#### APS1070

Foundations of Data Analytics and Machine Learning

Winter 2022

#### Week 10:

- Polynomial Regression
- Optimization and Convexity
- Regularization
- Classification
- Neural Networks



#### Slide Attribution

These slides contain materials from various sources. Special thanks to the following authors:

- Lisa Zhang
- Roger Grosse
- Jason Riordon

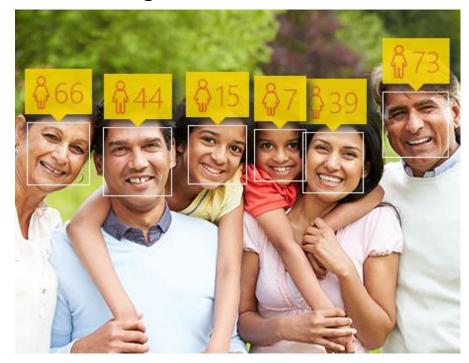
#### Last Time

- Linear Regression
  - Empirical Risk Minimization
  - Maximum Likelihood Estimation
    - ➤ Negative Log-likelihood

> Today we will continue with **nonlinear regression**.

## Nonlinear Regression

#### **Age Prediction**

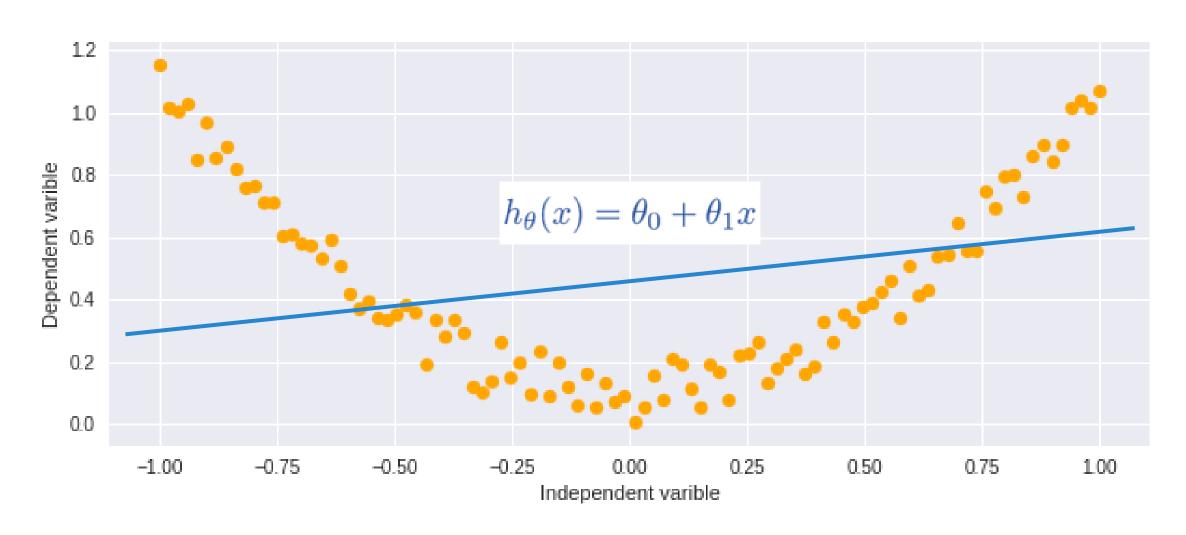


https://www.how-old.net/

#### **Stock Market Prediction**



#### Nonlinear Regression



### Agenda

- Polynomial Regression
- Convexity and Optimization
- Logistic Regression
- Gradient Descent
- Regularization
- Multiclass Classification
- Neural Networks

Theme:
Nonlinear Regression
(and Classification)

# Nonlinear Regression

#### Recap: Linear Regression

#### Hypothesis:

$$h_{\theta}(x) = \theta_0 + \theta_1 x$$

#### Parameters:

$$\theta_0, \theta_1$$

#### **Cost Function:**

$$J(\theta_0, \theta_1) = \frac{1}{2N} \sum_{i=1}^{N} (h_{\theta}(x^{(i)}) - y^{(i)})^2$$

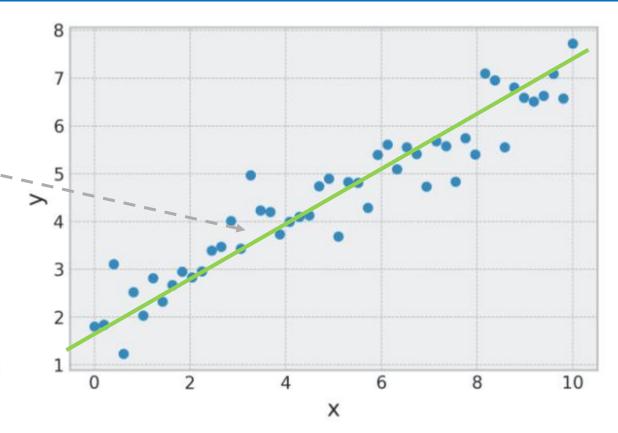
#### Goal:

minimize 
$$J(\theta_0, \theta_1)$$
  $\frac{dJ}{d\theta} = 0$  OR (2) gradient descent  $\theta \leftarrow \theta - \alpha \frac{\partial J}{\partial \theta}$ 

$$\frac{dJ}{d\theta} = 0$$

#### (2) gradient descent

$$\theta \leftarrow \theta - \alpha \frac{\partial J}{\partial \theta}$$



#### Recap: Vectorization

Hypothesis:

$$h_{\theta}(\mathbf{X}) = \mathbf{X}\mathbf{\theta}$$

Parameters:

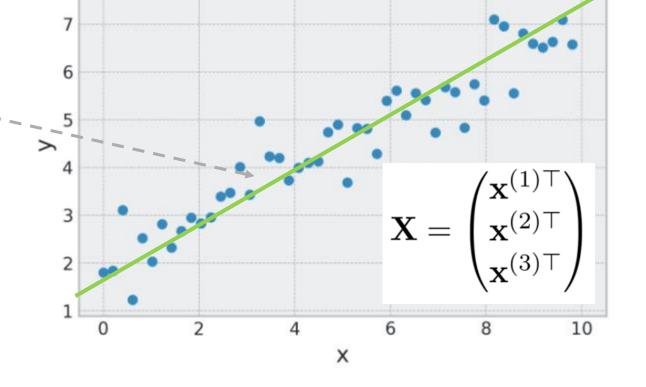
θ

**Cost Function:** 

$$\mathcal{J}(\theta) = \frac{1}{2N} \| \boldsymbol{y} - \widehat{\boldsymbol{y}} \|^2$$

Goal:

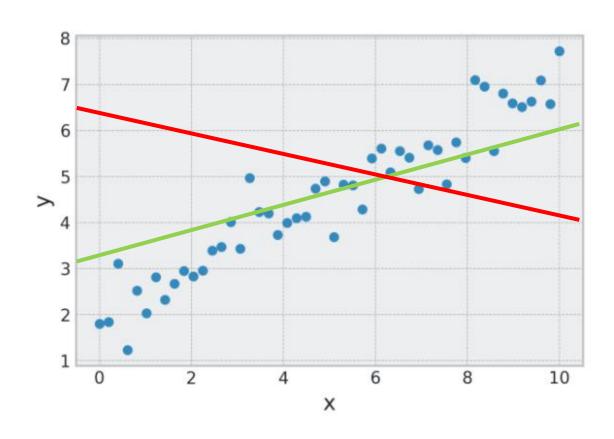
minimize 
$$J$$
 
$$\frac{dJ}{d\theta} = 0$$
 (1) direct solution

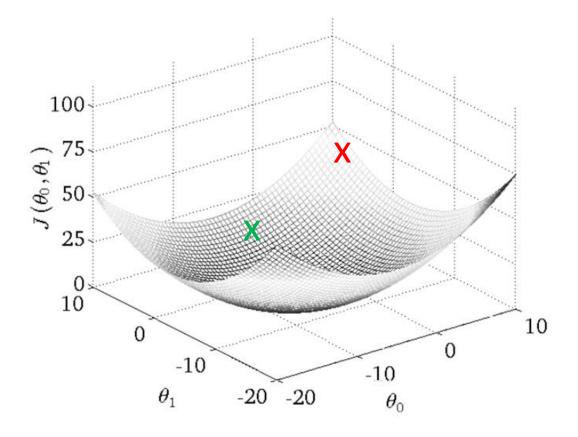


(2) gradient descent

$$\theta \leftarrow \theta - \alpha \frac{\partial J}{\partial \theta}$$

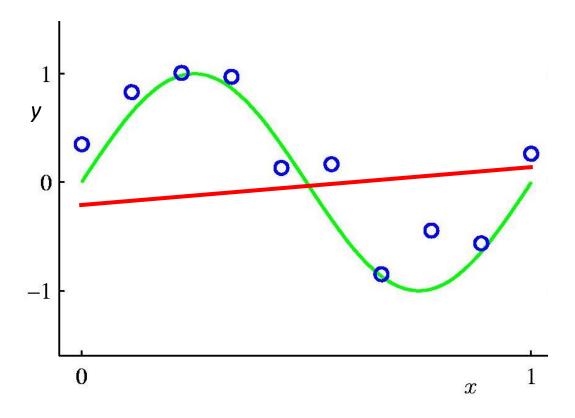
# Recap: Convexity





### Nonlinear Regression

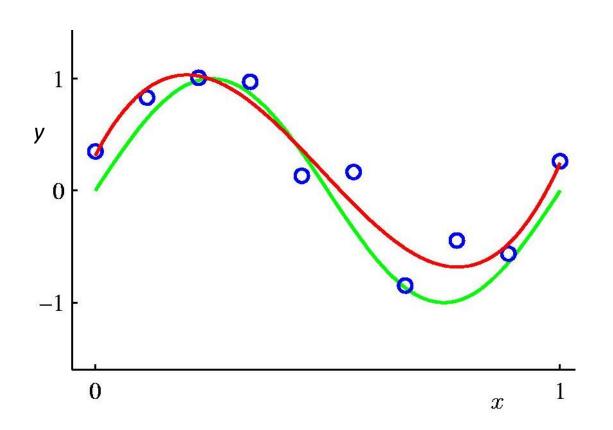
Suppose we want to model the following data



Given noisy sample data we want to find a hypothesis for what generated the data

> Cannot be fit with a linear model...

