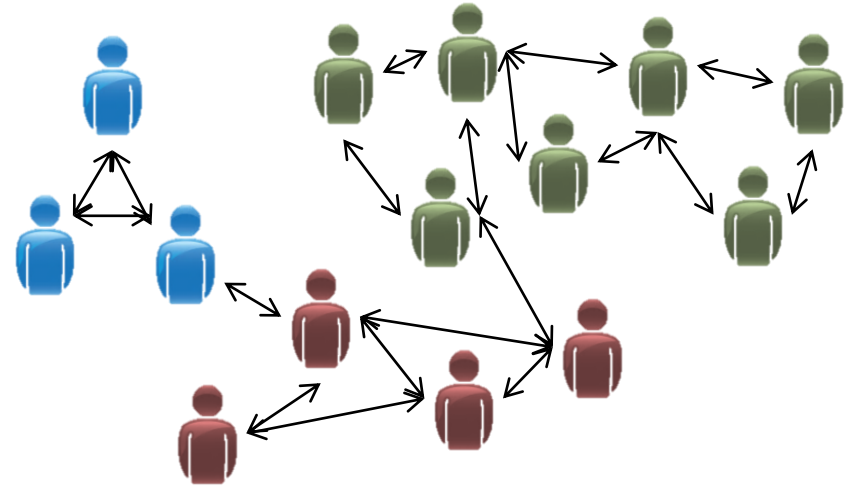
[Fitzgerald overstates claim on pork in COVID-19 relief bill](#)

[PolitiFact](#)

