APS1070

Foundations of Data Analytics and Machine Learning

Winter 2022

Week 10:

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

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Slide Attribution

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

- Lisa Zhang
- Roger Grosse
- Jason Riordon

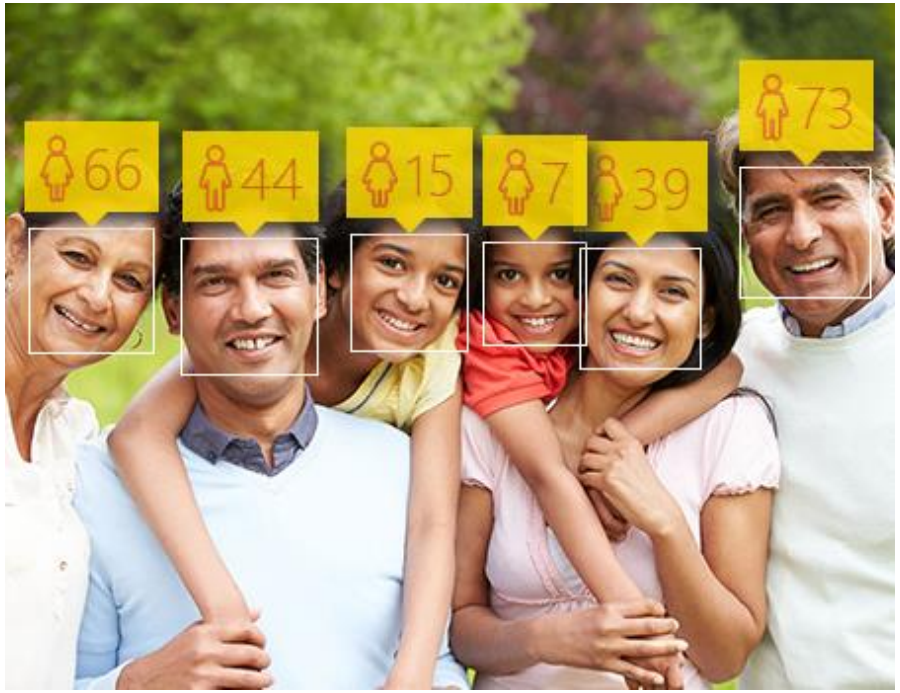
Last Time

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

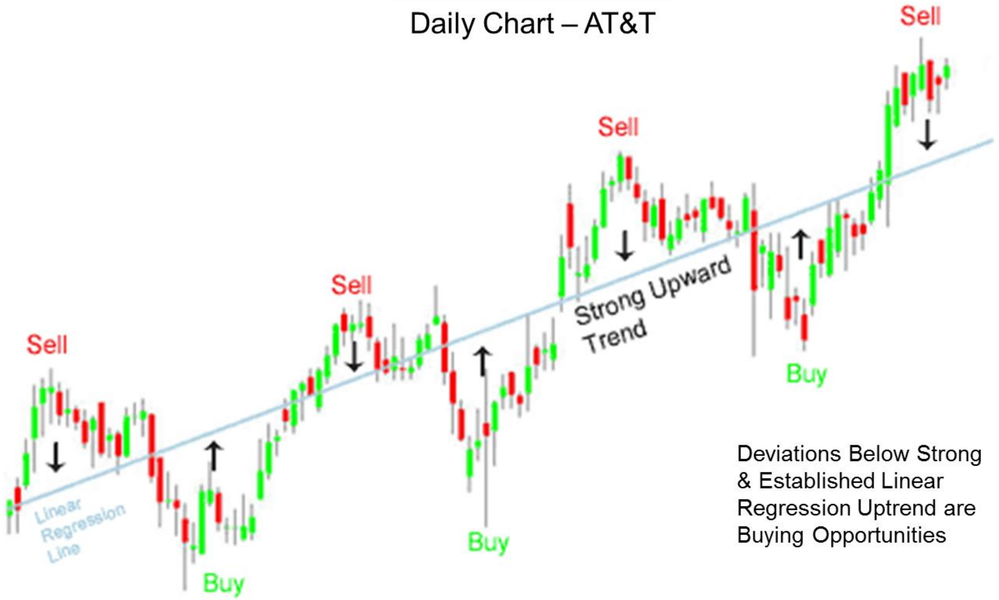
- Today we will continue with **nonlinear regression**.

Nonlinear Regression

Age Prediction



Stock Market Prediction



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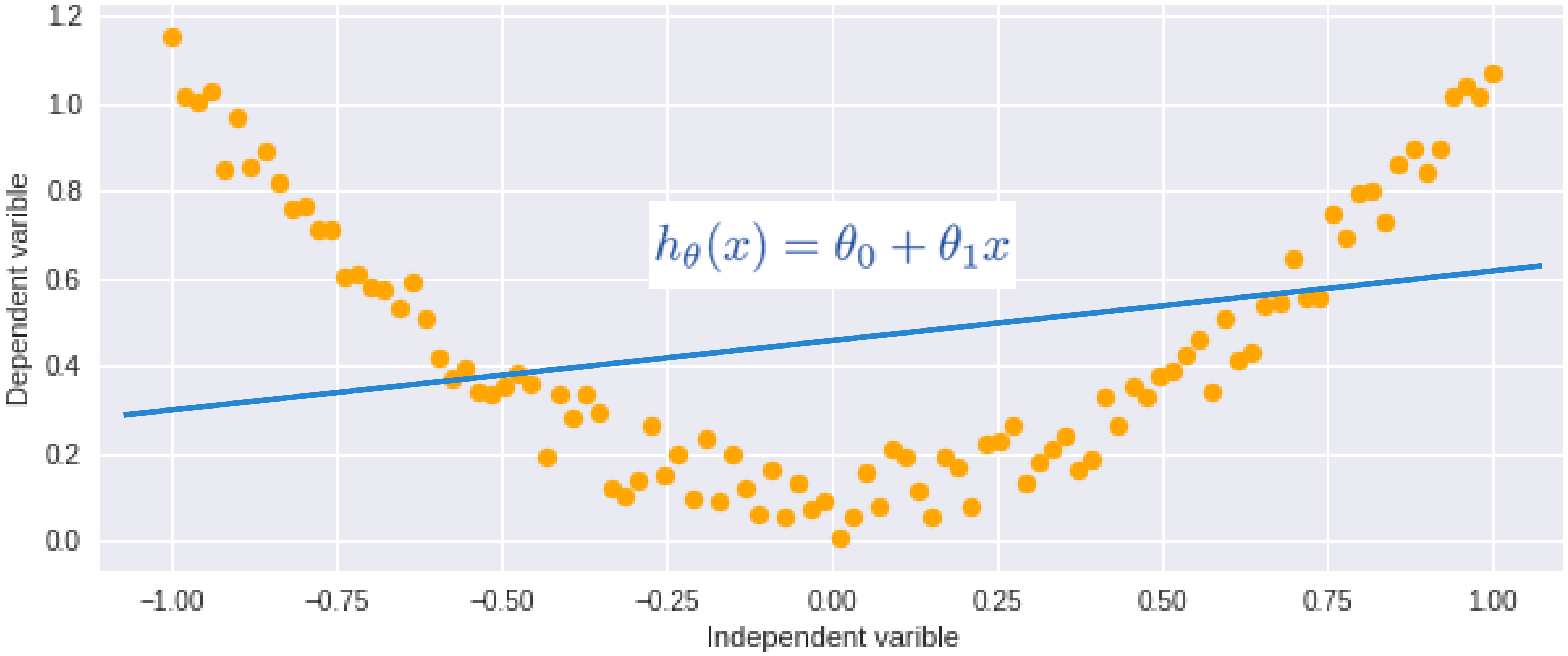
Nonlinear Regression



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:

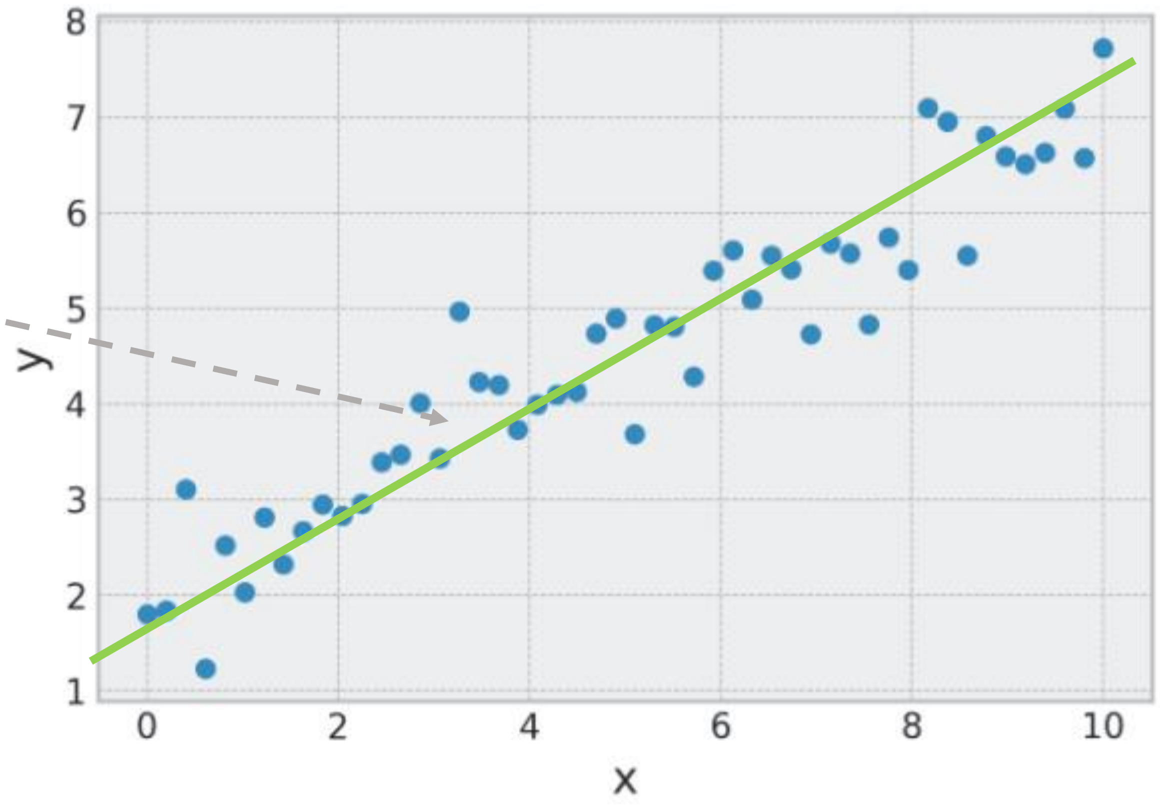
$$h_\theta(x) = \theta_0 + \theta_1 x$$

Parameters:

$$\theta_0, \theta_1$$

Cost Function:

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



Goal:

$$\underset{\theta_0, \theta_1}{\text{minimize}}\ J(\theta_0, \theta_1)$$

(1) direct solution

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

OR

(2) gradient descent

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

Recap: Vectorization

Hypothesis:

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

Parameters:

$$\theta$$

Cost Function:

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

Goal:

$$\underset{\theta}{\text{minimize}}\ J$$

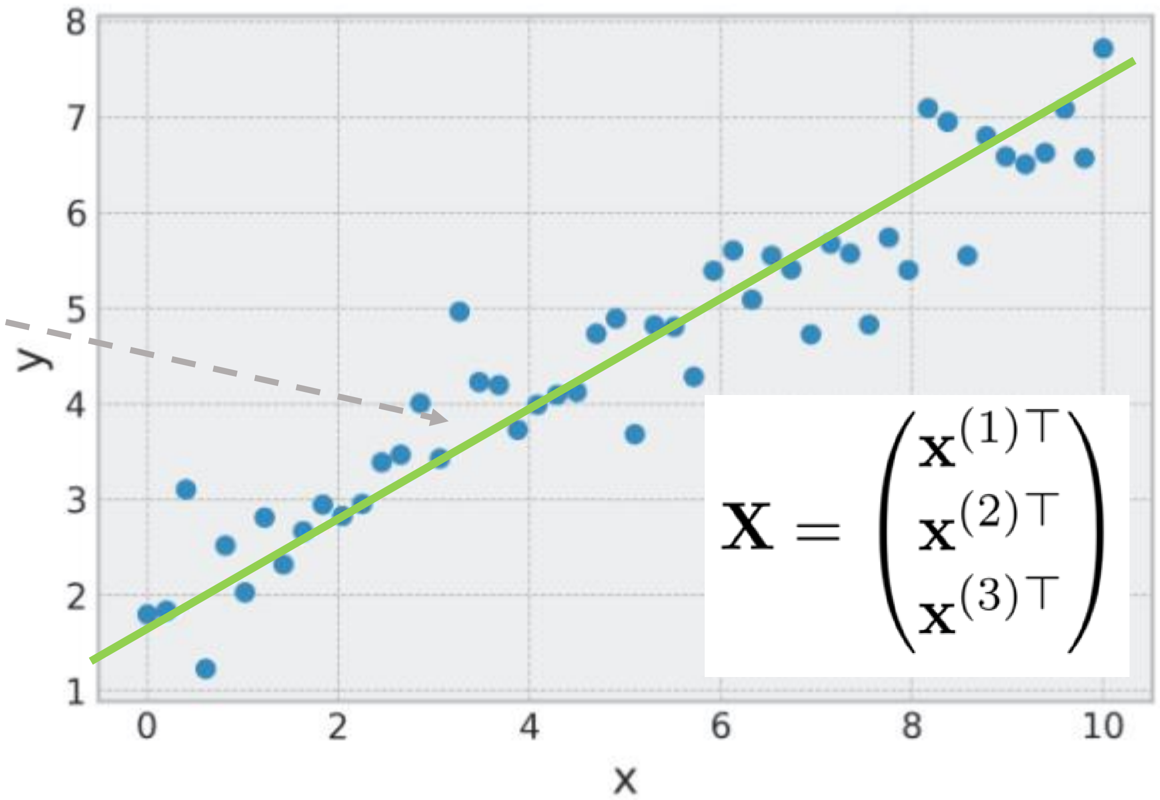
(1) direct solution

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

OR

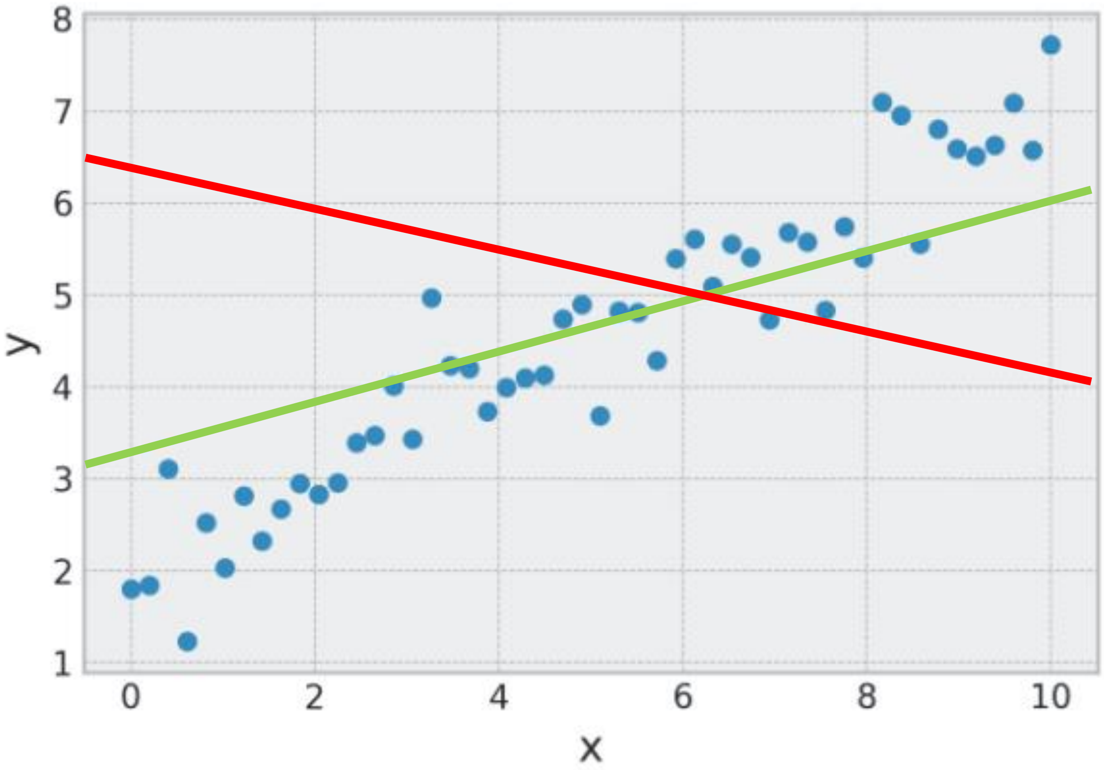
(2) gradient descent

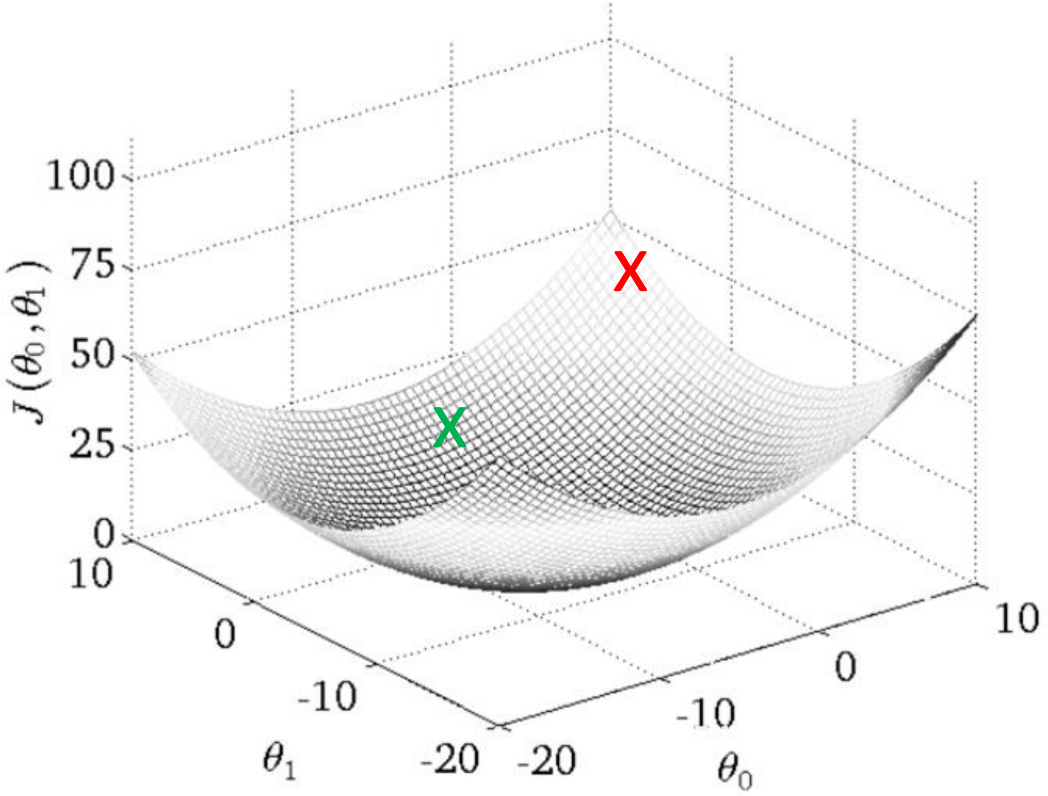
$$\theta \leftarrow \theta - \alpha\frac{\partial J}{\partial \theta}$$



$$\mathbf{X} = \begin{pmatrix} \mathbf{x}^{(1)\top} \\ \mathbf{x}^{(2)\top} \\ \mathbf{x}^{(3)\top} \end{pmatrix}$$

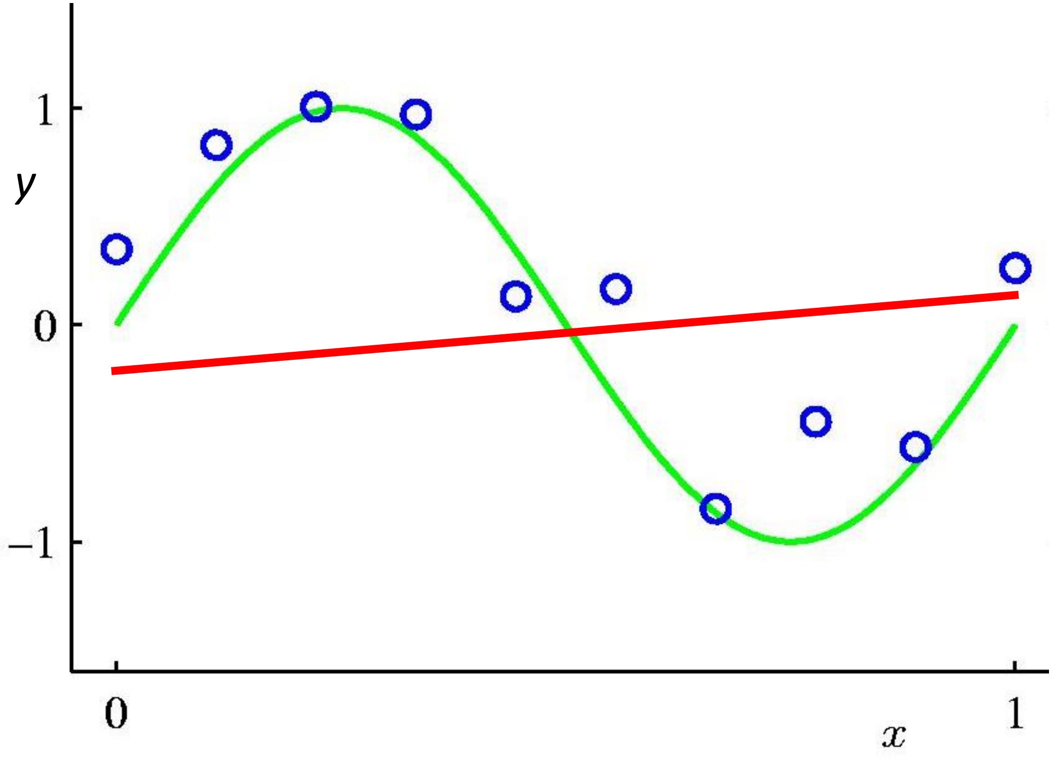
Recap: Convexity





Nonlinear Regression

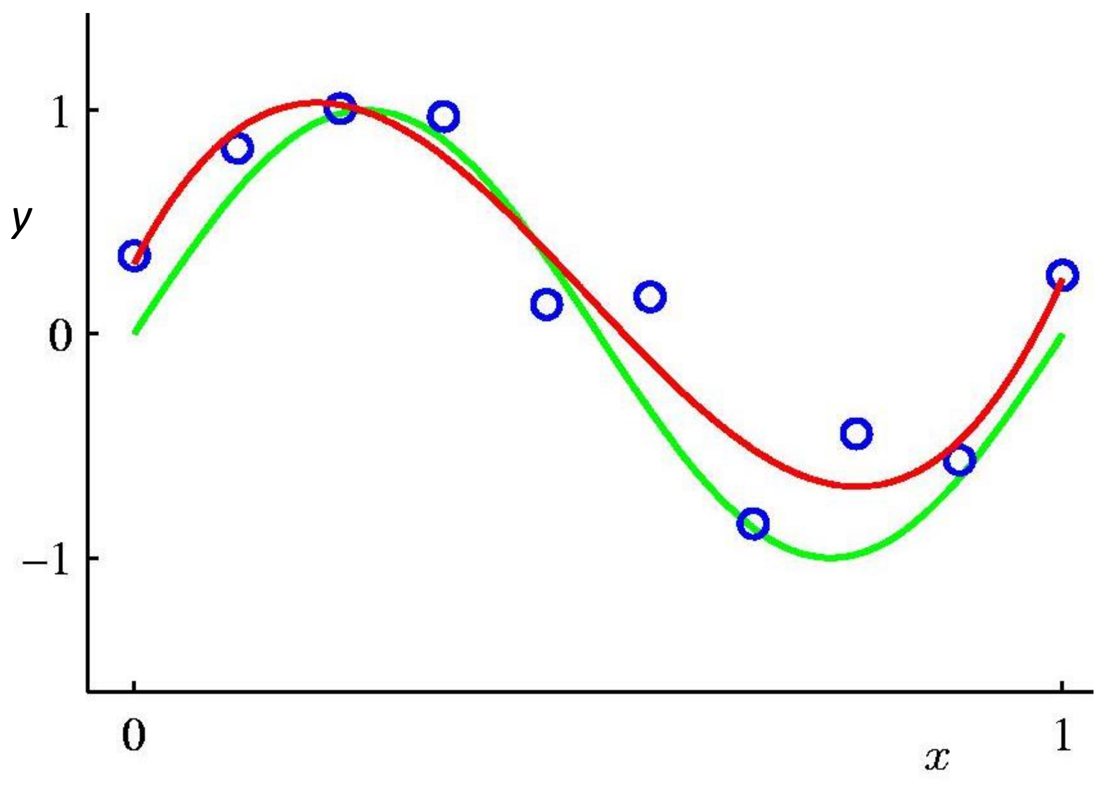
- Suppose we want to model the following data



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:

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

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

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

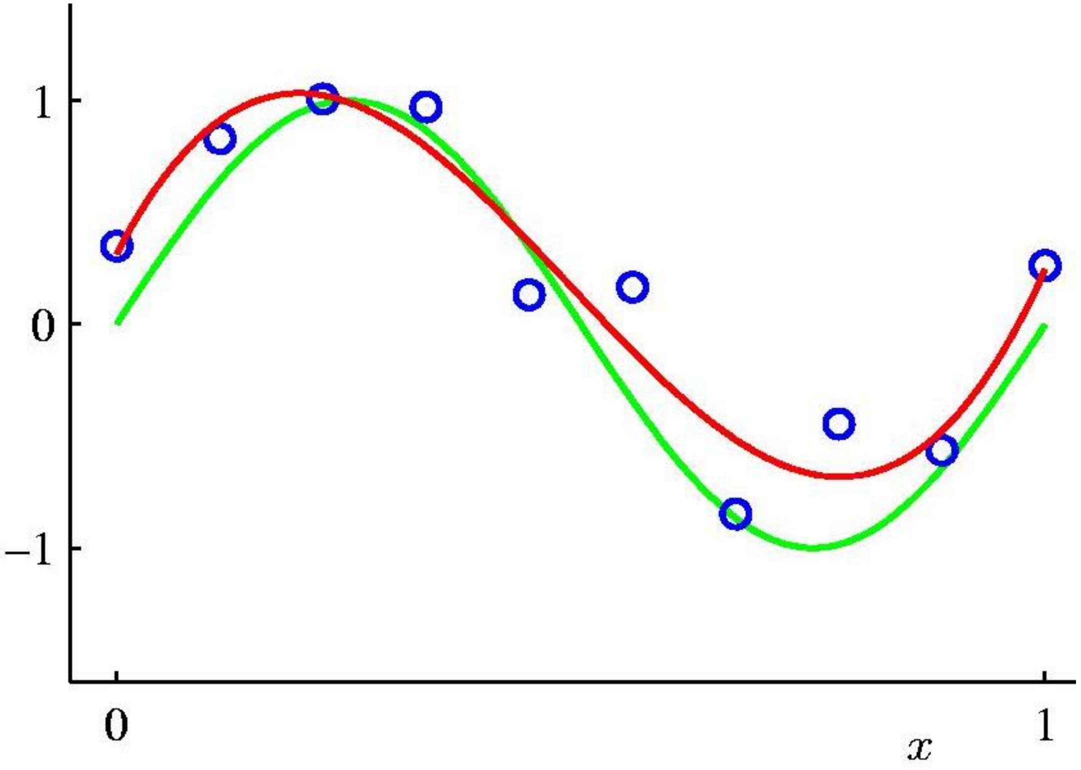
Polynomial Regression

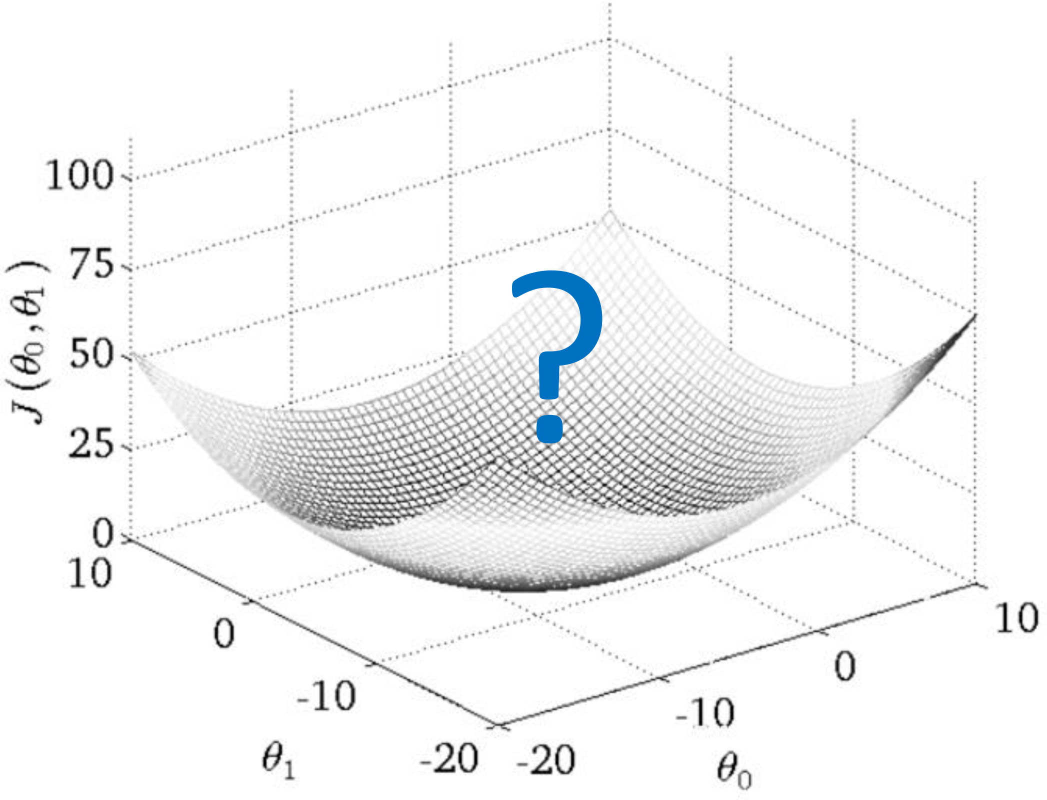
- This doesn't require changing the algorithm, just **pretend $\boldsymbol{\psi}(\boldsymbol{x})$ is the input vector**.