## Nonlinear Regression



**➢One option** is to fit a low-degree polynomial:

$$\hat{y} = \theta_3 x^3 + \theta_2 x^2 + \theta_1 x + \theta_0$$

This is known as polynomial regression

Q: Does this mean we have to derive a whole new algorithm?

#### Feature Mapping

➤ Implement a polynomial transformation (feature mapping) by replacing input with polynomial of increasing order:

$$\psi(x) = \begin{pmatrix} 1 \\ x \\ x^2 \\ x^3 \end{pmatrix}$$

Hence our hypothesis can be written as:

$$\hat{y} = \theta_3 x^3 + \theta_2 x^2 + \theta_1 x + \theta_0 (1)$$
$$\hat{y} = \mathbf{\theta}^T \psi(x)$$

The derivations and algorithms from last lecture remain the same! Why?

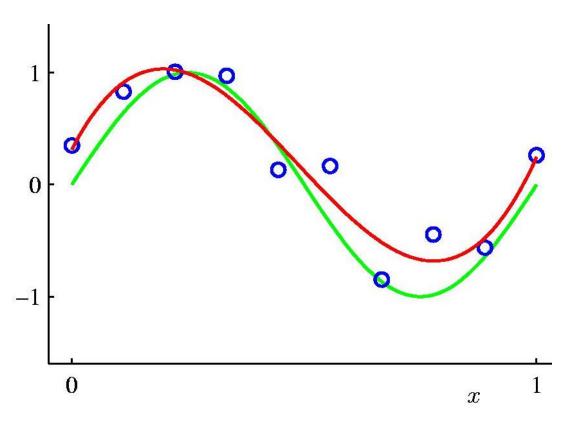
### Polynomial Regression

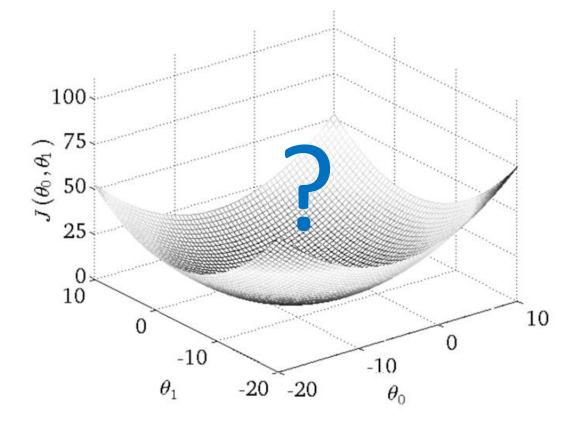
This doesn't require changing the algorithm, just **pretend**  $\psi(x)$  is the input vector.

$$\hat{y} = \theta^{\mathrm{T}} \psi(x) \qquad \psi(x) = \begin{pmatrix} 1 \\ x \\ x^2 \\ x^3 \end{pmatrix}$$

- > Feature maps let us fit nonlinear models
- ➤ Before deep learning, most of the effort in building a practical machine learning system was **feature engineering**.

# Q: Convexity of Polynomial Regression?





$$\hat{y} = \theta^{\mathrm{T}} \psi(x)$$

#### **Direct Solution**

➤ Polynomial regression is really a linear regression problem with some feature engineering.

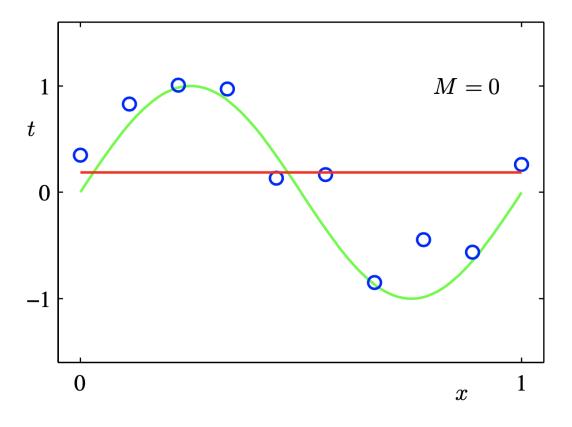
$$\widehat{y} = \theta^{T} \psi(x) \qquad \xrightarrow{\text{minimize cost}} \qquad \theta = (\psi^{T} \psi)^{-1} \psi^{T} y$$

$$\mathcal{J}(\theta) = \frac{1}{2N} \|y - \widehat{y}\|^{2} \qquad \qquad Requires that all columns are linearly independent$$

Require that  $\psi^T \psi \in \mathbb{R}^{D \times D}$  to be invertible. This is the case if and only if rank  $(\psi) = D$ .

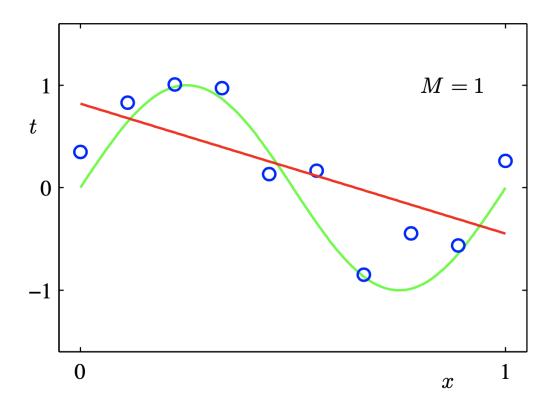
## Fitting Polynomial (M = 0)

$$\hat{y} = w_0$$



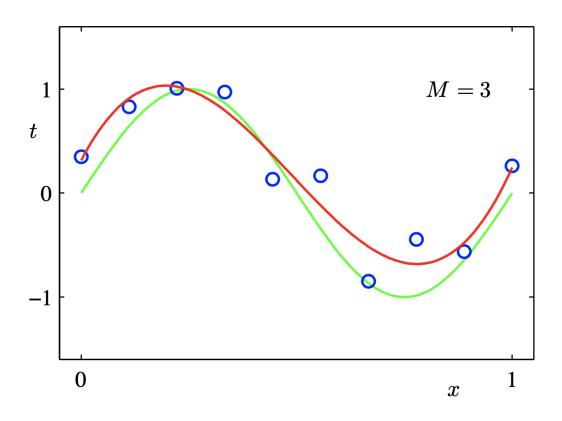
## Fitting Polynomial (M = 1)

$$\hat{y} = w_0 + w_1 x$$



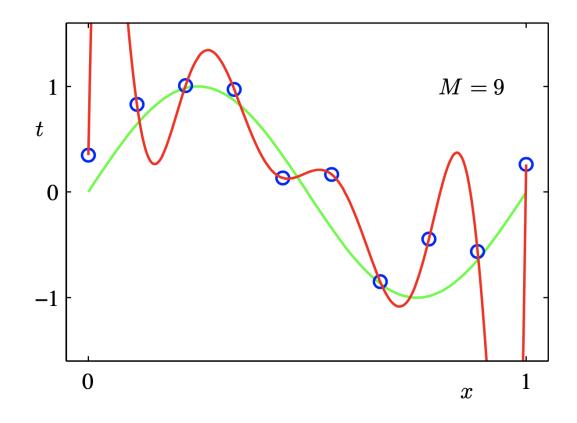
## Fitting Polynomial (M = 3)

$$\hat{y} = w_0 + w_1 x + w_2 x^2 + w_3 x^3$$



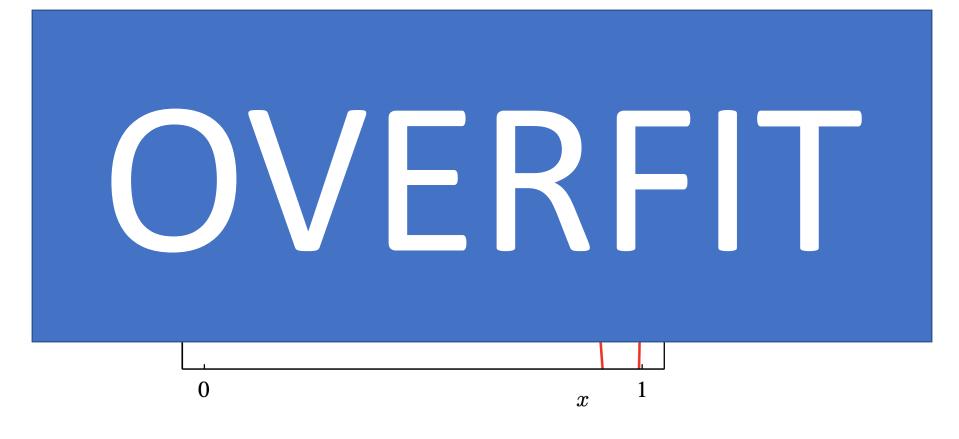
# Fitting Polynomial (M = 9)

$$\hat{y} = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + \ldots + w_9 x^9$$