Other Examples



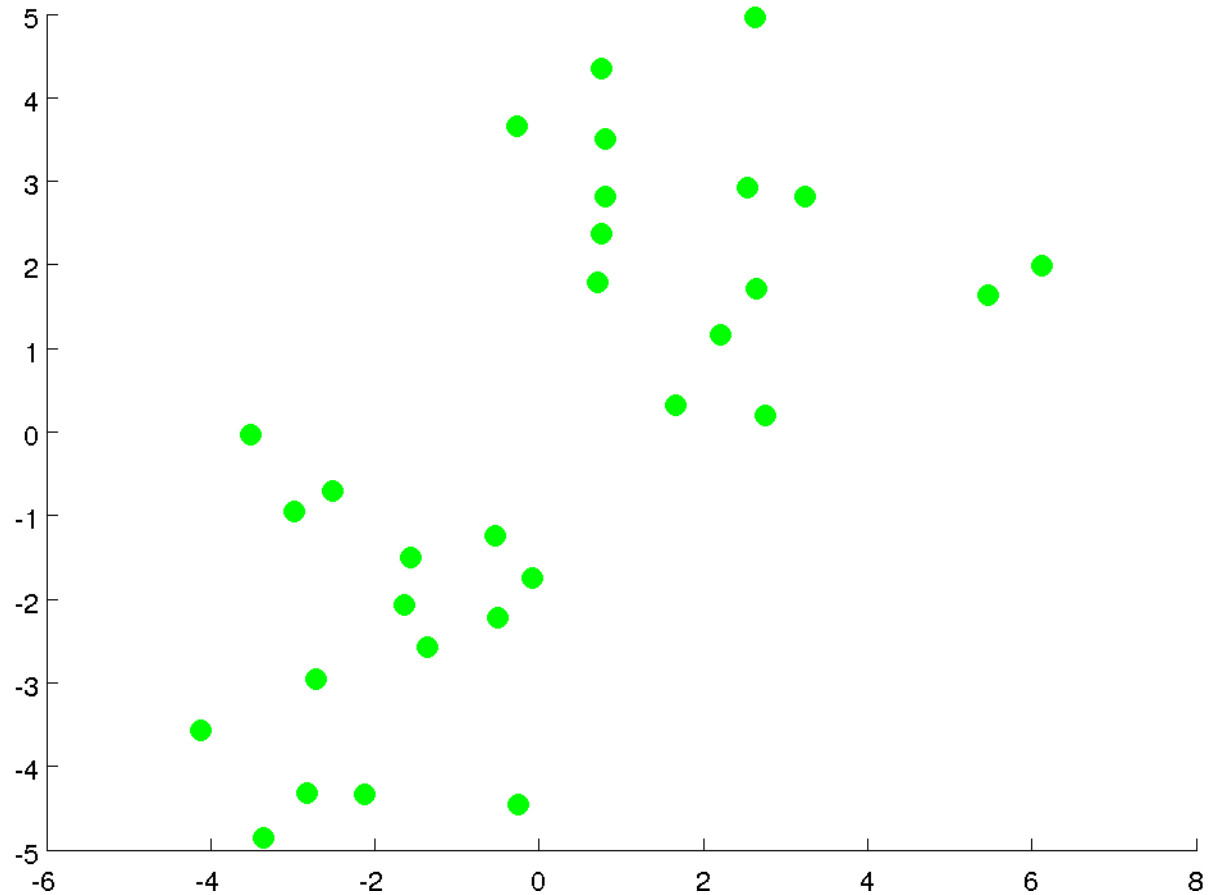
Clustering computer servers



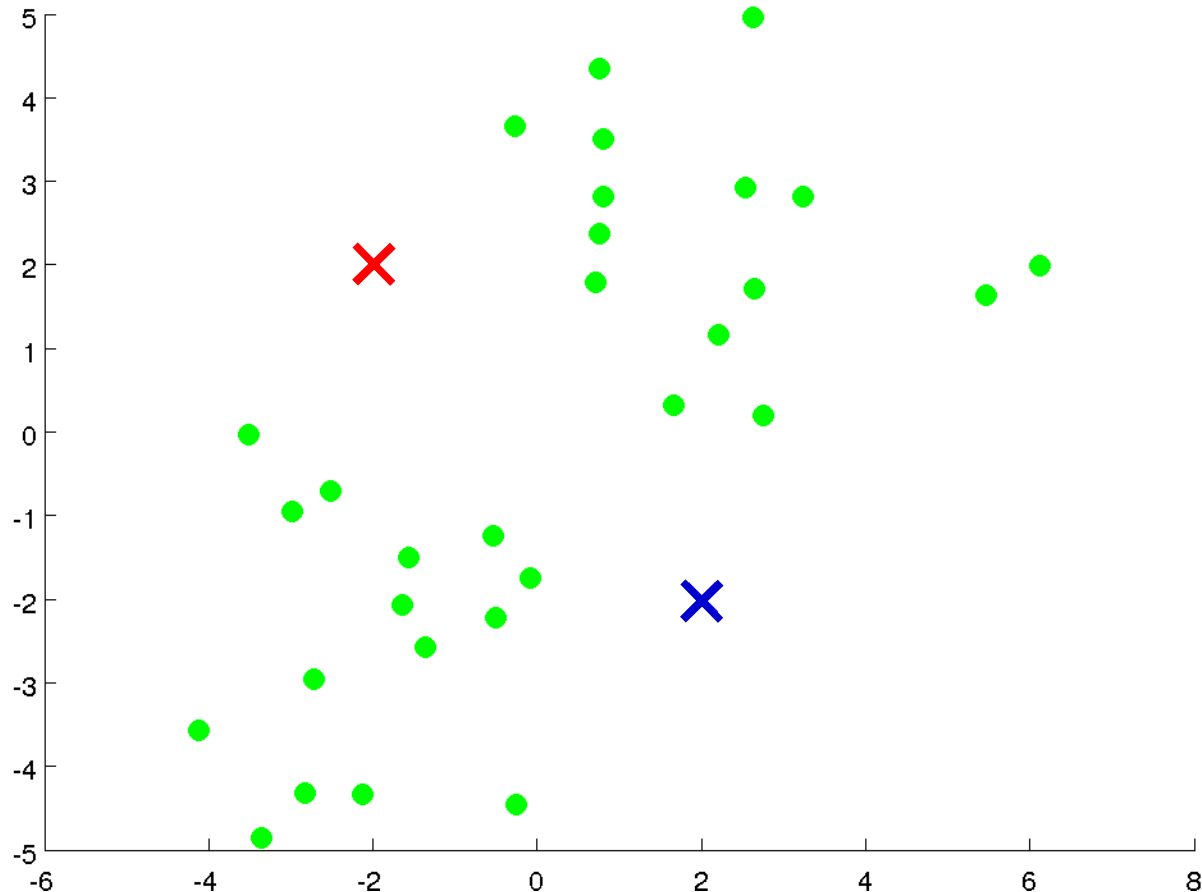
Clustering users in a
social network

K-means Clustering Algorithm