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

- 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.

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

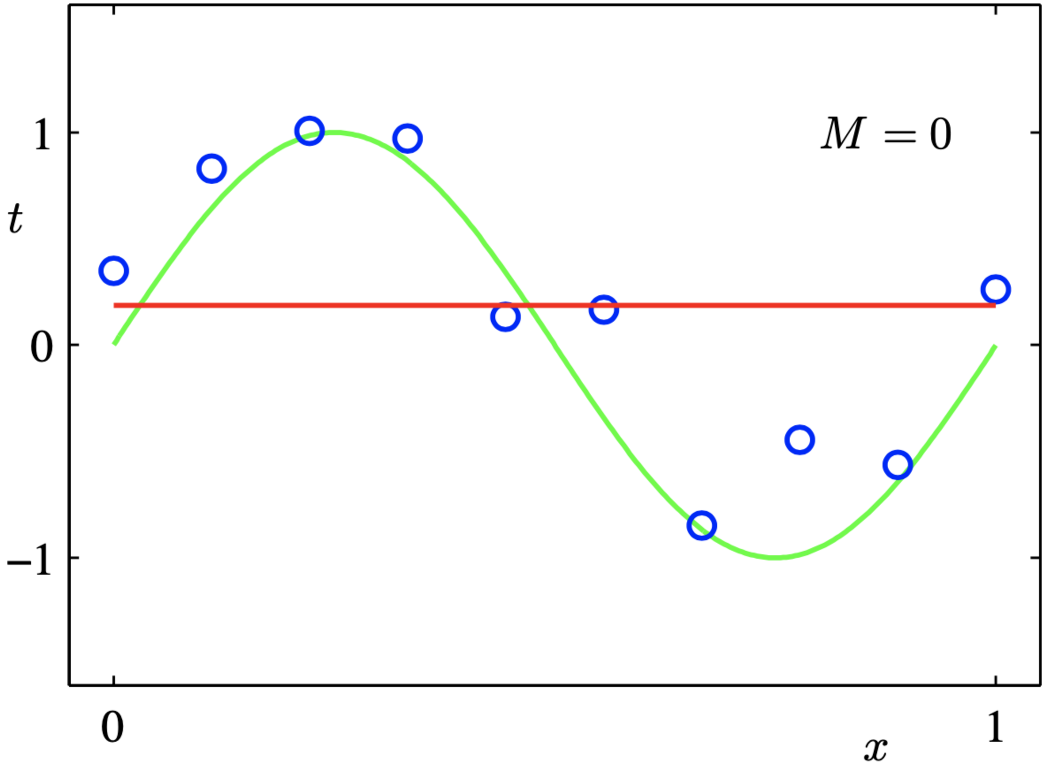
$$\mathcal{J}(\theta) = \frac{1}{2N}||\boldsymbol{y} - \hat{\boldsymbol{y}}||^2 \xrightarrow{\text{minimize cost}} \theta = (\psi^T\psi)^{-1}\psi^T \mathrm{y}$$

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 (ψ) = D.

Fitting Polynomial (M = 0)

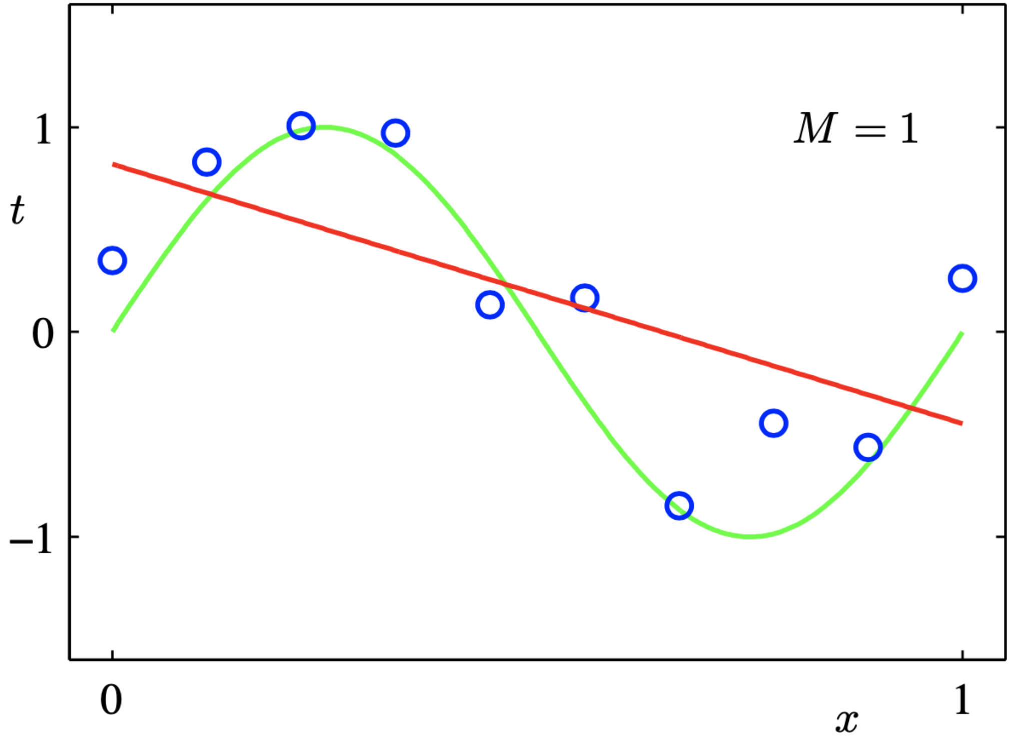
$$\hat{y} = w_0$$



-Pattern Recognition and Machine Learning, Christopher Bishop.

Fitting Polynomial (M = 1)

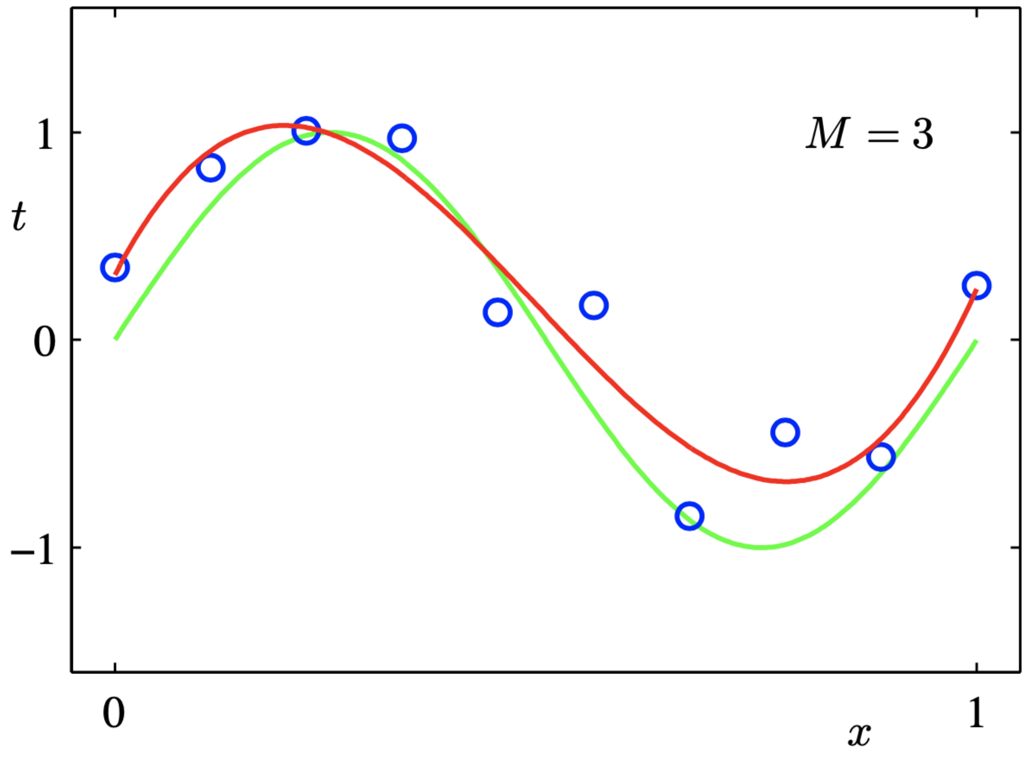
$$\hat{y} = w_0 + w_1 x$$



-Pattern Recognition and Machine Learning, Christopher Bishop.

Fitting Polynomial (M = 3)

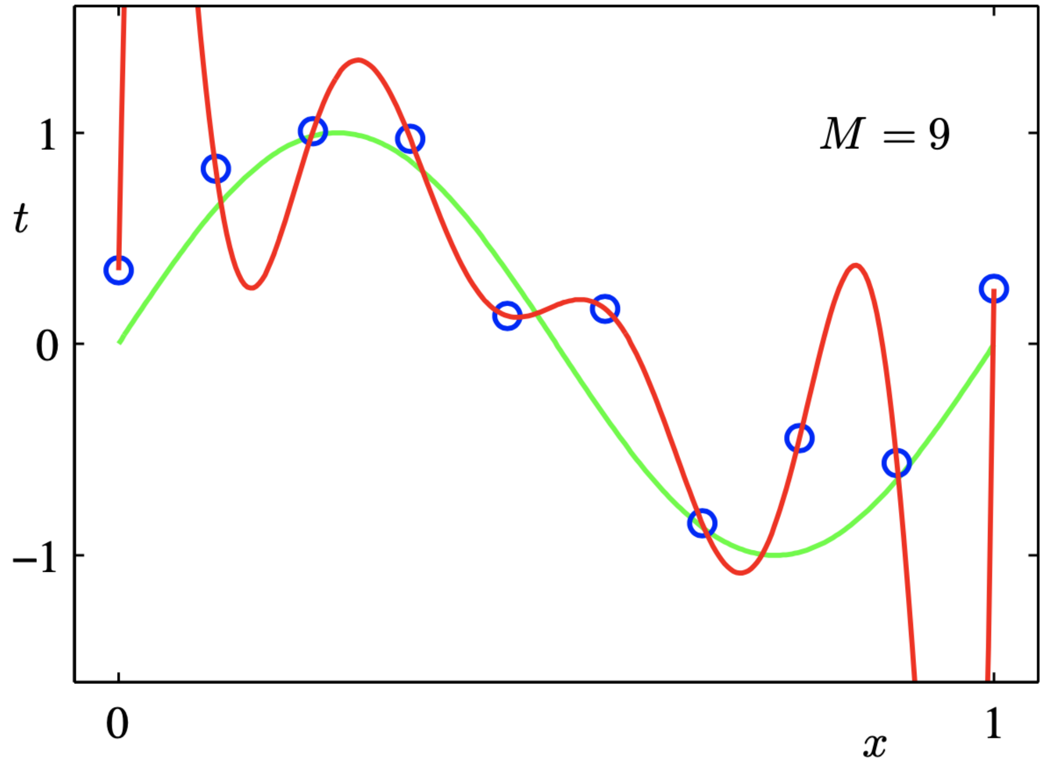
$$\hat{y} = w_0 + w_1 x + w_2 x^2 + w_3 x^3$$



-Pattern Recognition and Machine Learning, Christopher Bishop.

Fitting Polynomial (M = 9)

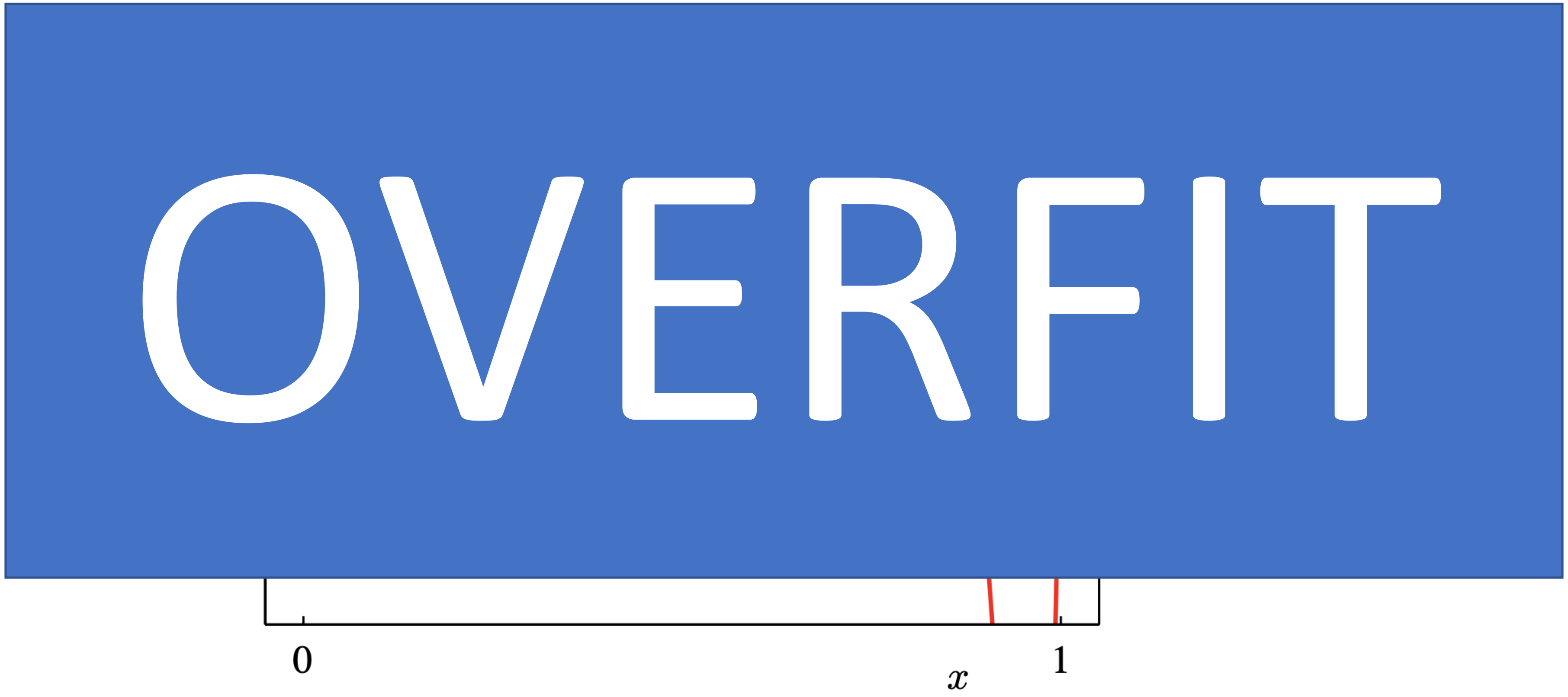
$$\hat{y} = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + \ldots + w_9 x^9$$



-Pattern Recognition and Machine Learning, Christopher Bishop.