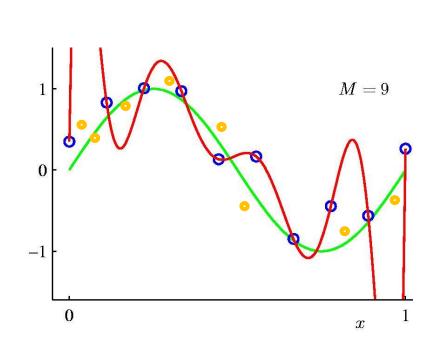
## Fitting Polynomial (M = 9)

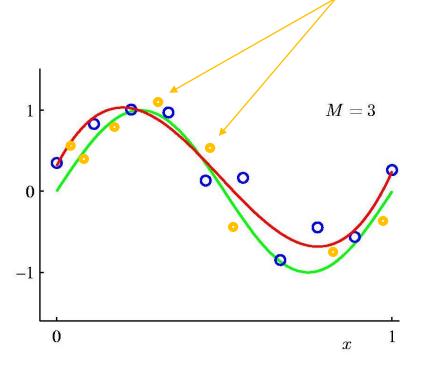
$$\hat{y} = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + \ldots + w_9 x^9$$



#### Generalize to New Samples

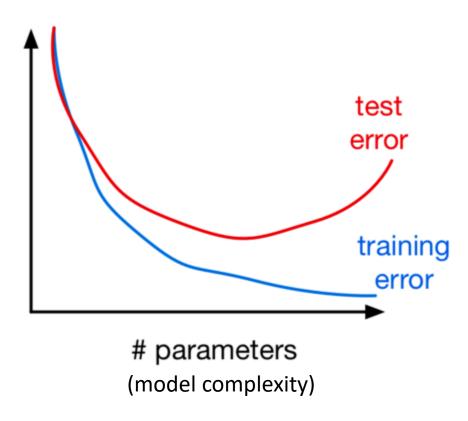
➤ We could give the hypothesis a higher complexity, or capacity to fit the data, but this may not generalize well to new samples





#### Generalization

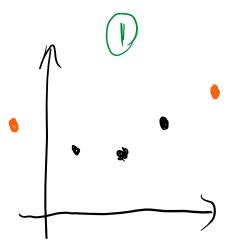
> Training and test error as a function of # parameters:



#### Generalization

> Training and test error as a function of # training examples:

Fixed model: Polynomial of degree 2



Training error: Zero

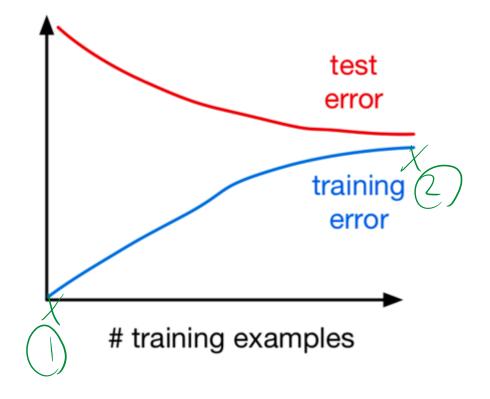
Test error: >>> 0

Their difference: Huge

Training error: Some nonzero value a

Test error: a+ε

Their difference: ε



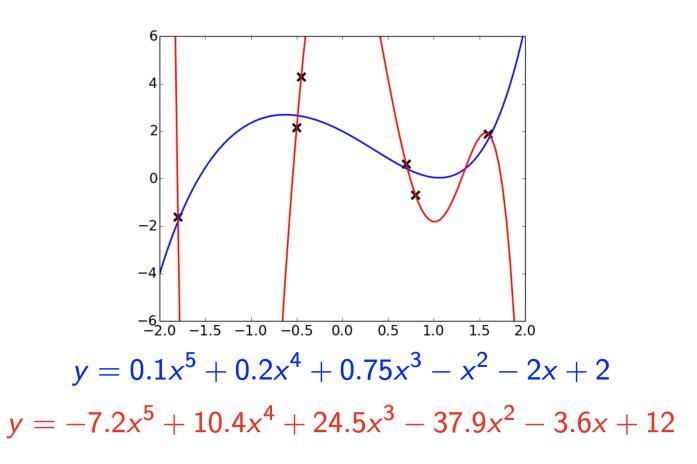
## Regularization

- The degree of the polynomial is a hyperparameter, just like k in KNN. We can tune it using a validation set.
- ➤ But restricting the size of a model is a crude solution, since you'll never be able to learn a more complex model, even if the data support it.

- >Another approach: keep the model flexible, but regularize it
  - Regularizer: a function that quantifies how much we prefer one hypothesis vs another

#### **Observation:**

polynomials that overfit often have large coefficients



- >Another reason we want parameters (weights) to be small:
  - Suppose inputs  $x_1$  and  $x_2$  are nearly identical for all training examples. The following two hypotheses make nearly the same predictions:

$$\mathbf{\theta}_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \mathbf{\theta}_2 = \begin{pmatrix} -9 \\ 11 \end{pmatrix}$$

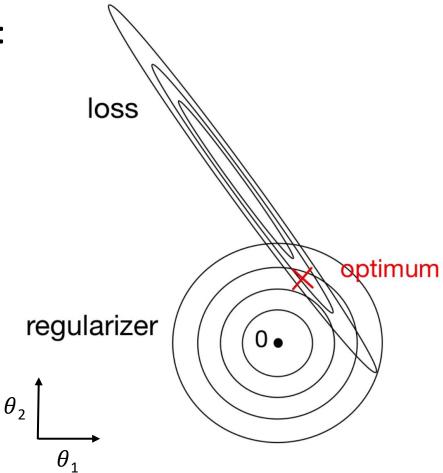
 $\triangleright$  But the second model might make weird predictions if the test distribution is slightly different (e.g.  $x_1$  and  $x_2$  match less closely).

We can encourage the parameters to be small by adding an  $L^2$  penalty (regularizer) to our cost function:

$$\frac{1}{2}\|\mathbf{\theta}\|^2 = \frac{1}{2}\sum_{j}\theta_{j}^2$$
 hyperparameter to be tuned 
$$\mathcal{J}_{reg} = \mathcal{J} + \frac{\lambda}{2}\sum_{j}\theta_{j}^2$$

The regularized cost function makes a tradeoff between fit to the data and the norm of the weights vector.

> The geometric picture:



$$\mathcal{J}(w,b) = \frac{1}{2N} \sum_{i=1}^{N} (y^{(i)} - t^{(i)})^2$$

• We can encourage the weights to be small by choosing as our regularizer the  $L^2$  penalty.

$$\mathcal{R}(\mathbf{w}) = \frac{1}{2} \|\mathbf{w}\|^2 = \frac{1}{2} \sum_j w_j^2.$$

- Note: to be pedantic, the  $L^2$  norm is Euclidean distance, so we're really regularizing the squared  $L^2$  norm.
- The regularized cost function makes a tradeoff between fit to the data and the norm of the weights.

$$\mathcal{J}_{ ext{reg}} = \mathcal{J} + \lambda \mathcal{R} = \mathcal{J} + rac{\lambda}{2} \sum_{j} w_{j}^{2}$$

• Here,  $\lambda$  is a hyperparameter that we can tune using a validation set.

• Recall the gradient descent update:

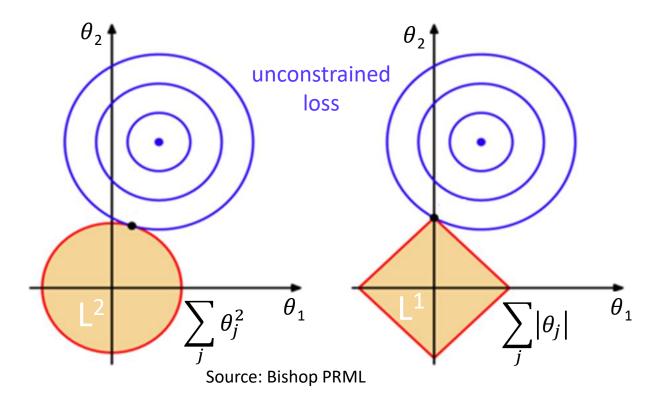
$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \frac{\partial \mathcal{J}}{\partial \mathbf{w}}$$

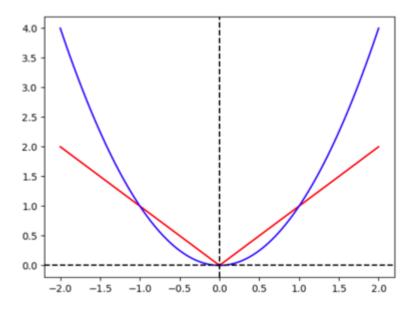
 The gradient descent update of the regularized cost has an interesting interpretation as weight decay:

$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \left( \frac{\partial \mathcal{J}}{\partial \mathbf{w}} + \lambda \frac{\partial \mathcal{R}}{\partial \mathbf{w}} \right)$$
$$= \mathbf{w} - \alpha \left( \frac{\partial \mathcal{J}}{\partial \mathbf{w}} + \lambda \mathbf{w} \right)$$
$$= (1 - \alpha \lambda) \mathbf{w} - \alpha \frac{\partial \mathcal{J}}{\partial \mathbf{w}}$$

### L<sup>1</sup> vs L<sup>2</sup> Regularization

 $\triangleright$  The  $L^1$  norm (or sum of absolute values) is another regularizer that encourages weights to be exactly zero.