K-means Clustering

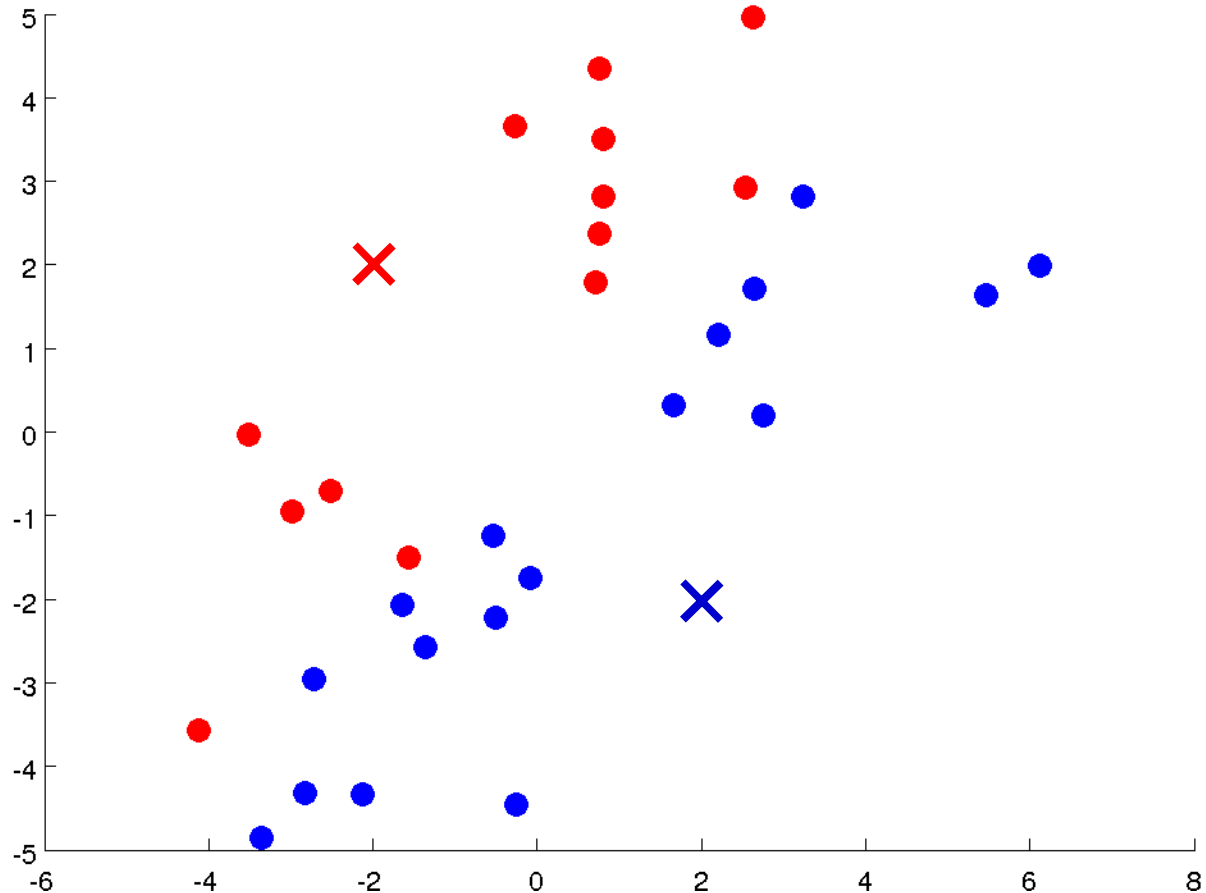


K-means Clustering



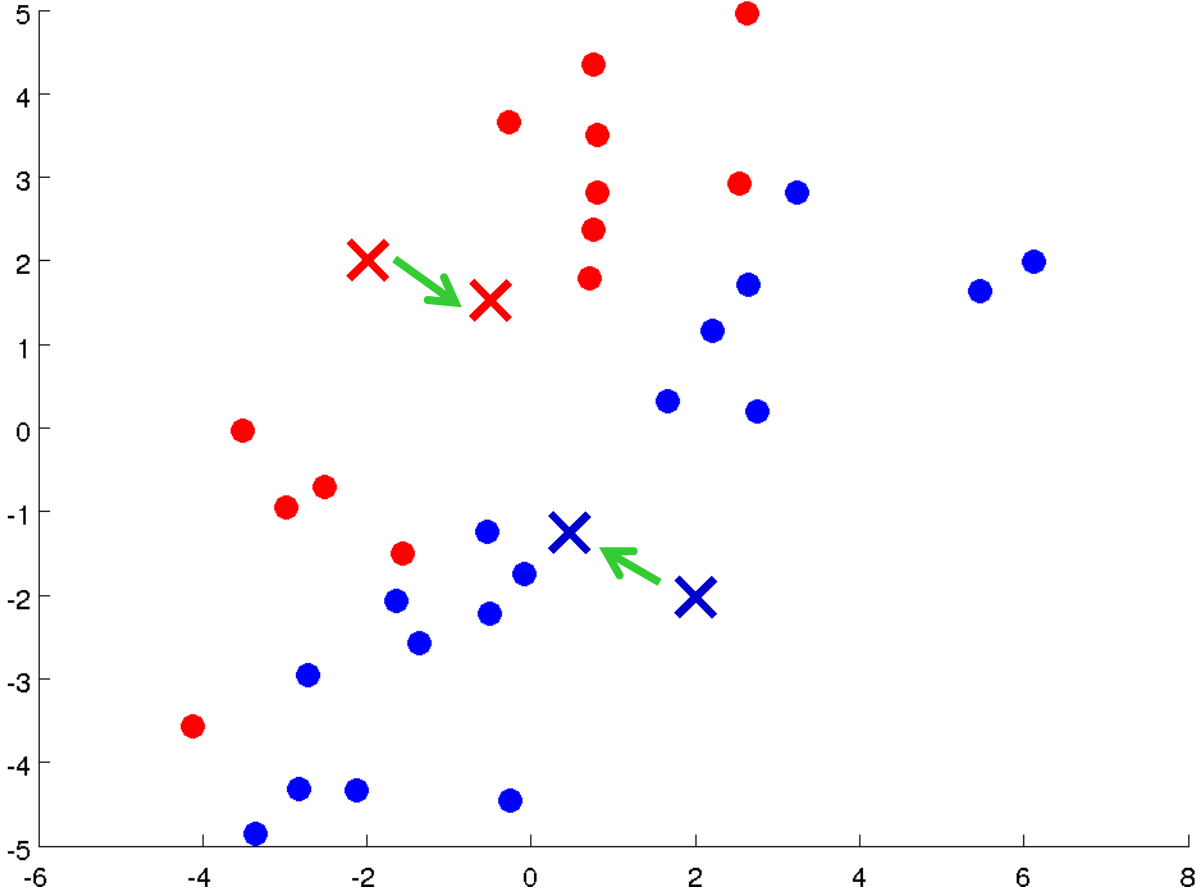
K= number of clusters. Start with centroid for each.