Fitting Polynomial (M = 9)

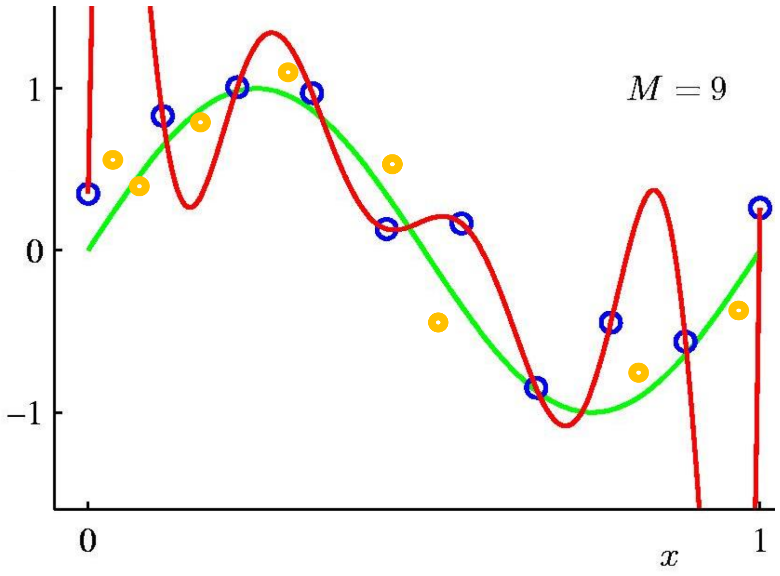
$$\hat{y} = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + \ldots + w_9 x^9$$

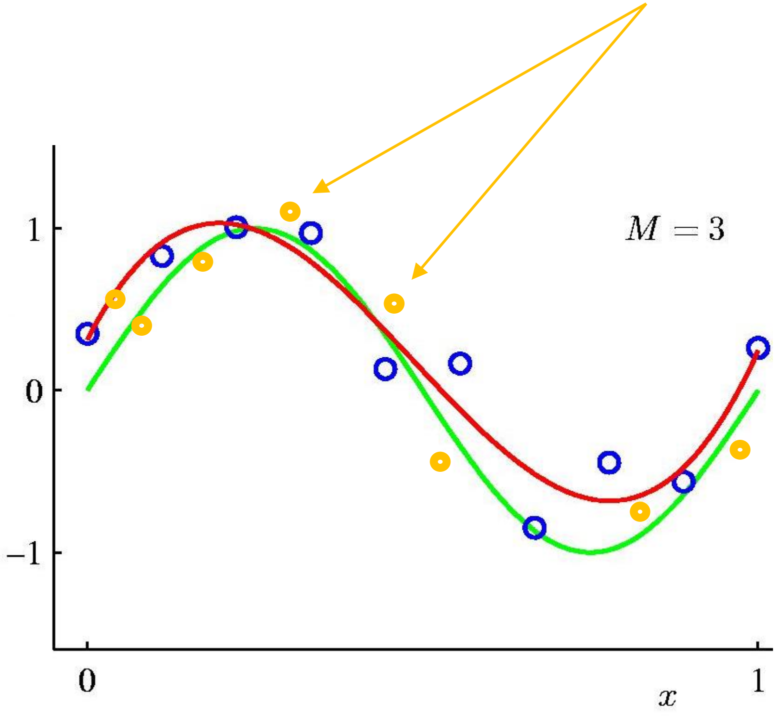


-Pattern Recognition and Machine Learning, Christopher Bishop.

Generalize to New Samples

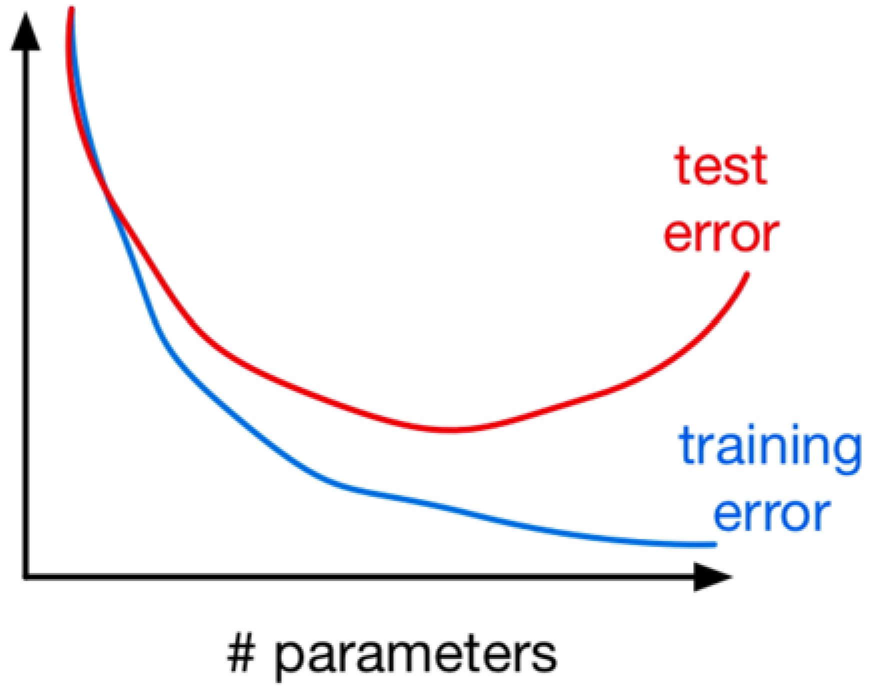
- We could give the hypothesis a higher complexity, or capacity to fit the data, but this may not generalize well to **new samples**





Generalization

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

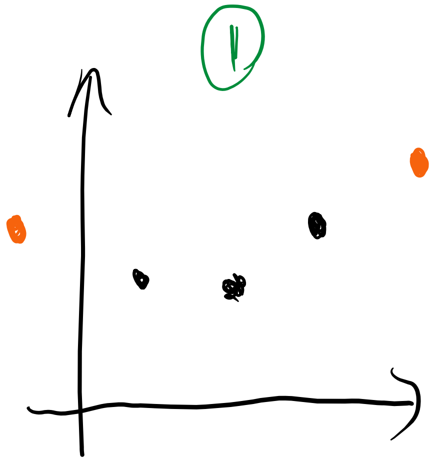


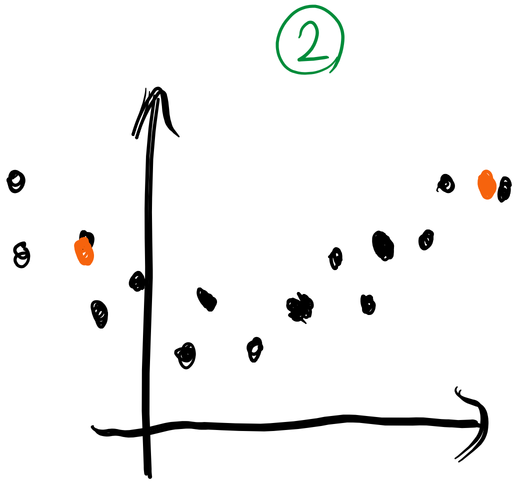
(model complexity)

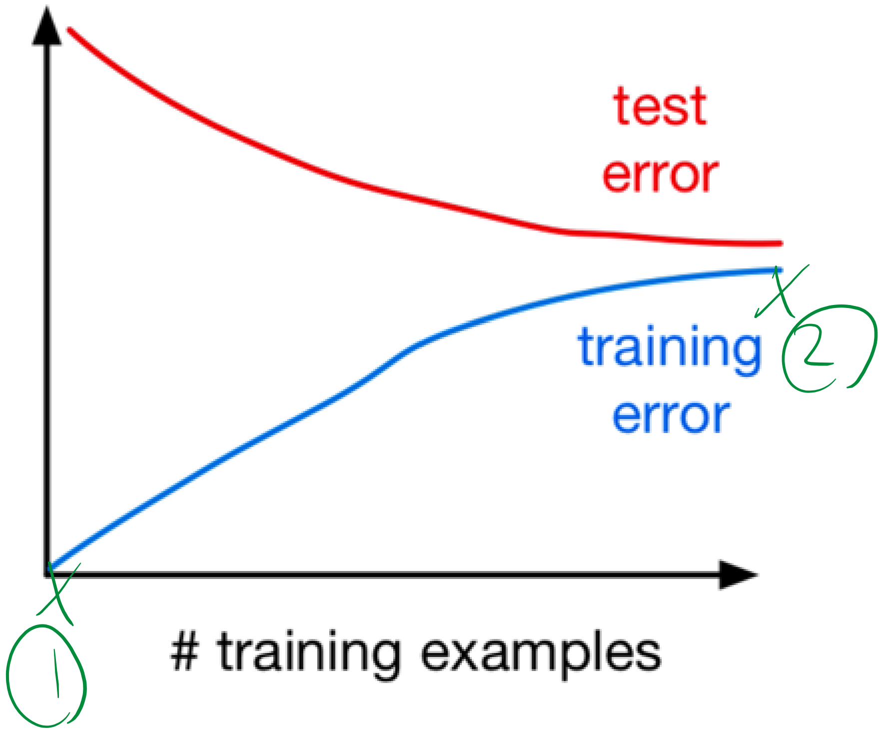
Generalization

➤ 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

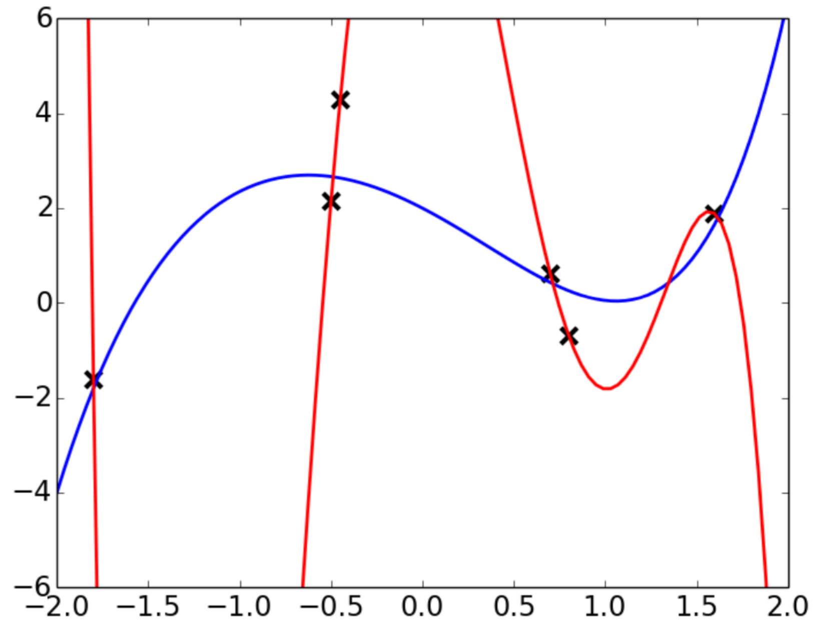
- The degree of the polynomial is a hyperparameter, just like k in KNN. We can tune it using a validation set.
- But restricting the size of a model is a crude solution, since you'll never be able to learn a more complex model, even if the data support it.

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

L^2 Regularization

Observation:

polynomials that overfit often have large coefficients



$$y = 0.1x^5 + 0.2x^4 + 0.75x^3 - x^2 - 2x + 2$$

$$y = -7.2x^5 + 10.4x^4 + 24.5x^3 - 37.9x^2 - 3.6x + 12$$

L^2 Regularization

- **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:

$$\boldsymbol{\theta} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \boldsymbol{\theta} = \begin{pmatrix} -9 \\ 11 \end{pmatrix}$$