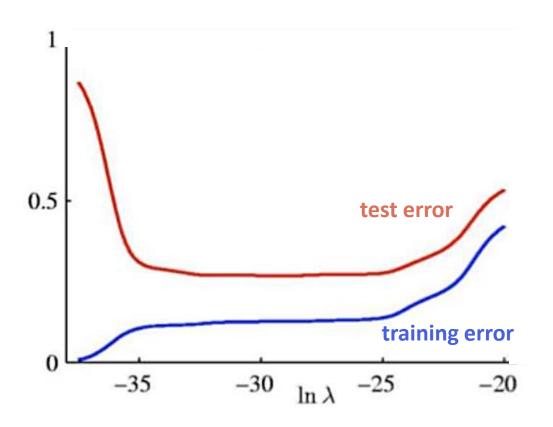




L1-regularization tends to push parameters to zero

#### Generalization

 $\triangleright$  Training and test error as a function of regularization parameter  $\lambda$ :



	$\ln \lambda = -\infty$	$\ln \lambda = -18$	$\ln \lambda = 0$
$\theta_0$	0.35	0.35	0.13
$ heta_{ exttt{1}}$	232.37	4.74	-0.05
$\theta_2$	-5321.83	-0.77	-0.06
$\theta_3$	48568.31	-31.97	-0.05
$ heta_4$	-231639.30	-3.89	-0.03
$\theta_{5}$	640042.26	55.28	-0.02
$ heta_{6}$	-1061800.52	41.32	-0.01
$\theta_7$	1042400.18	-45.95	-0.00
$\theta_8$	-557682.99	-91.53	0.00
$\theta_9$	125201.43	72.68	0.01

#### Ineffective Batch Size

> Q: What happens if the batch size is too small? Too large?

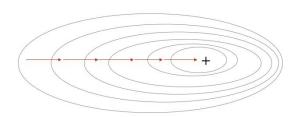
#### > Too large:

- Computationally expensive
- Average loss might not change very much as batch size grows

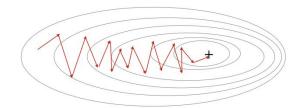
#### > Too small:

- We optimize a (possibly very) different loss function at each iteration
- Noisy
- SGD may actually take longer

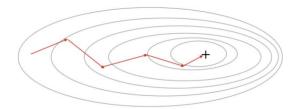
Gradient Descent



Stochastic Gradient Descent



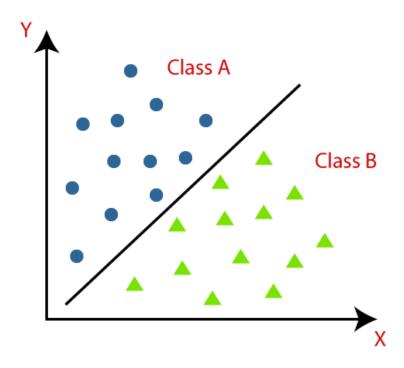
Mini-Batch Gradient Descent



#### Classification

#### Overview

- Classification: predicting a discretevalued target
- ➤ Binary classification: number of target values is 2 (binary-valued)
- > Examples:
  - predict where a patient has a disease given presence or absence of various symptoms
  - classify e-mails as spam or non-spam
  - predict whether a financial transaction is fraudulent



# Binary Classification

➤ We can start with our linear function of x, but now we introduce a threshold :

$$\mathbf{z} = \mathbf{\theta}^{\mathrm{T}} \mathbf{x} + b$$

$$\hat{y} = \begin{cases} 1 & \text{if } z \ge r \\ 0 & \text{if } z < r \end{cases}$$

# **Binary Classification**

- Eliminating the threshold
  - $\triangleright$  Can make the threshold r = 0 without loss of generality.

$$\mathbf{\theta}^{\mathrm{T}}\mathbf{x} + b \ge 0 \qquad \mathbf{\theta}^{\mathrm{T}}\mathbf{x} + b - r \ge 0$$

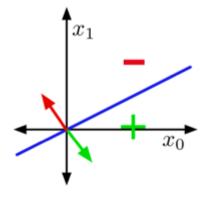
- Eliminating the bias
  - $\triangleright$  Add a dummy feature  $x_0$  which always takes the value 1. The weight  $\theta_0$  is equivalent to the bias.

$$\mathbf{z} = \mathbf{\theta}^{\mathrm{T}} \mathbf{x} \qquad \qquad \hat{y} = \begin{cases} 1 & \text{if } z \ge 0 \\ 0 & \text{if } z < 0 \end{cases}$$

### The Geometric Picture

- > Here we're visualizing the logical NOT example
- Training examples are points
- Hypothesis are half-spaces whose boundaries pass through the origin
- > This boundary is the decision boundary
  - In 2-D it's a line, but think of it as a hyperplane
- ➤ If the training examples can be separated by a linear decision rule, they are linearly separable.

Input Space, or Data Space:



#### NOT

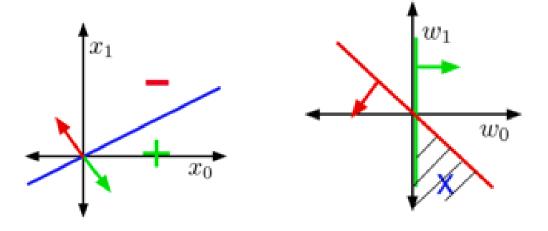
<i>X</i> <sub>0</sub>	<i>x</i> <sub>1</sub>	t
1	0	1
1	1	0

### The Geometric Picture

- Hypotheses are points
- Training examples are half-spaces whose boundaries pass through the origin
- The region satisfying all the constraints is the feasible region; if this region is nonempty, the problem is feasible

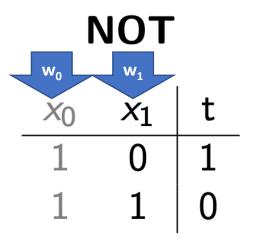
How do you optimize?

Weight Space



$$w_0 > 0$$

# Example 1



# Example 2

#### **AND**

<i>X</i> <sub>0</sub>	$x_1$	<i>X</i> <sub>2</sub>	t
1	0	0	0
1	0	1	0
1	1	0	0
1	1	1	1

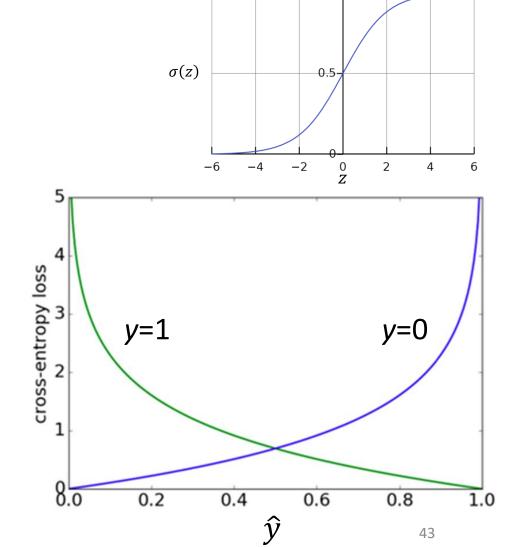
# Logistic Regression

$$\mathbf{z} = \mathbf{\theta}^{\mathrm{T}} \mathbf{x}$$

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

- Because the prediction  $\hat{y} \in [0, 1]$ , we can interpret it as the estimated probability that the label is positive (y = 1).
- Cross-entropy loss captures this intuition:

$$\mathcal{L}_{CE}(\hat{y}, y) = \begin{cases} -\log \hat{y} & \text{if } y = 1\\ -\log(1 - \hat{y}) & \text{if } y = 0 \end{cases}$$
$$= -y \log \hat{y} - (1 - y) \log(1 - \hat{y})$$



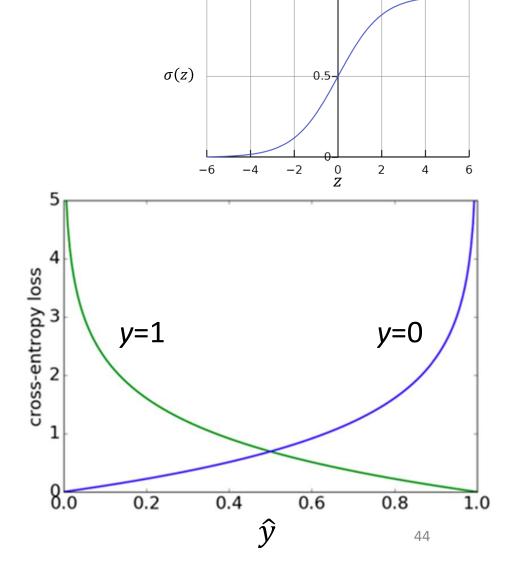
# Logistic Regression with Cross-entropy Loss

$$z = \mathbf{\theta}^{T} \mathbf{x}$$

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

➤ Being 99% confident in the wrong answer is much more wrong than being only 90% confident.

$$\mathcal{L}_{CE}(\hat{y}, y) = -y \log \hat{y} - (1 - y) \log(1 - \hat{y})$$



# Logistic Regression with Cross-entropy Loss

**Computation Problem:** 

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

If  $\hat{y} = \sigma(z)$  gets too close to 0 or 1, it may cause very subtle and hard-to-find bugs:

$$\hat{y} = \sigma(z)$$
  $\Rightarrow \hat{y} \approx 0$   $\mathcal{L}_{CE}(\hat{y}, y) = -y \log \hat{y} - (1 - y) \log(1 - \hat{y}) \Rightarrow \text{computes log } 0$ 

➤ Instead, we combine the activation function and the loss into a single logistic-cross-entropy function.