K-means Clustering



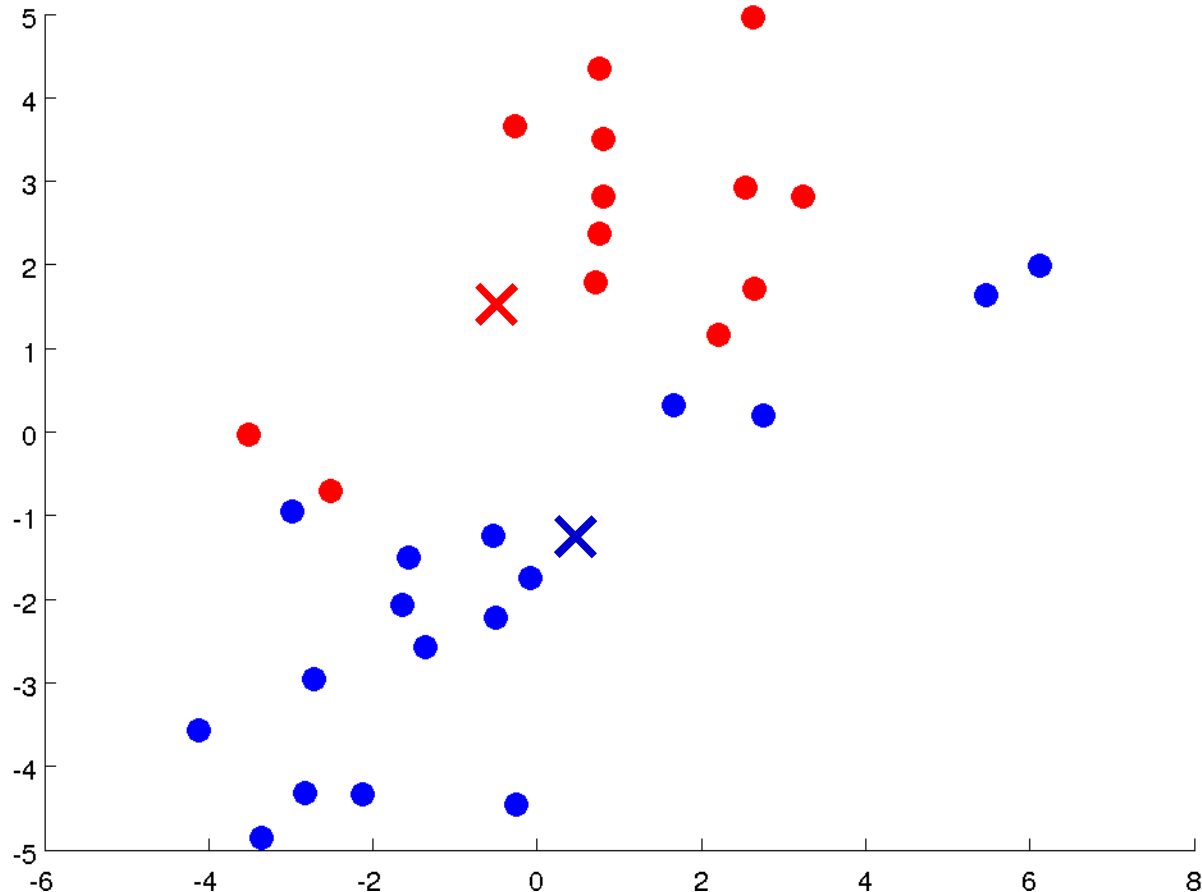
Match each point to the centroid which is “closer”