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

L^2 Regularization

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

$$\frac{1}{2}\|\boldsymbol{\theta}\|^2 = \frac{1}{2}\sum_j \theta_j^2$$

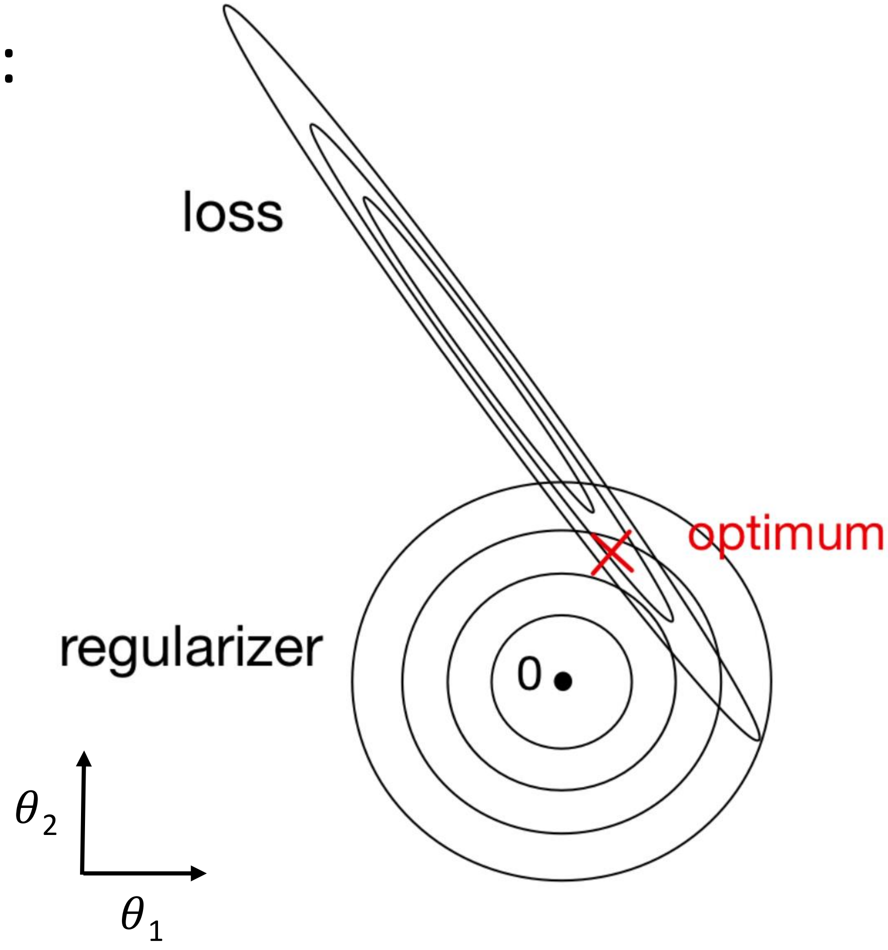
hyperparameter to be tuned

$$\mathcal{J}_{reg} = \mathcal{J} + \frac{\lambda}{2}\sum_j \theta_j^2$$

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

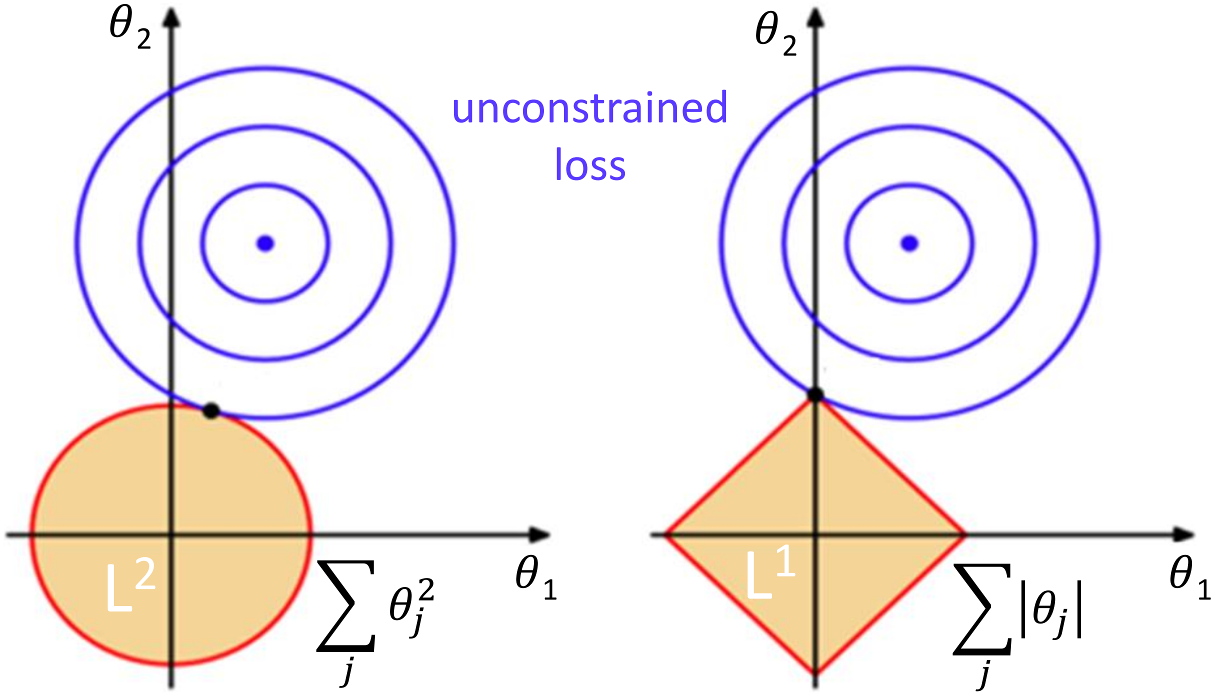
L^2 Regularization

- The geometric picture:

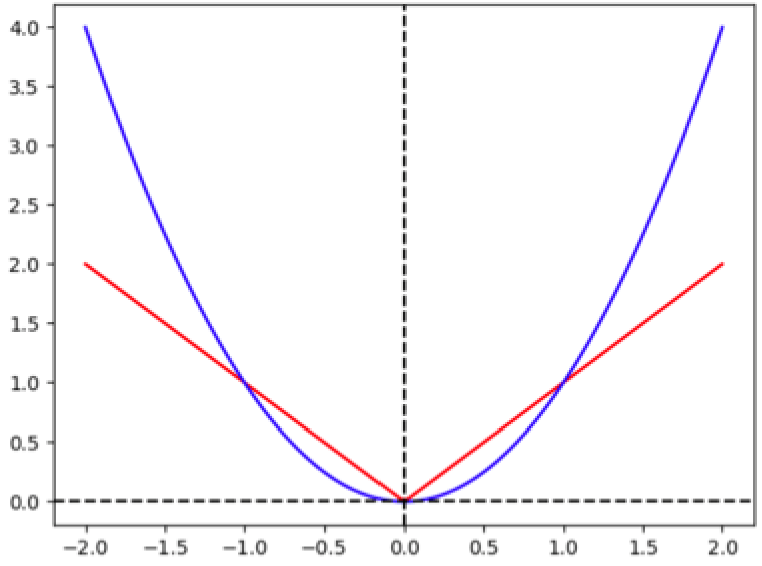


L^1 vs L^2 Regularization

➤ The L^1 norm (or sum of absolute values) is another regularizer that encourages weights to be exactly zero. (How can you tell?)



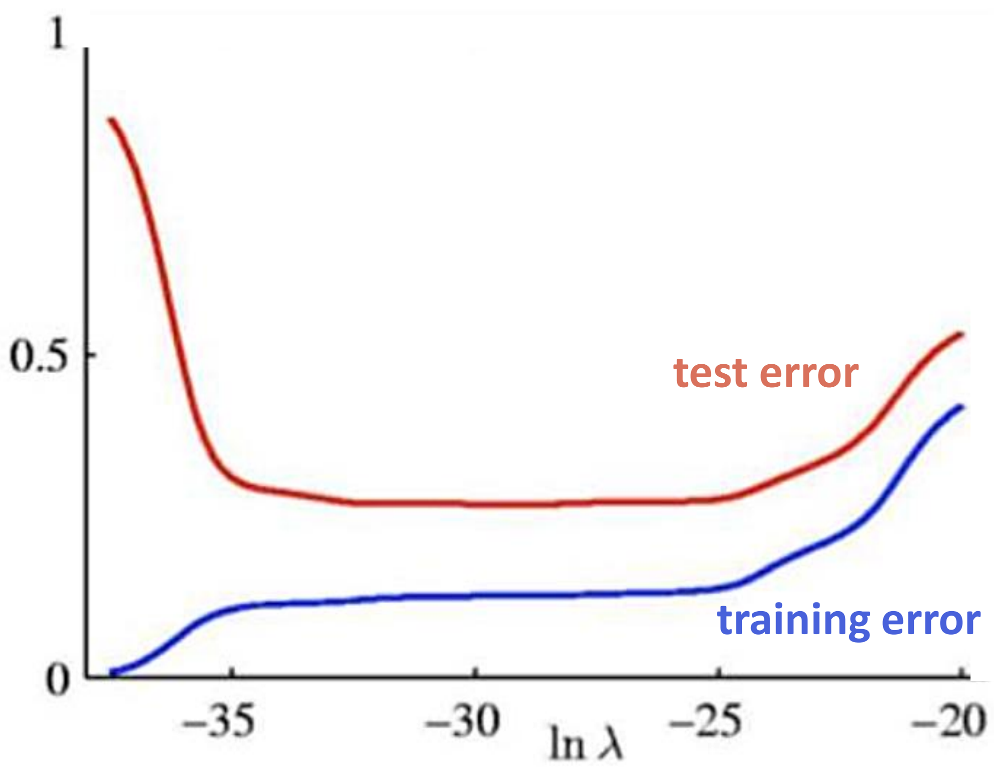
Source: Bishop PRML



L1-regularization tends to push parameters to zero

Generalization

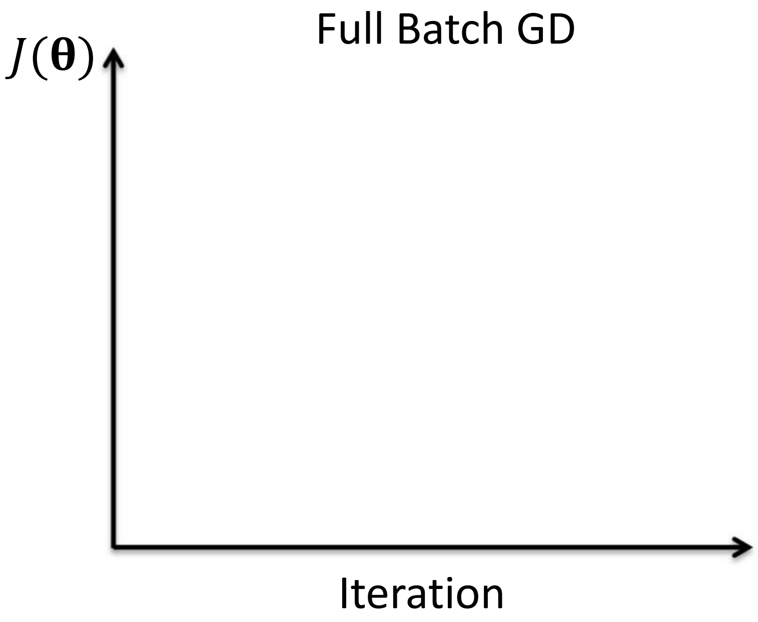
➢ Training and test error as a function of regularization parameter λ:

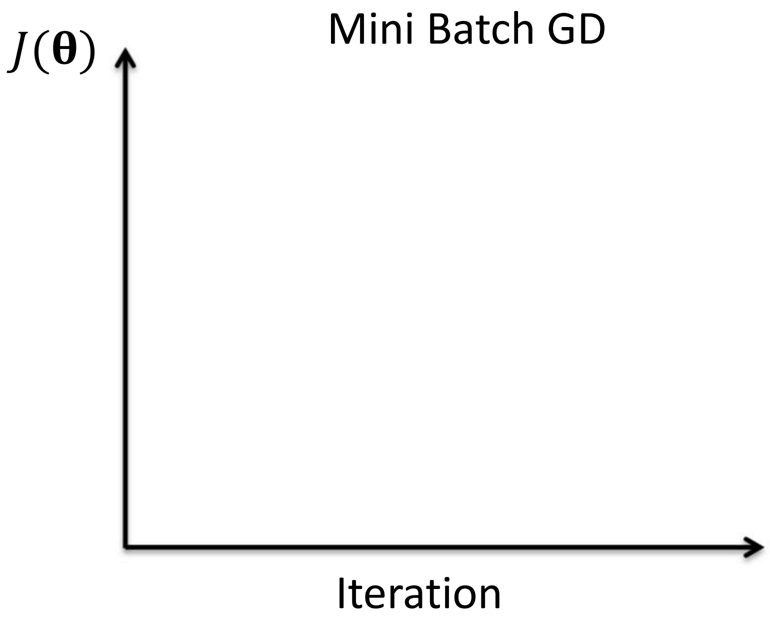


	$\ln\lambda = -\infty$	$\ln\lambda = -18$	$\ln\lambda = 0$
θ_0	0.35	0.35	0.13
θ_1	232.37	4.74	-0.05
θ_2	-5321.83	-0.77	-0.06
θ_3	48568.31	-31.97	-0.05
θ_4	-231639.30	-3.89	-0.03
θ_5	640042.26	55.28	-0.02
θ_6	-1061800.52	41.32	-0.01
θ_7	1042400.18	-45.95	-0.00
θ_8	-557682.99	-91.53	0.00
θ_9	125201.43	72.68	0.01

Batch Size

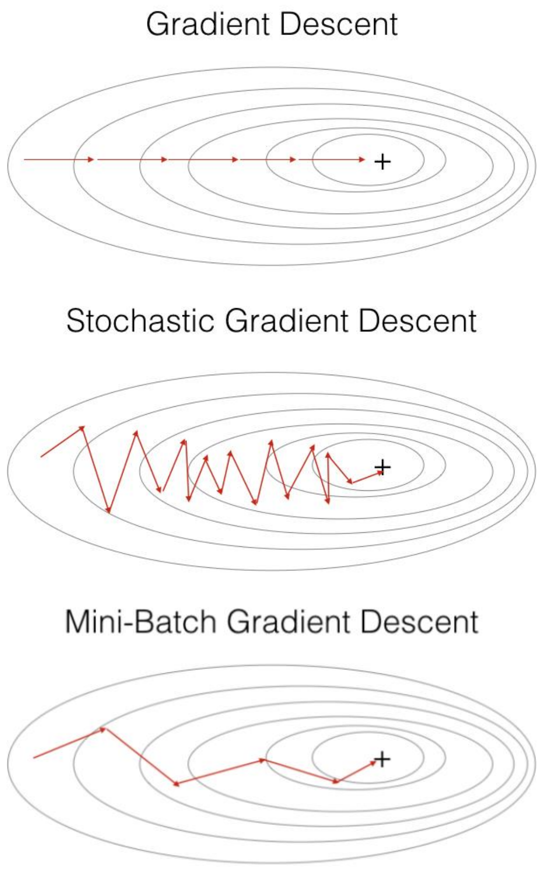
- Q: How much (training) data do you consider when performing a step?
  - Stochastic Gradient Descent – 1 data point
  - Mini-batch – part of your data
  - Full batch – all data





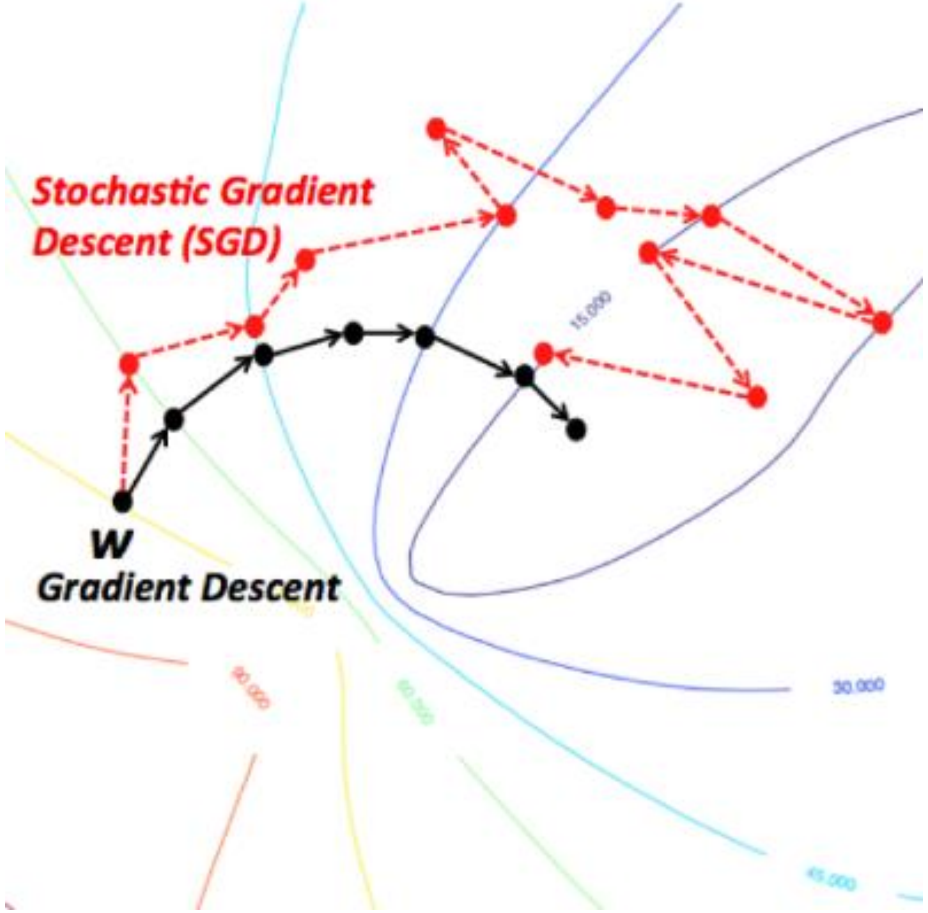
Ineffective Batch Size

- Q: What happens if the batch size is too small? Too large?
- **Too small:**
  - We optimize a (possibly very) different function loss at each iteration
  - Noisy
- **Too large:**
  - Expensive
  - Average loss might not change very much as batch size grows



Stochastic Gradient Descent

- For each iteration evaluate a training sample from the dataset
  taken at random.
- Computing the gradient takes less time, but… may not actually be faster…
- Optimization path that looks rather erratic
  - SGD allows you to do **more of a global search for an optimum**, often results in a better set of parameters for your model!