$$\mathcal{L}_{LCE}(\sigma(z), y) = y \log(1 + e^{-z}) + (1 - y) \log(1 + e^{z})$$

# Example:

$$\mathcal{L}_{CE}(\hat{y}, y) = -y \log \hat{y} - (1 - y) \log(1 - \hat{y})$$
  $\sigma(z) = \frac{1}{1 + e^{-z}}$ 

$$\mathcal{L}_{LCE}(\sigma(z), y) = y \log(1 + e^{-z}) + (1 - y) \log(1 + e^{z})$$

# Weight Updates

- Comparison of gradient descent updates:
  - > Linear regression:

$$\mathbf{\theta} \leftarrow \mathbf{\theta} - \frac{\alpha}{N} \sum_{i=1}^{N} (\hat{y}^{(i)} - y^{(i)}) \mathbf{x}^{(i)}$$

Logistic regression:

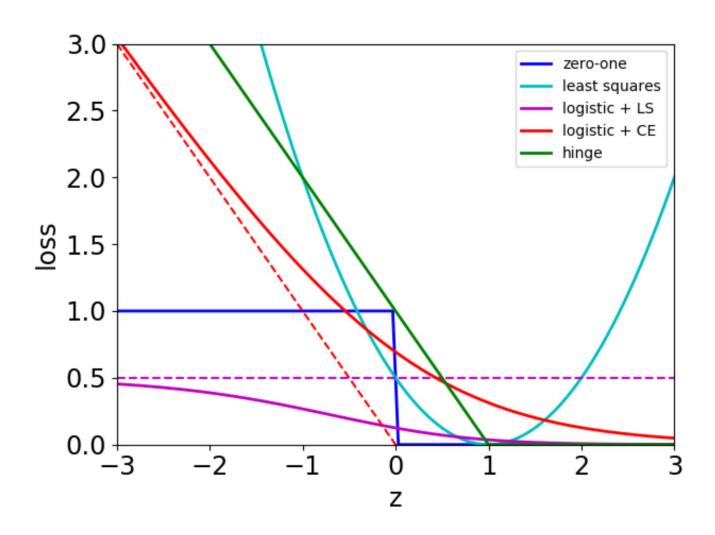
$$\mathbf{\theta} \leftarrow \mathbf{\theta} - \frac{\alpha}{N} \sum_{i=1}^{N} (\hat{y}^{(i)} - y^{(i)}) \mathbf{x}^{(i)}$$

$$z = \mathbf{\theta}^{\mathrm{T}} \mathbf{x} + b$$

Using activation function

$$\hat{y} = \frac{1}{1 + e^{-z}}$$

# Loss Summary

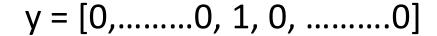


## Multiclass Classification

### **Multiclass Classification**

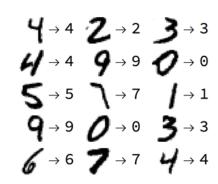
➤ What about classification task with more than two categories?

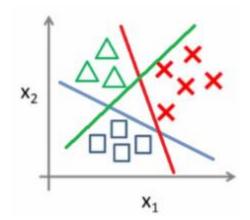
- Targets form a discrete set {1, ..., K}
- It's often more convenient to represent them as one-hot vectors or a one-of-K encoding:











### Multiclass Classification

- Now there are D input dimensions and K output dimensions, so we need  $K \times D$  parameters, which we arrange as a matrix  $\Theta$ .
- > Also, we have a K-dimensional vector **b** of biases.
- Linear predictions:

$$z_k = \sum_j \theta_{kj} x_j + b_k$$

➤ Vectorized:

$$z = \theta x + \mathbf{b}$$

### **Activation Function**

A natural activation function to use is the softmax function, a multivariable generalization of the logistic (sigmoid) function:

$$\hat{y}_k = \operatorname{softmax}(z_1, \dots, z_K)_k = \frac{e^{z_k}}{\sum_{k'} e^{z_{k'}}}$$

Softmax makes differences larger – pushes values close to 1 to 1, values close to 0 to 0

- ➤ The input are called the logits.
- Outputs are positive and sum to 1 (interpreted as probabilities)

### **Loss Function**

If a model outputs a vector of class probabilities, we can use cross-entropy as the loss function:

**Binary** 

$$\mathcal{L}_{CE}(\hat{y}, y) = -y \log \hat{y} - (1 - y) \log(1 - \hat{y})$$

Multi-class

$$\mathcal{L}_{CE}(\hat{\mathbf{y}}, \mathbf{y}) = -\sum_{k=1}^{K} y_k \log \hat{y}_k$$
$$= -\mathbf{y}^T \log \hat{\mathbf{y}}$$

# Softmax Regression

➤ Softmax regression:

$$z = \mathbf{\theta} \mathbf{x} + \mathbf{b}$$

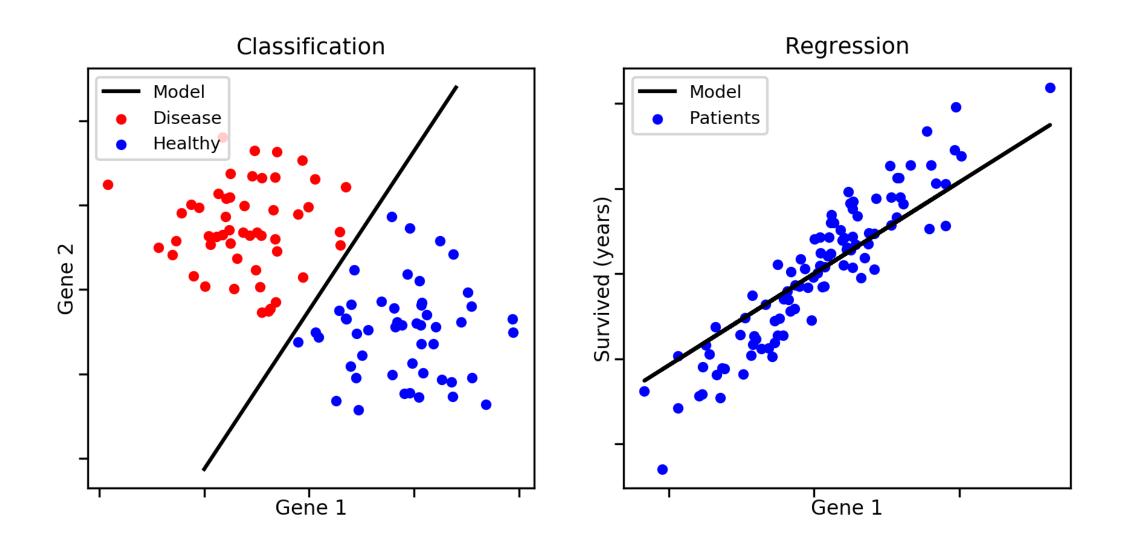
$$\hat{\mathbf{y}} = \operatorname{softmax}(\mathbf{z})$$

$$\mathcal{L}_{CE}(\hat{\mathbf{y}}, \mathbf{y}) = -\mathbf{y}^T \log \hat{\mathbf{y}}$$

Gradient descent updates:

$$\frac{\partial \mathcal{L}_{CE}}{\partial \mathbf{z}} = \hat{\mathbf{y}} - \mathbf{y}$$

# Summary



# Practice in Google Colab

### Neural Networks

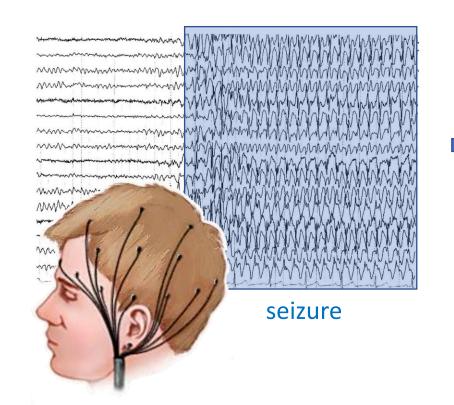
# Challenges with Feature Maps

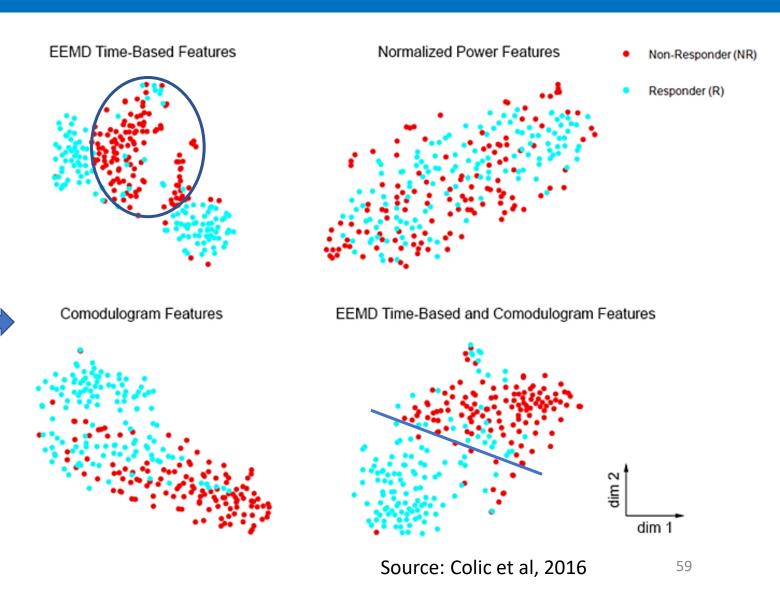
Feature maps can be useful for solving nonlinear regression and classification problems.