K-means Clustering



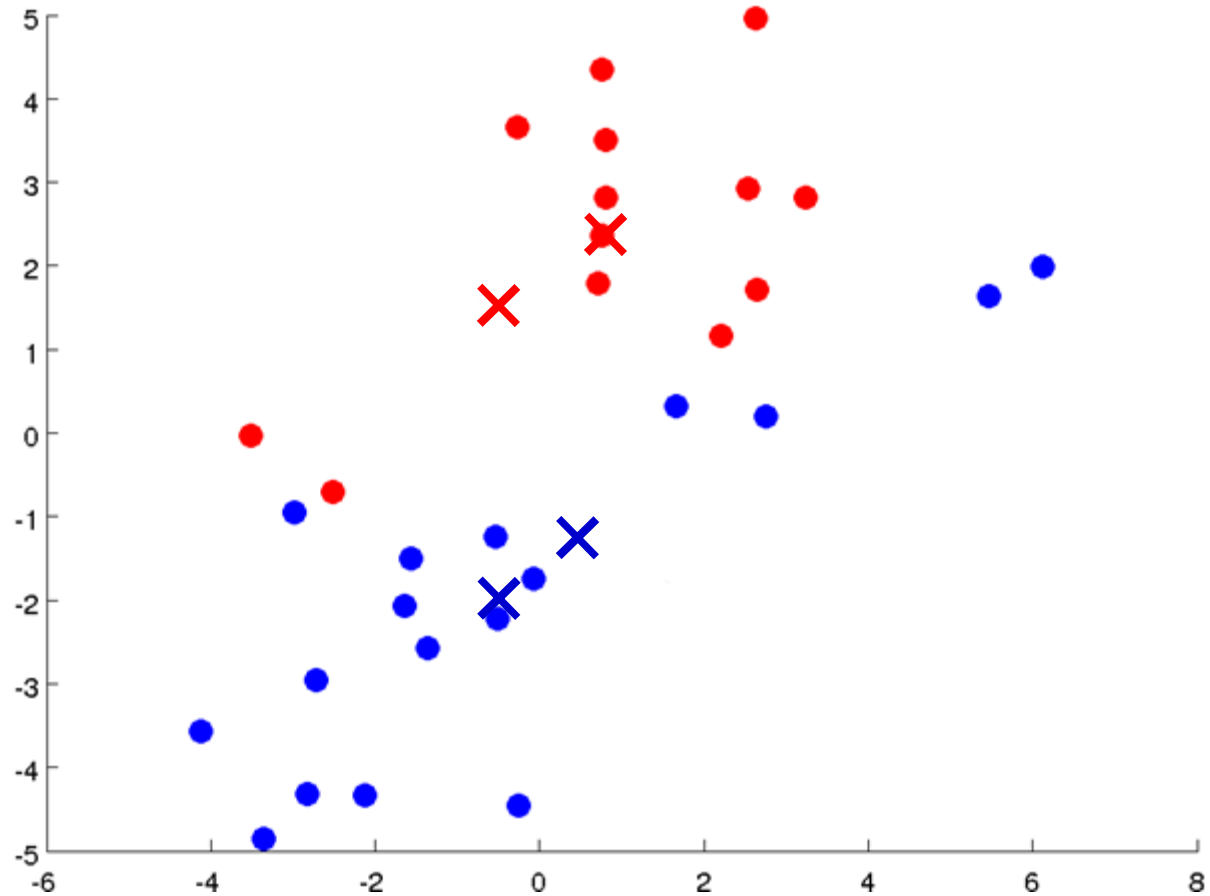
Compute new centroids as the “average” of each cluster