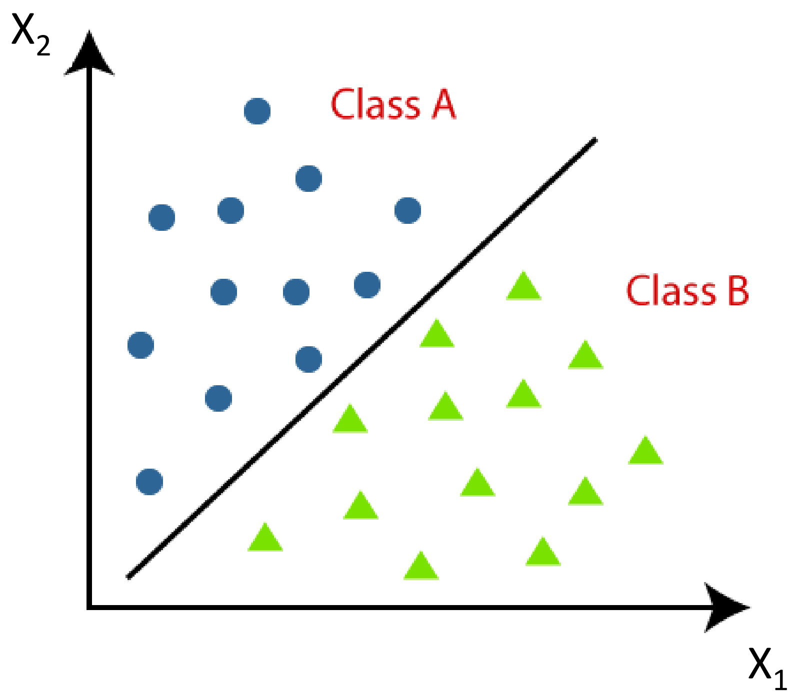


Classification

Overview

- **Classification:** predicting a discrete-valued 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 :

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

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

Binary Classification

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

$$\boldsymbol{\theta}^{\mathrm{T}}\mathbf{x} + b \geq 0 \longleftarrow \boldsymbol{\theta}^{\mathrm{T}}\mathbf{x} + \underbrace{b - r}_{\triangleq b'} \geq 0$$

- Eliminating the bias
  - Add a dummy feature x_0 which always takes the value 1. The weight θ_0 is equivalent to a bias.

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

The Geometric Picture

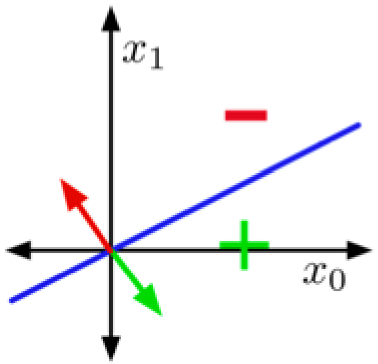
- Training examples are points
- Hypothesis are half-spaces whose boundaries pass through the origin
- The boundary is the decision boundary
  - In 2-D it's a line, but think of it as a hyperplane
- If the training examples can be separated by a linear decision rule, they are linearly separable.

Let us visualize the NOT example

NOT

x_0	x_1	t
1	0	1
1	1	0

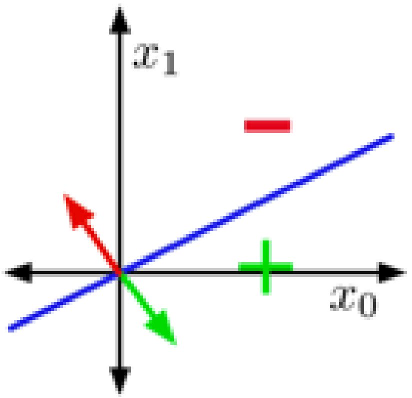
- Input Space, or Data Space:



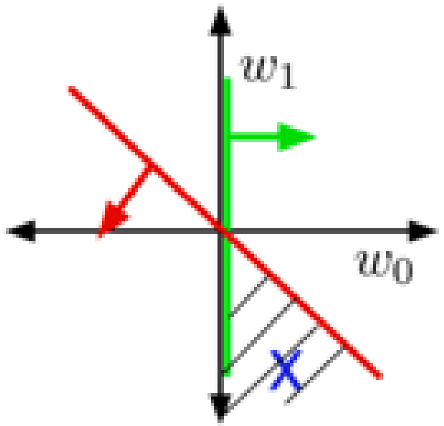
The Geometric Picture

- 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



$$w_0 > 0$$
$$w_0 + w_1 < 0$$

What is the loss function?

- Recall: binary linear classifiers. Target $y \epsilon \{0,1\}$

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

- Seemingly obvious loss function 0-1 loss:

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

Attempt: 0-1 loss

- Problem: How to optimize?
- Chain rule:

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

$$\frac{\partial \mathcal{L}_{0-1}}{\partial \theta_j} = \frac{\partial \mathcal{L}_{0-1}}{\partial z} \frac{\partial z}{\partial \theta_j}$$

- But $\frac{\partial \mathcal{L}_{0-1}}{\partial z}$ is zero everywhere it's defined!
- $\frac{\partial \mathcal{L}_{0-1}}{\partial z} = 0$ means that changing the parameters by a very small amount probably has no effect on the loss.
- Cannot use gradient descent to optimize.

Attempt: 2: Linear Regression

- Sometimes we can replace the loss function we care about with one which is easier to optimize.
- We already know how to fit a linear regression model. Can we use squared error loss instead?

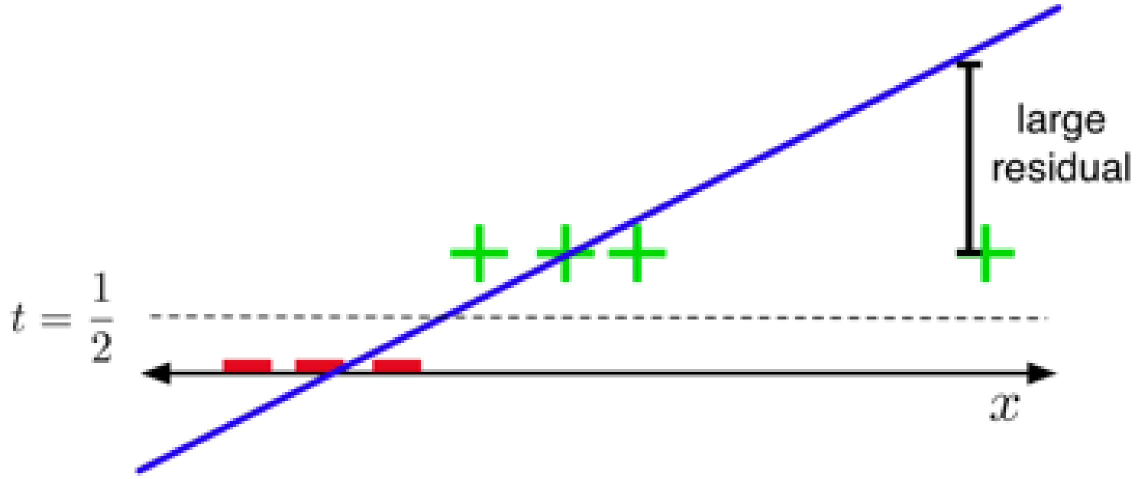
$$\hat{y} = \boldsymbol{\theta}^{\mathrm{T}}\mathbf{x} + b \qquad \mathcal{L}_{SE}(\hat{y}, y) = \frac{1}{2}(y - \hat{y})^2$$

- Doesn’t matter that the targets are actually binary
- Threshold predictions at y = 1/2.

Attempt: 2: Linear Regression

- The Problem:

$$\mathcal{L}_{SE}(\hat{y}, y) = \frac{1}{2}(y - \hat{y})^2$$



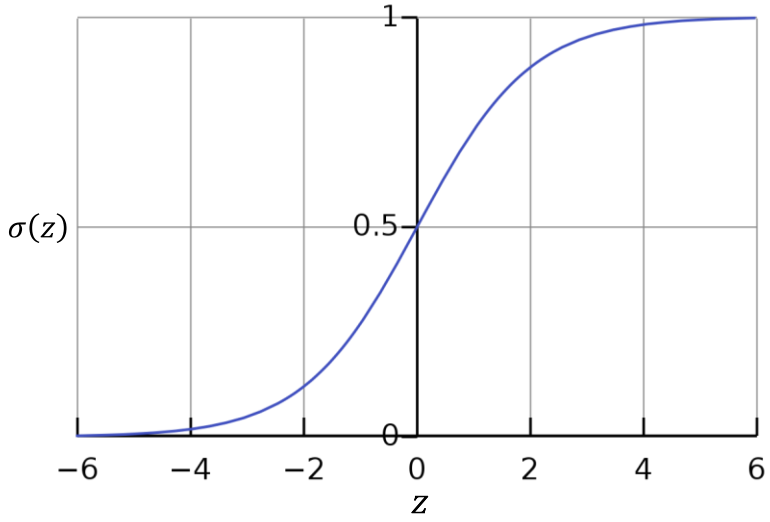
How do we avoid this issue?

- The loss function hates when you make correct predictions with high confidence!
- If label y=1, it's more unhappy about predictions $\hat{y}$ = 10 than $\hat{y}$ = 0

Attempt: 3: Logistic Activation Function

- There's obviously no reason to predict values outside [0, 1].
- We can squash $\hat{y}$ into this interval using a logistic function:

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



$$z = \boldsymbol{\theta}^{\mathrm{T}}\mathbf{x} + b$$
$$\hat{y} = \sigma(z)$$
$$\mathcal{L}_{SE}(\hat{y}, y) = \frac{1}{2}(y - \hat{y})^2$$

- Used in this way, σ is called an activation function, and z is called the logit.

What's the issue with this?

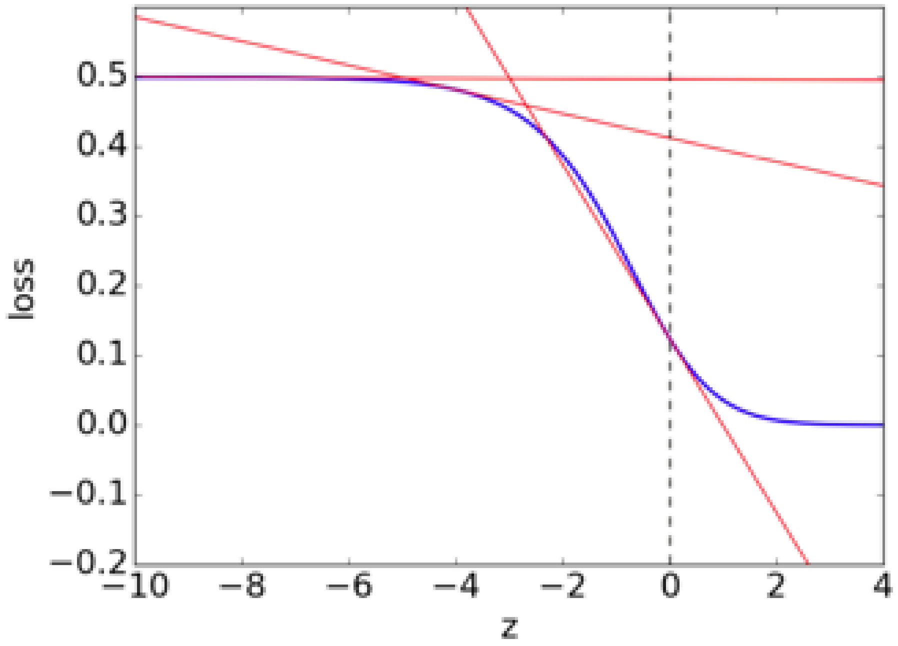
Attempt: 3: Logistic Activation Function

- The problem:
  - In gradient descent, a small gradient (in magnitude) implies a small step.
  - If the prediction is really wrong, shouldn't you take a large step?

$$\frac{\partial \mathcal{L}_{SE}}{\partial \theta_j} = \frac{\partial \mathcal{L}_{SE}}{\partial z} \frac{\partial z}{\partial \theta_j}$$

$$\theta_i \leftarrow \theta_i - \alpha \frac{\partial \mathcal{L}_{SE}}{\partial \theta_i}$$

Plot loss $\mathcal{L}_{SE}$ as a function of z



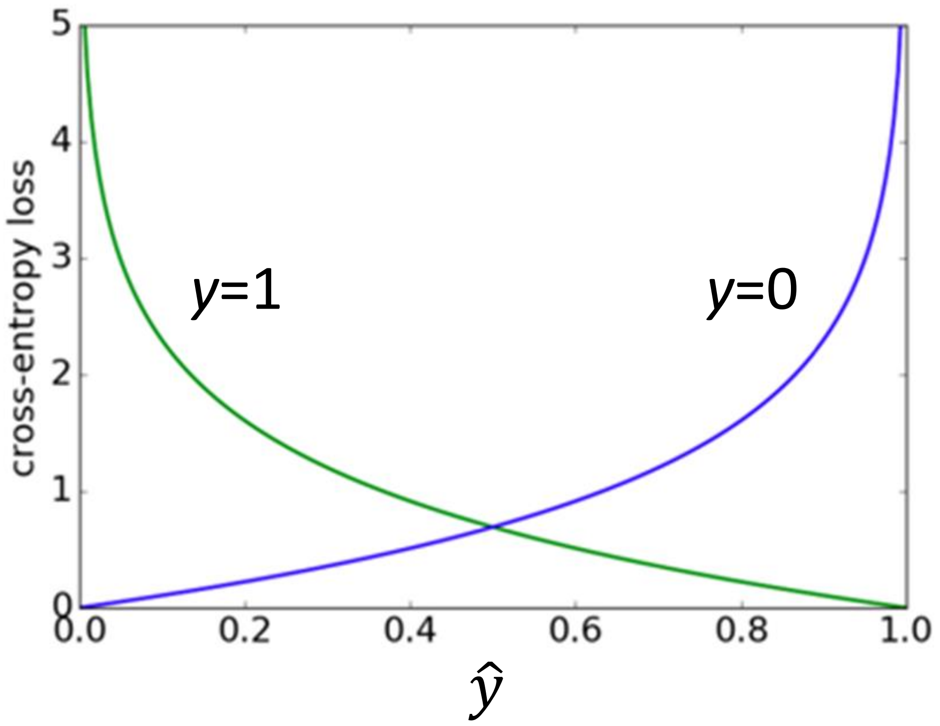
What should loss look like?

Logistic Regression

- Because the prediction $\hat{y} \epsilon$ [0, 1], we can interpret it as the estimated probability that the label is positive (y = 1).
- Being 99% confident in the wrong answer is much more wrong than being only 90% confident.
- **Cross-entropy loss captures** this intuition:

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

$$= -\mathrm{y} \log \hat{y} - (1-\mathrm{y}) \log(1-\hat{y})$$



Logistic Regression

- **Computation Problem:** what if y = 1 but you're really confident it's a negative example (z << 0)?