- ➤ Have several limitations:
  - > The feature maps must be selected in advance
  - Not always easy to pick a good feature map and can take a long time to craft
  - > In high dimensions the feature representations can explode

# Example of Feature Engineering:

**Objective:** Predict **responders** from **non-responders** given raw electroencephalogram data.





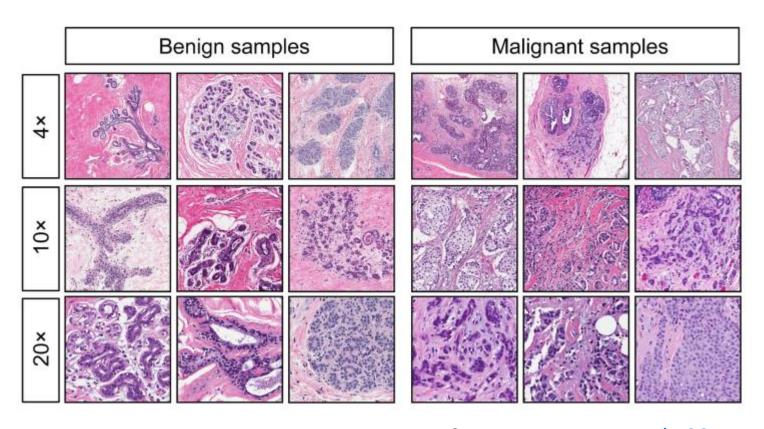
# Challenges with Feature Maps

We need an algorithm that can learn good features for nonlinear regression and classification.

# Motivating Example: Tumor Classification

**Objective:** Classify an image of a biopsy as cancerous (malignant) or benign (tumor)

- Pathologists/radiologists train for years to do this!
- How would you solve this problem?

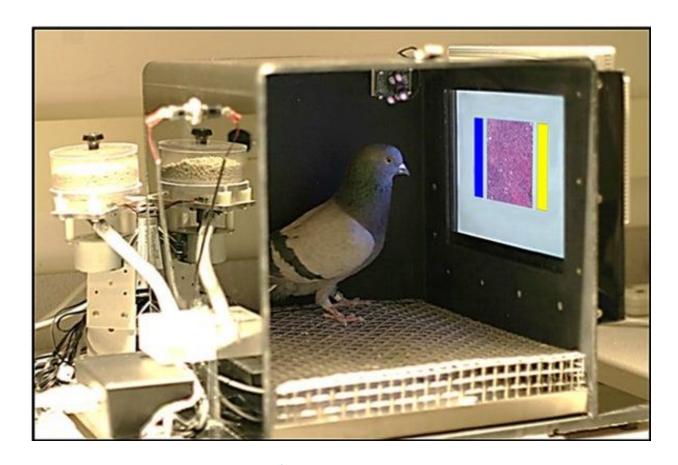


Source: <u>Levenson et al., 2015</u>

# Maybe We Can Use Pigeons

#### Train a Pigeon!

A 2015 study suggests that the common pigeon can reliably distinguish between benign versus malignant tumors and, in doing so, could help researchers develop better cancer screening technologies.

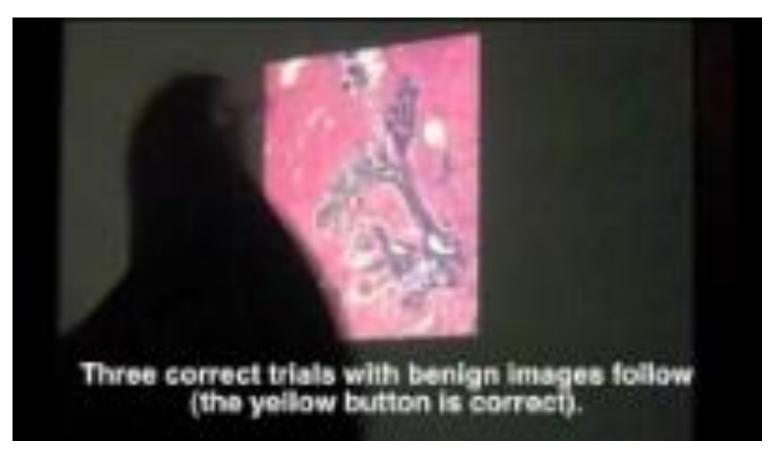


Source: <u>Levenson et al., 2015</u>

# Maybe We Can Use Pigeons

#### Training Algorithm:

- Show an image of a magnified biopsy to pigeon
- 2. Pigeon pecks at one of two answer buttons on sides for malignant/benign
- 3. Correct classifications are rewarded with food pellets



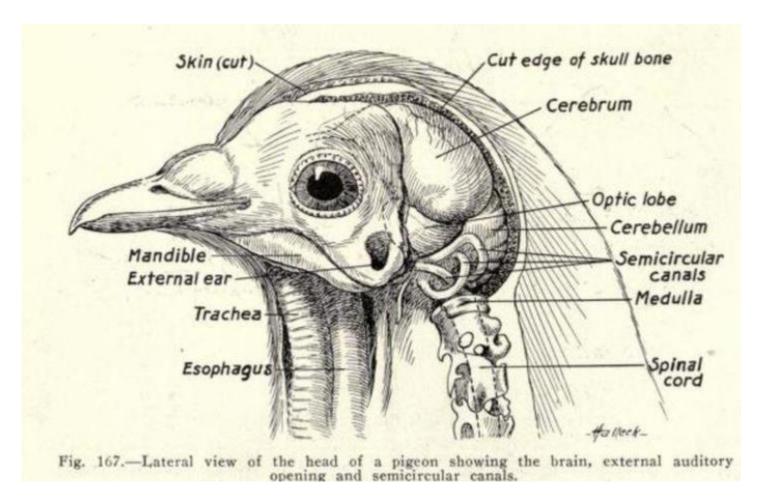
**Video:** https://www.youtube.com/watch?v=flzGjnJLyS0

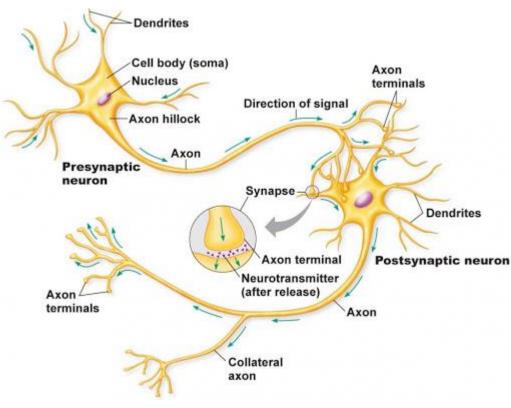
# Why are we talking about pigeons?

We need to answer similar questions in training a pigeon/artificial neural network:

- How will we reward correct responses?
- How do we train the neural network efficiently?
- How do we know the pigeon didn't just memorize the images we showed it?
- What are the ethics of trusting a pigeon to detect cancer?

# How do Pigeons Work?

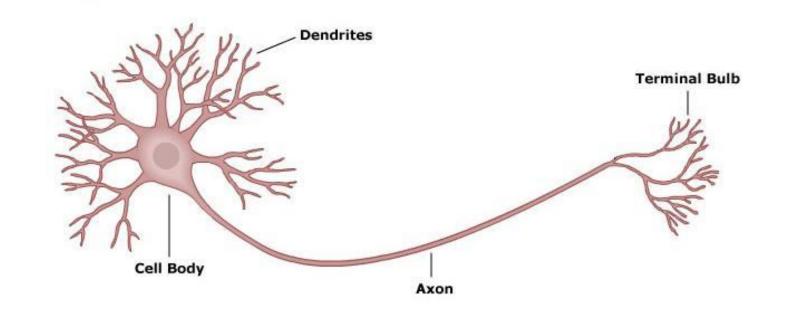




Source: Letsmaketech

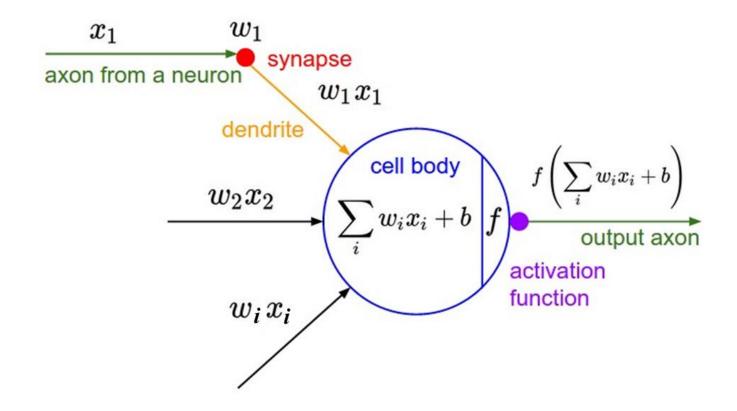
# Simplified Neuron Anatomy

- Dendrites: are connected to other cells that provide information.
- Cell body: consolidates information from dendrites.
- Axon: an extension from the cell body that passes information to other neurons.
- > **Synapse:** the area where the axon of one neuron and the dendrite of another connect.