K-means Clustering

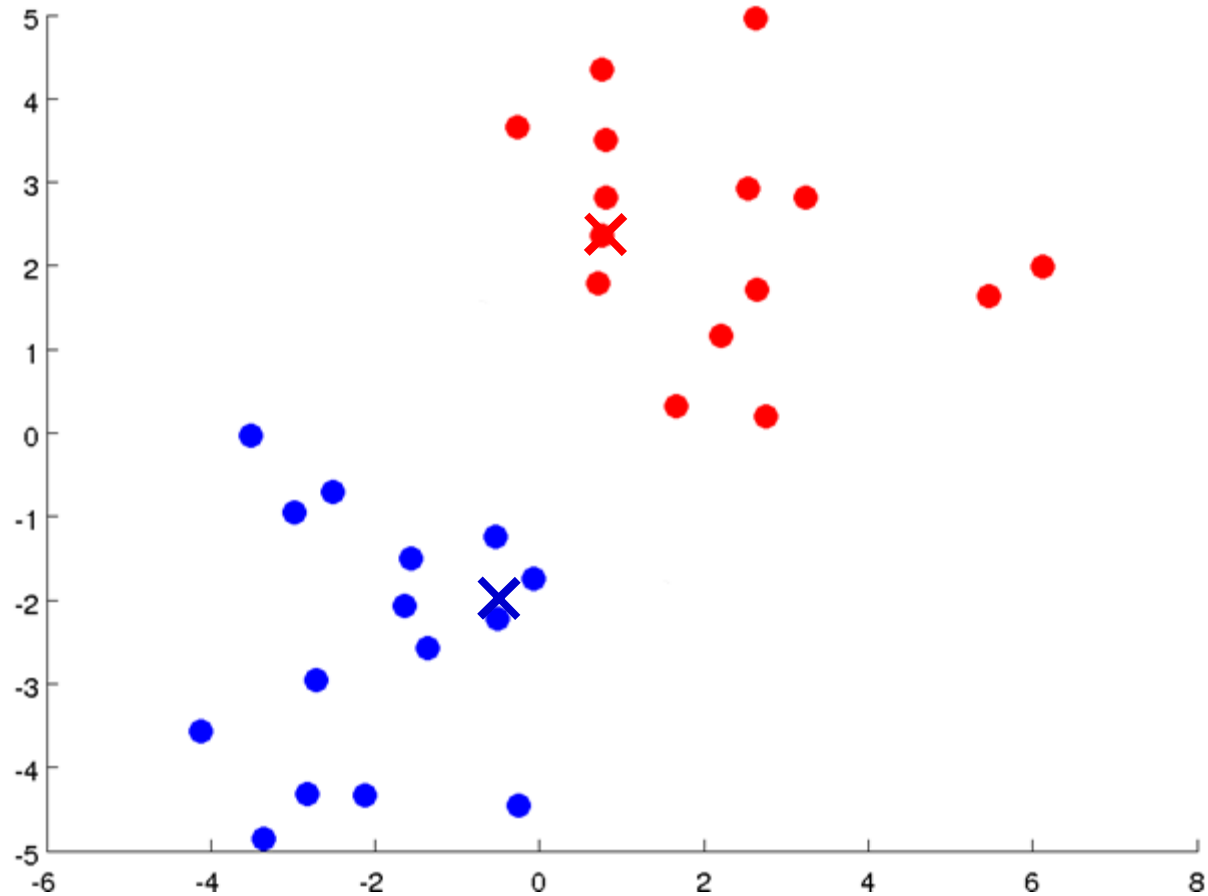


Restart with new centroids: Match each point to the centroid which is “closer”