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

- If y is small enough, it may be numerically zero. This can cause very subtle and hard-to-find bugs:

$$\hat{y} = \sigma(z) \qquad \Rightarrow \hat{y} \approx 0$$

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

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

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

Example:

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

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

$$= -y\log\left(\frac{1}{1+e^{-z}}\right) - (1-y)\log\left(1-\frac{1}{1+e^{-z}}\right)$$

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

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

$$\frac{\partial L_{LCE}}{\partial \theta} = \frac{\partial L_{LCE}}{\partial z} \cdot \frac{\partial z}{\partial \theta} \checkmark$$

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

$$\frac{\partial L_{LCE}}{\partial z} = \frac{\partial}{\partial z} y\log(1+e^{-z}) + \frac{\partial}{\partial z}(1-y)\log(1+e^{z})$$

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

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

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

$$= -y(1-\hat{y}) + (1-y)\hat{y}$$

$$= -y + \cancel{y\hat{y}} + \hat{y} - \cancel{y\hat{y}}$$

$$= \underline{\underline{\hat{y} - y}}$$

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

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

$$\frac{\partial L_{LCE}}{\partial \theta_j} = (\hat{y}-y) \cdot \frac{\partial z}{\partial \theta}$$

$$= \underline{(\hat{y}-y)\, x_j}$$

Weight Updates

- Comparison of gradient descent updates:
  - Linear regression:

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

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

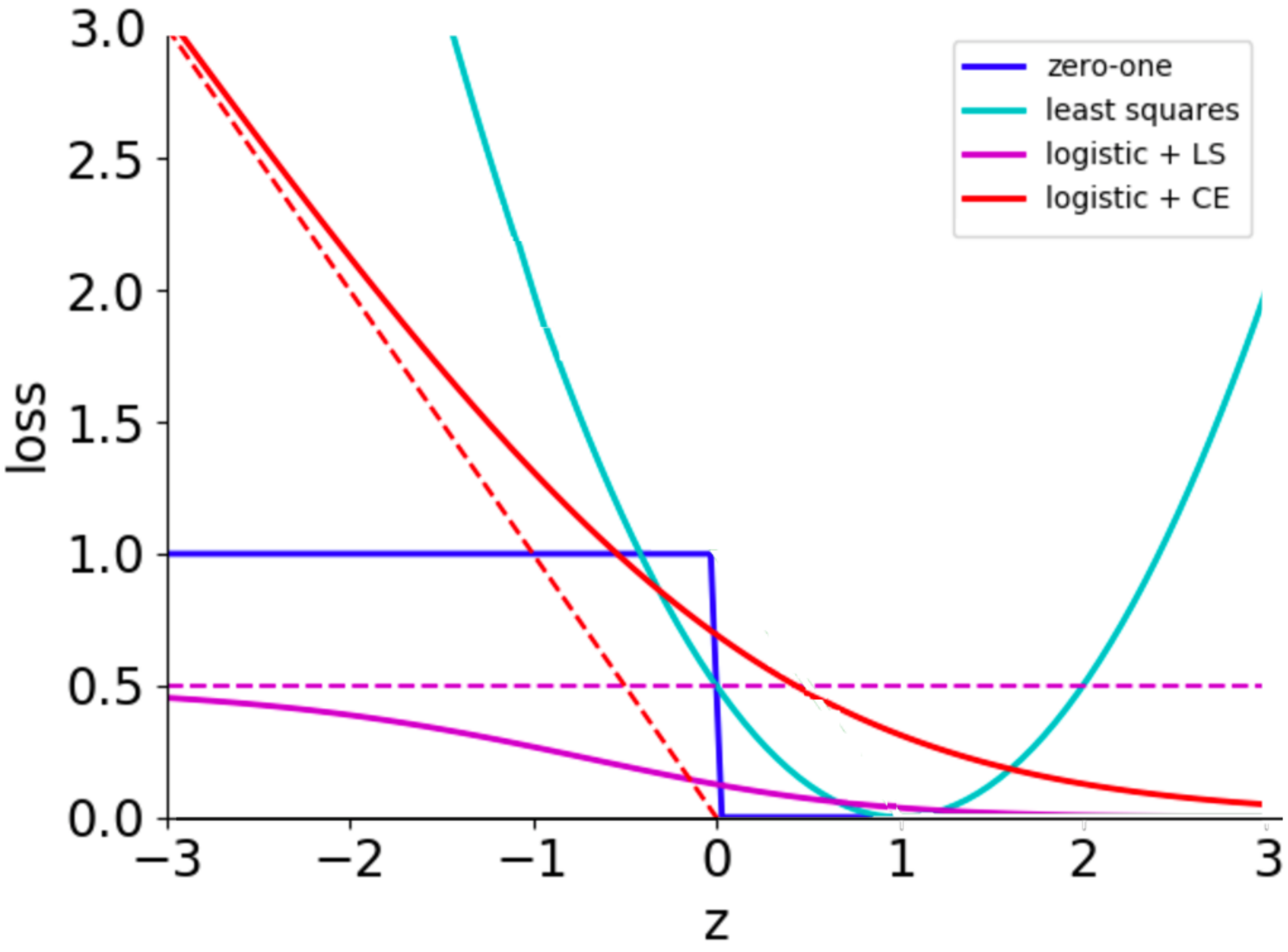
  - Logistic regression:

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

Using activation function

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

Loss Summary



Assume this is for a binary classification problem where the sample assessed has a ground truth of “1” i.e. positive class

Multiclass Classification

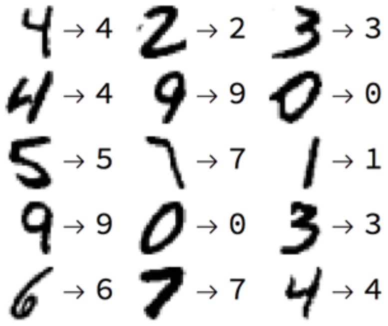
Multiclass Classification

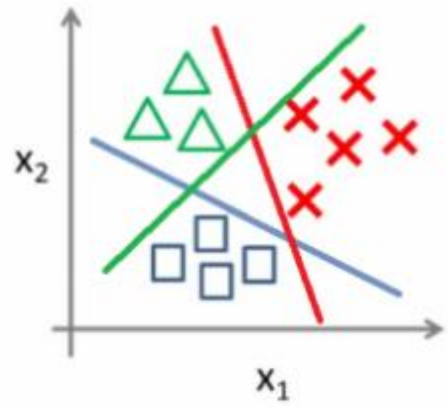
- What about classification task with more than two categories?

- 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:

$$y = [0, \ldots\ldots\ldots 0,\ 1,\ 0,\ \ldots\ldots\ldots 0]$$

entry k is a 1, all others are 0





Multiclass Classification

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

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

- Vectorized:

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

Activation Function

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

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

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

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

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:

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

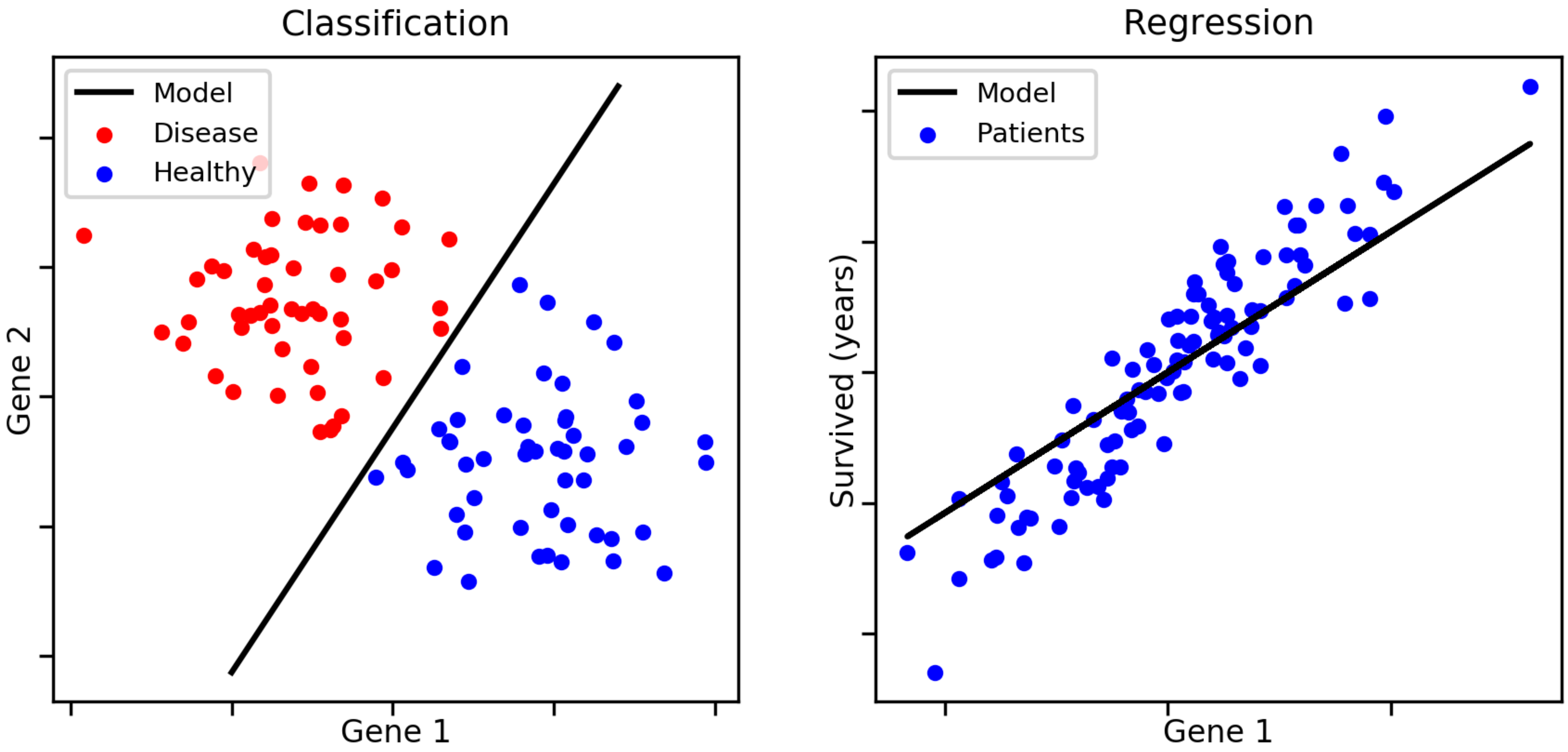
$$\hat{\mathbf{y}} = \mathrm{softmax}(\mathbf{z})$$

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

- Gradient descent updates:

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

Summary


Classification
Model
Disease
Healthy
Gene 2
Gene 1
Regression
Model
Patients
Survived (years)
Gene 1

Neural Networks

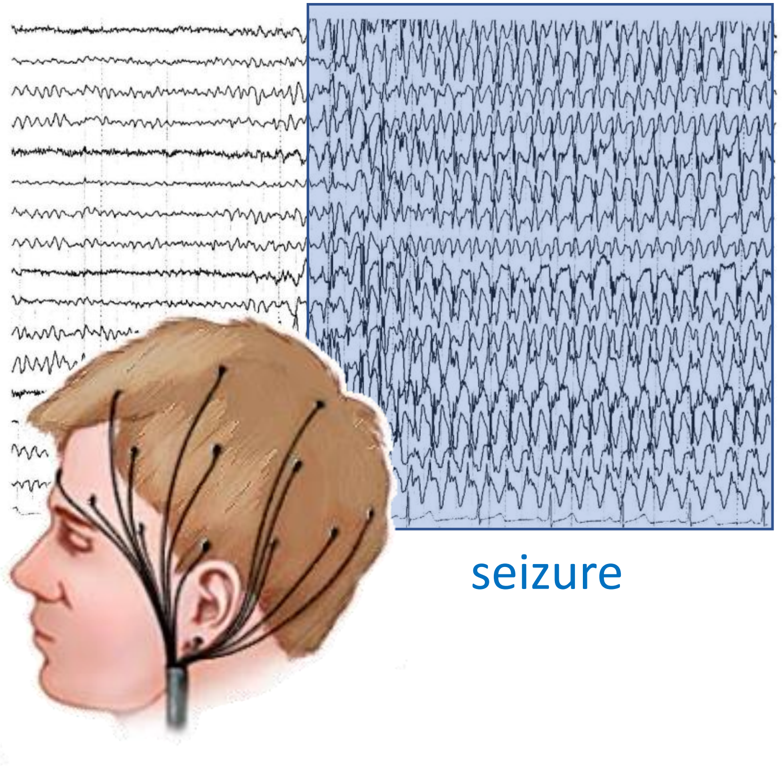
Challenges with Feature Maps

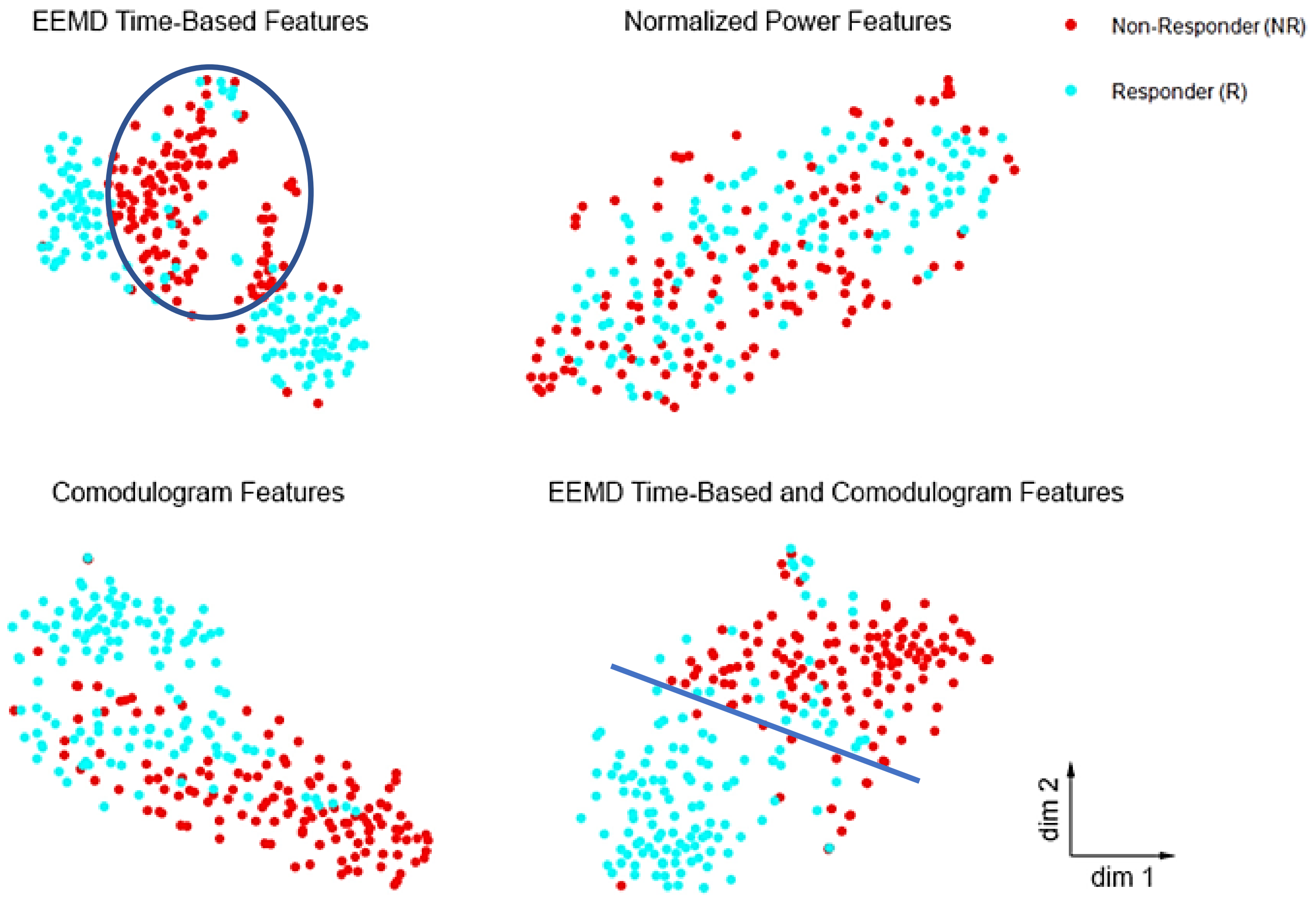
- Feature maps can be useful for solving nonlinear regression and classification problems.