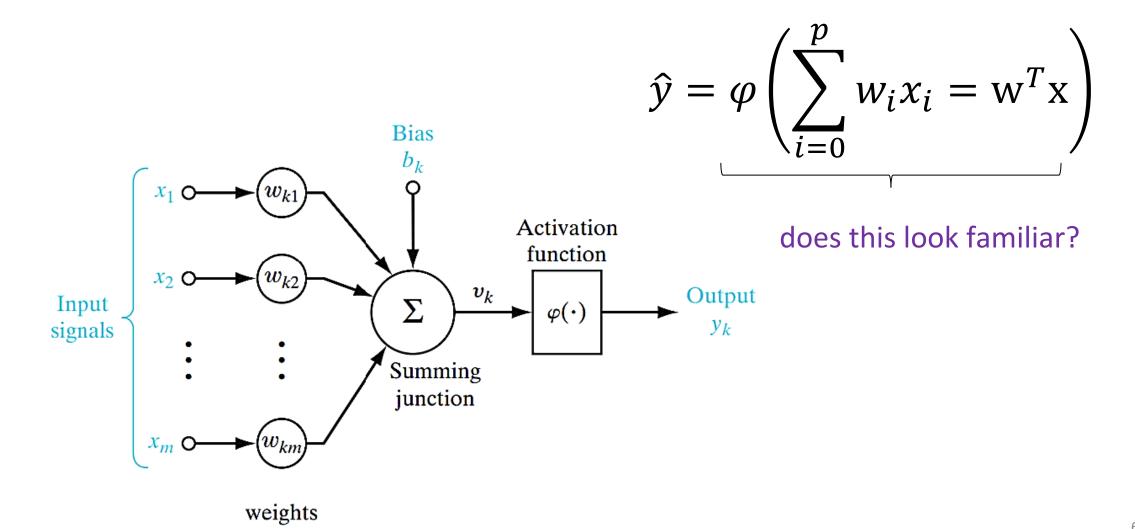


### Artificial Neural Network

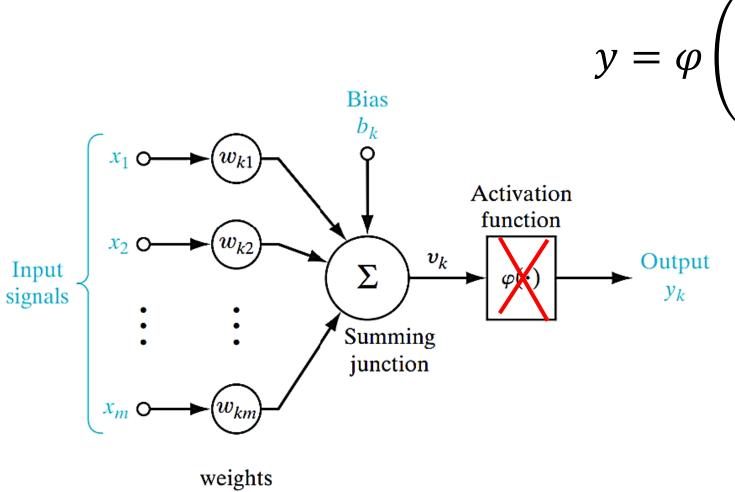
Maybe we're note quite ready for pigeon doctors, but we can use the next best thing... an artificial pigeon (artificial neural network)



### Artificial Neural Network



### Artificial Neural Network



# $y = \varphi\left(\sum_{i=0}^{r} w_i x_i = \mathbf{w}^T \mathbf{x} + \mathbf{b}\right)$

#### **Logistic Regression!**

What will we have if we exclude the activation function?

# Training / Learning Parameters

- > In order to train an ANN we should define the error on our predictions.
- > This is the same as with linear regression and logistic regression:

#### **Mean Squared Error**

(regression)

$$\frac{1}{2N} \sum_{n=1}^{N} \|\hat{y}_n - y_n\|^2$$

**Cross-Entropy Loss** 

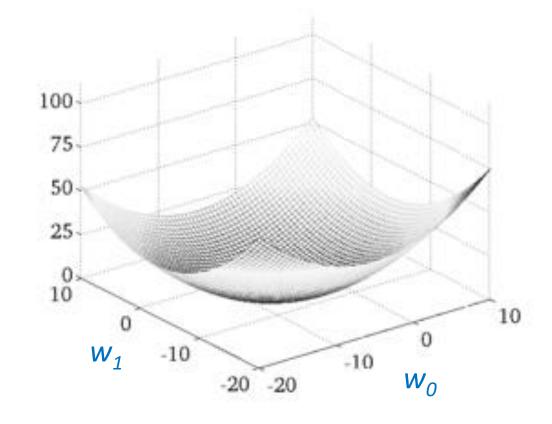
(classification)

$$-\frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K}y_{n,k}\log(\hat{y}_{n,k})$$

implement gradient descent to learn parameters!

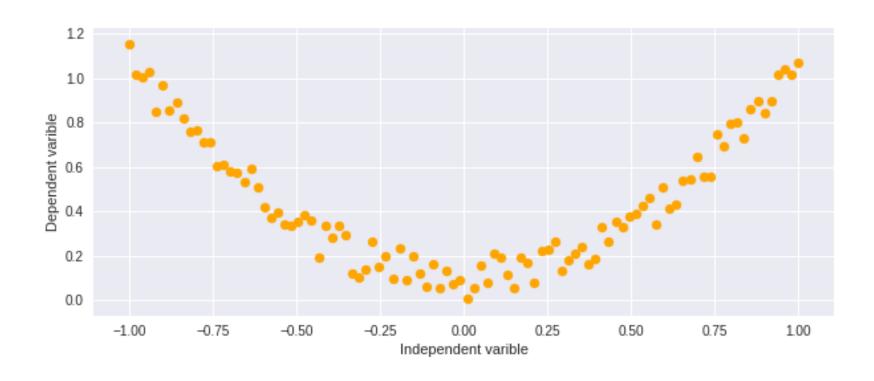
### Gradients

- For this simple version of neural networks all the gradient calculations are the same as we've seen earlier...
- ➤ It probably wouldn't be a surprise to find out that to train this simple ANN is a convex problem (not true for all ANNs).

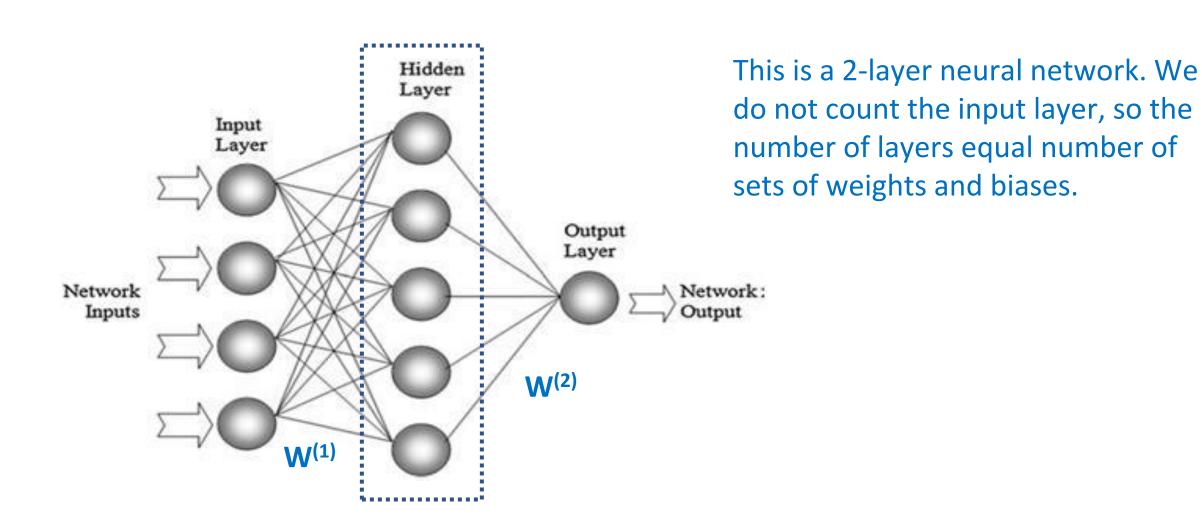


parameters (w) can be multidimensional

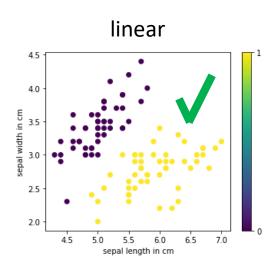
# **Achieving Nonlinearity**

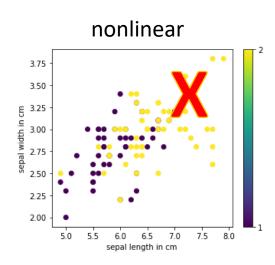


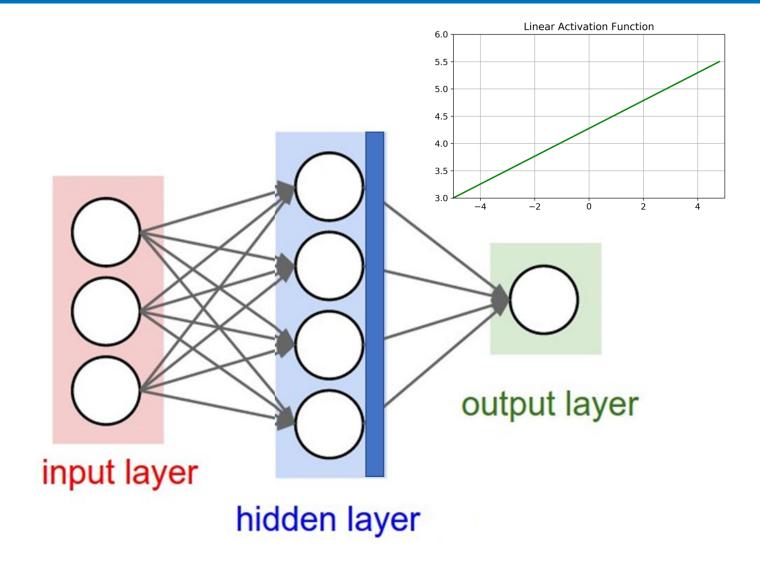
### Add More Neurons?