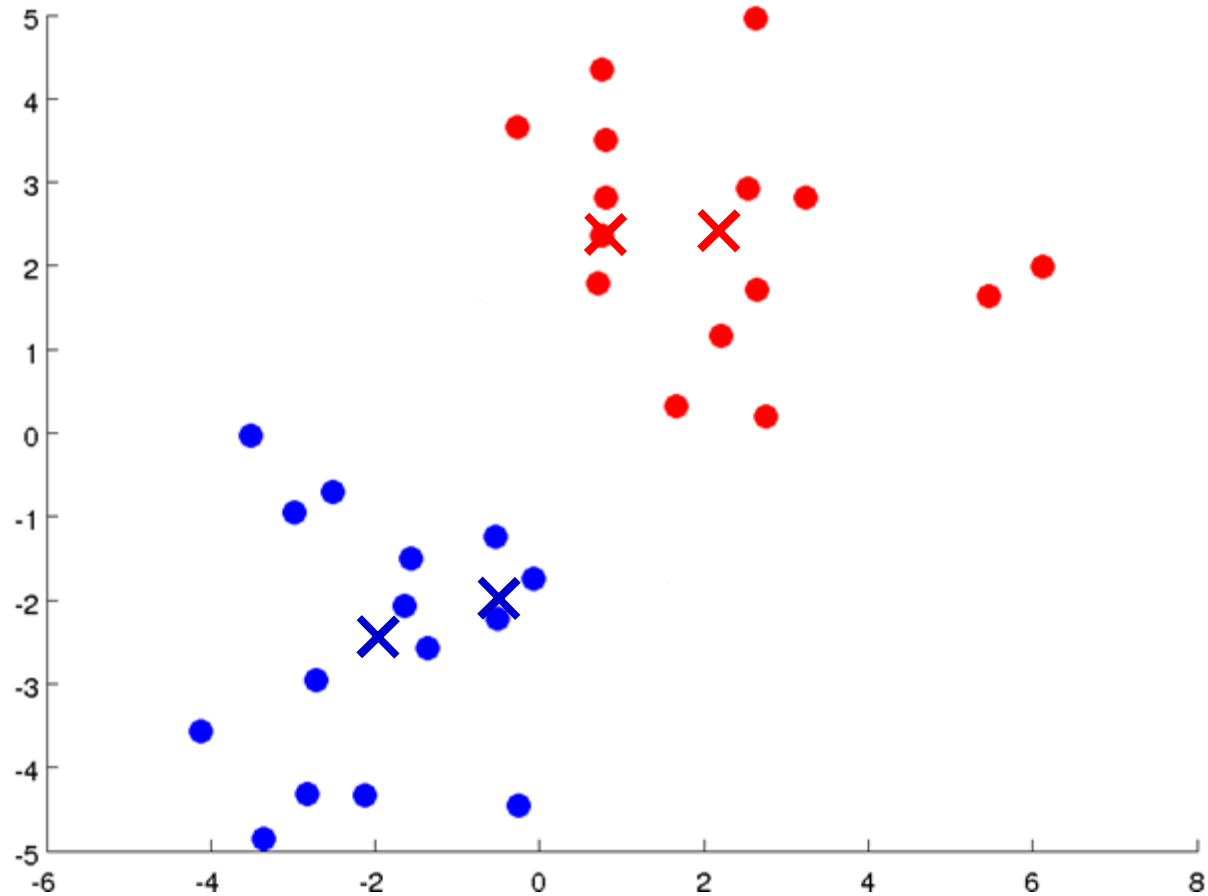
K-means Clustering



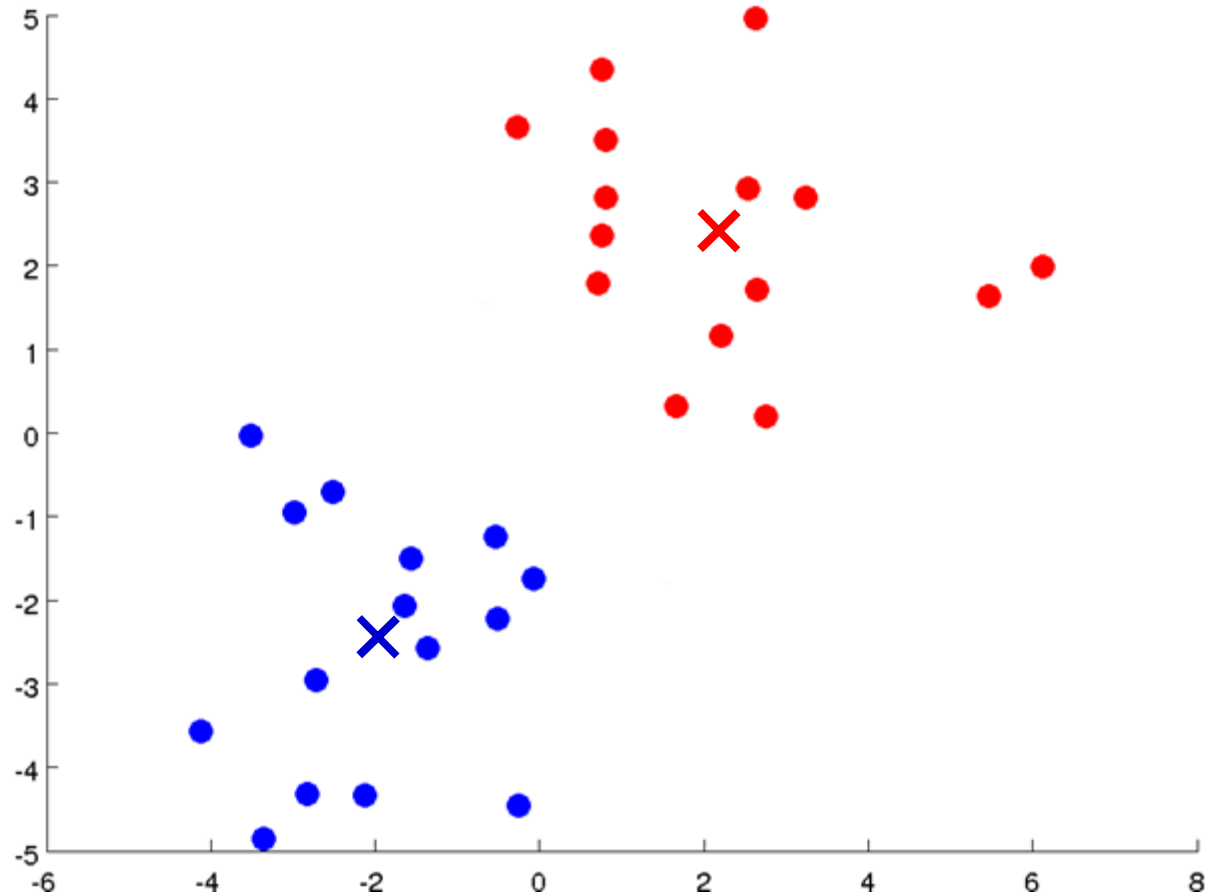
K-means Clustering



K-means Clustering



K-means Clustering



K-means Concepts

Input:

- K (number of clusters)
- Training set $\{x^{(1)}, x^{(2)}, \dots, x^{(m)}\}$ $x^{(i)} \in R^n$

(Algorithm running in n-dimensional space)

Compute distance: Take L_2 or Euclidean norm of the difference

$$x = (x_1, x_2, \dots, x_n)$$

$$y = (y_1, y_2, \dots, y_n)$$

$$\|x - y\| = \sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2 + \dots + (x_n - y_n)^2}$$