# 2-layer ANN with Linear Activation







# **Expressive Power**

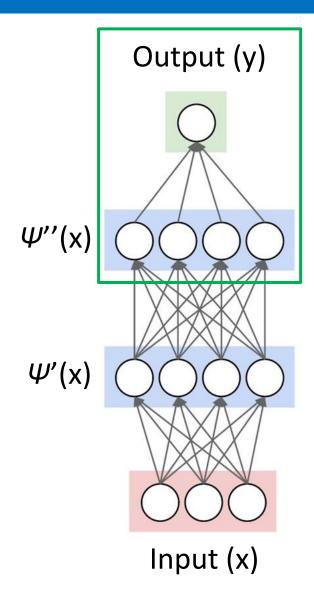
- Adding more linear layers does not help increase the capacity of the model.
- Any sequence of linear layers can be equivalently represented with a single linear layer.

$$\hat{\mathbf{y}} = \mathbf{W}^{(1)}\mathbf{W}^{(2)}\mathbf{W}^{(3)}\mathbf{x}$$

$$\mathbf{W}'\mathbf{x}$$

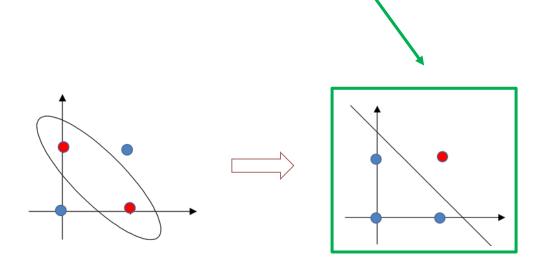
Deep linear networks are no more expressive than linear regression!

### Need an Activation Function

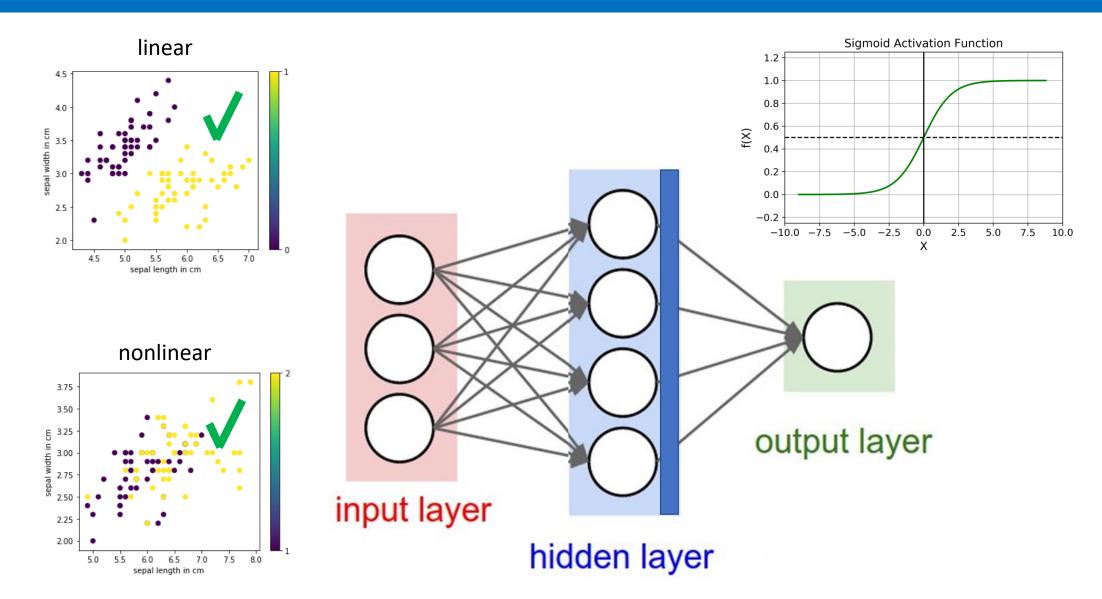


- Neural Networks can be viewed as a way of learning features
- ➤ The goal being that the final layer is presented with linearly separable

feature data



# 2-layer ANN with Nonlinear Activation

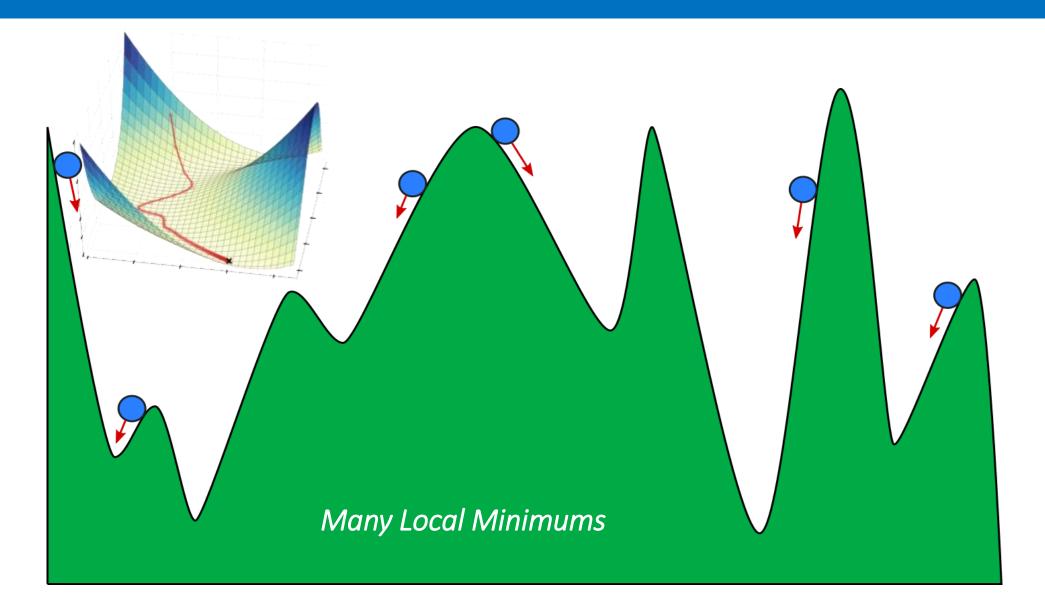


# **Expressive Power**

Multilayer feed-forward neural nets with nonlinear activation functions are universal function approximators.

➤ They can approximate any function arbitrarily well, but this comes at a cost...

### **Cost Function is Non-Convex!**



Nonlinear activations introduce non-convex surface!

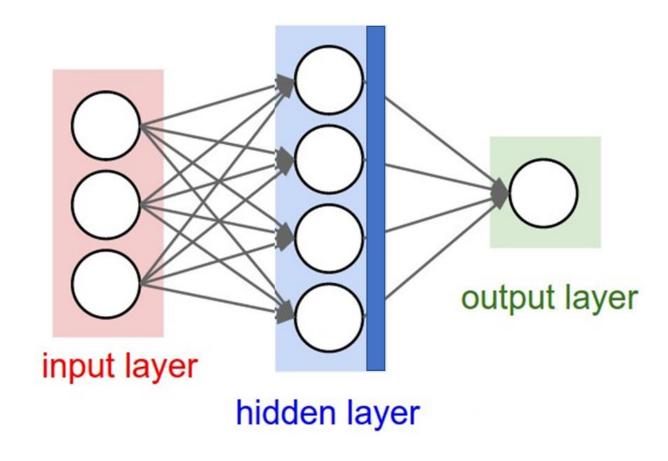
# Tuning Neural Networks

#### **Changing ANN Architecture:**

- Number of hidden units
- Weights
- > Activation Functions

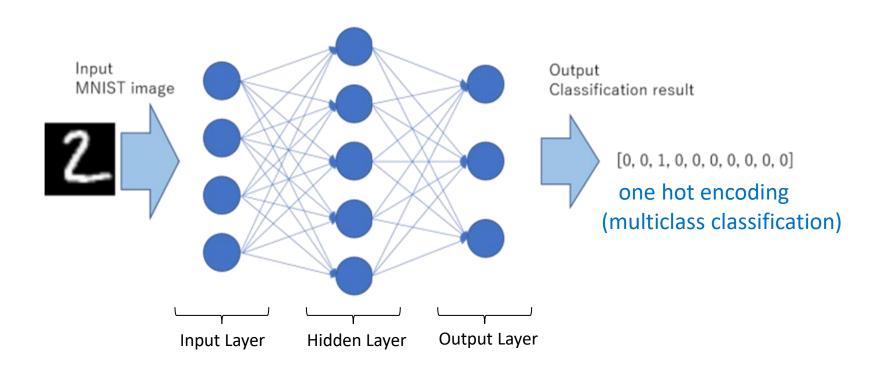
#### **Applying Different Training Techniques:**

- Number of iterations
- Learning rate and adaptive learning rate
- **≻** Momentum
- Batching of Data
- Regularization
- Dropout
- > Feature Augmentation
- Many more...



### Take-home Exercise: Discuss on Piazza

Q: Determine the gradients for a 2-layer artificial neural network with sigmoid activation on the hidden and output layers. The error is computed using mean squared error loss.



### **Next Time**

- Week 10 Q&A session: Thursday and Friday
  - Project 4 is due on April 1<sup>st</sup>

- Week 11 Lecture Deep Learning (and More)
  - Neural Network Architectures
  - > Automatic Differentiation
  - Discrete Optimization