K-means Concepts

Input:

- K (number of clusters)
- Training set $\{x^{(1)}, x^{(2)}, \dots, x^{(m)}\}$ $x^{(i)} \in R^n$

(Algorithm running in n-dimensional space)

Taking average: Average of each coordinate

$$x = (x_1, x_2, \dots, x_n)$$

$$y = (y_1, y_2, \dots, y_n)$$

$$\text{average} = \left(\frac{x_1 + y_1}{2}, \frac{x_2 + y_2}{2}, \dots, \frac{x_n + y_n}{2} \right)$$

K-means Algorithm

Randomly initialize K cluster centroids $\mu_1, \mu_2, \dots, \mu_k \in R^n$

Repeat {

 for $i = 1$ to m

$c^{(i)} :=$ index (from 1 to K) of cluster centroid
 closest to $x^{(i)}$

 for $k = 1$ to K

$\mu_k :=$ average (mean) of points assigned to cluster k

}

K-means Optimization Objective

$c^{(i)}$ = index of cluster (1, 2,..., K) to which example $x^{(i)}$ is currently assigned

μ_k = cluster centroid k ($\mu_k \in R^n$)

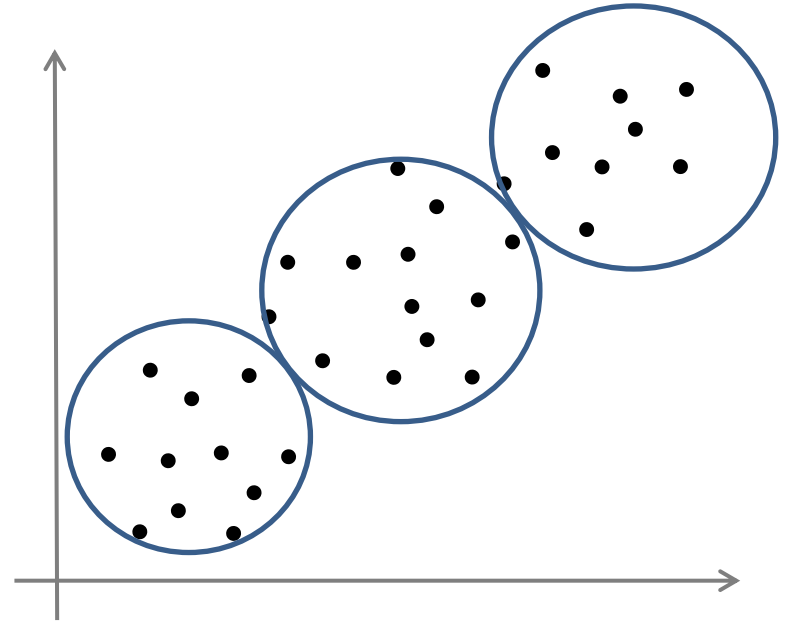
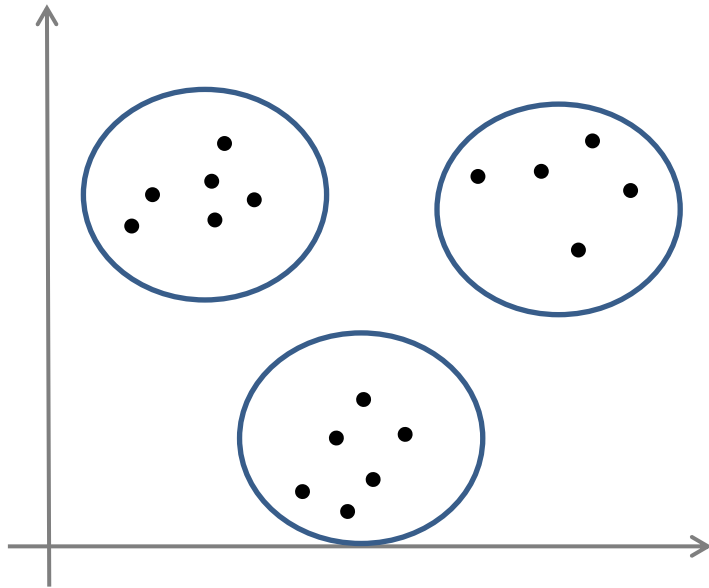
$\mu_{c^{(i)}}$ = cluster centroid of cluster to which example $x^{(i)}$ has been assigned

Optimization objective:

$$J(c^{(1)}, \dots, c^{(m)}, \mu_1, \dots, \mu_k) = \frac{1}{m} \sum_{i=1}^m \|x^{(i)} - \mu_{c^{(i)}}\|^2$$

$$\min_{\substack{c^{(1)}, \dots, c^{(m)}, \\ \mu_1, \dots, \mu_k}} J(c^{(1)}, \dots, c^{(m)}, \mu_1, \dots, \mu_k)$$

No Natural Clusters?



Questions?