- 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.





Source: Colic et al, 2016

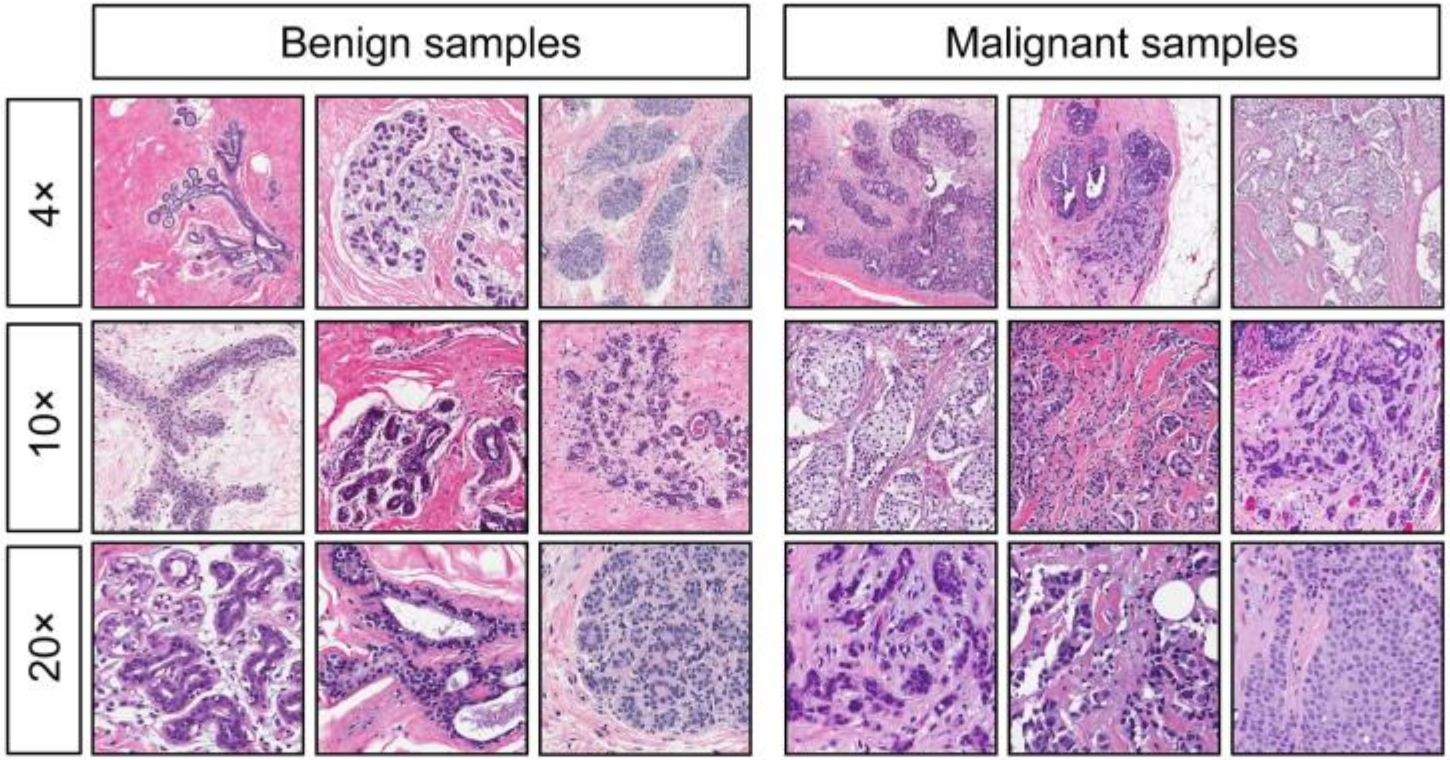
Challenges with Feature Maps

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)

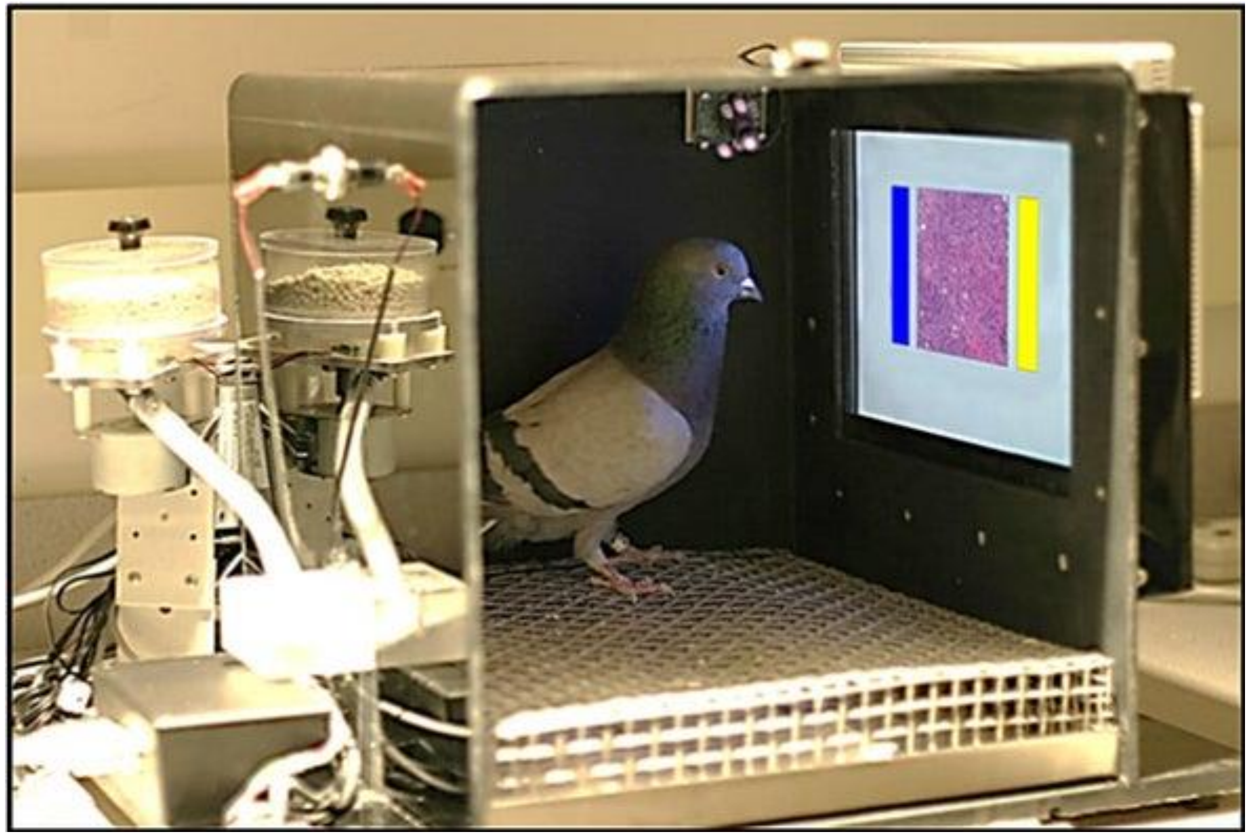
- Pathologists/radiologists train for years to do this!
- How would you solve this problem?



Source: [Levenson et al., 2015]

Maybe We Can Use Pigeons

- **Train a Pigeon!**
- A new 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: Levenson et al., 2015

Maybe We Can Use Pigeons

Training Algorithm:

1. 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?

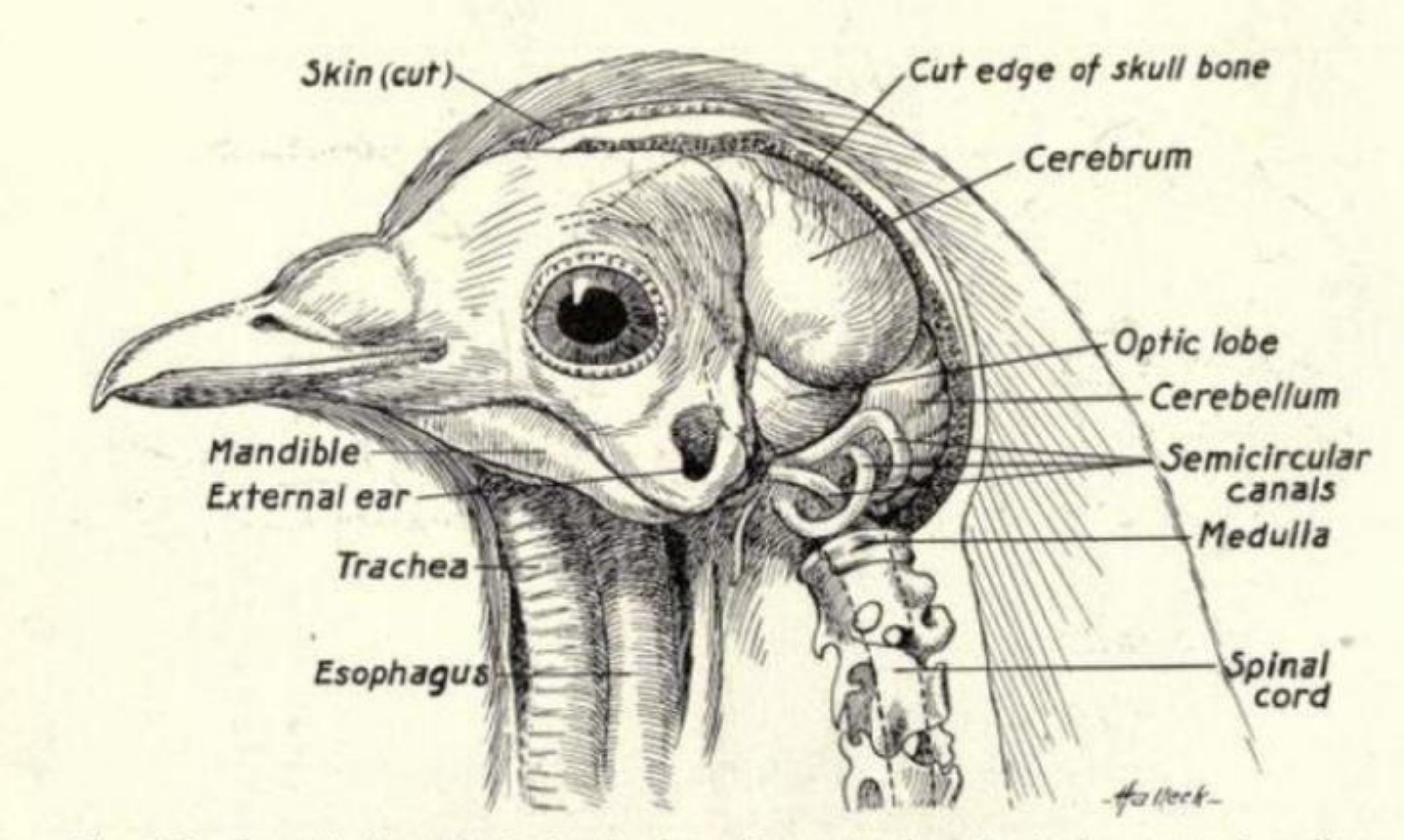
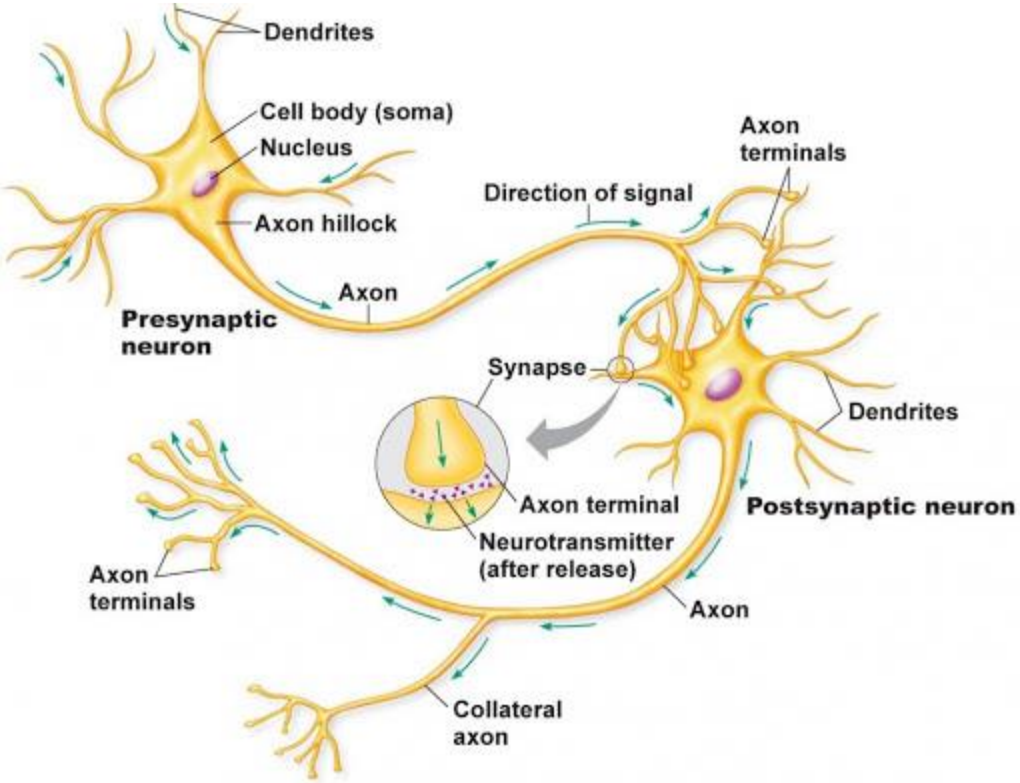


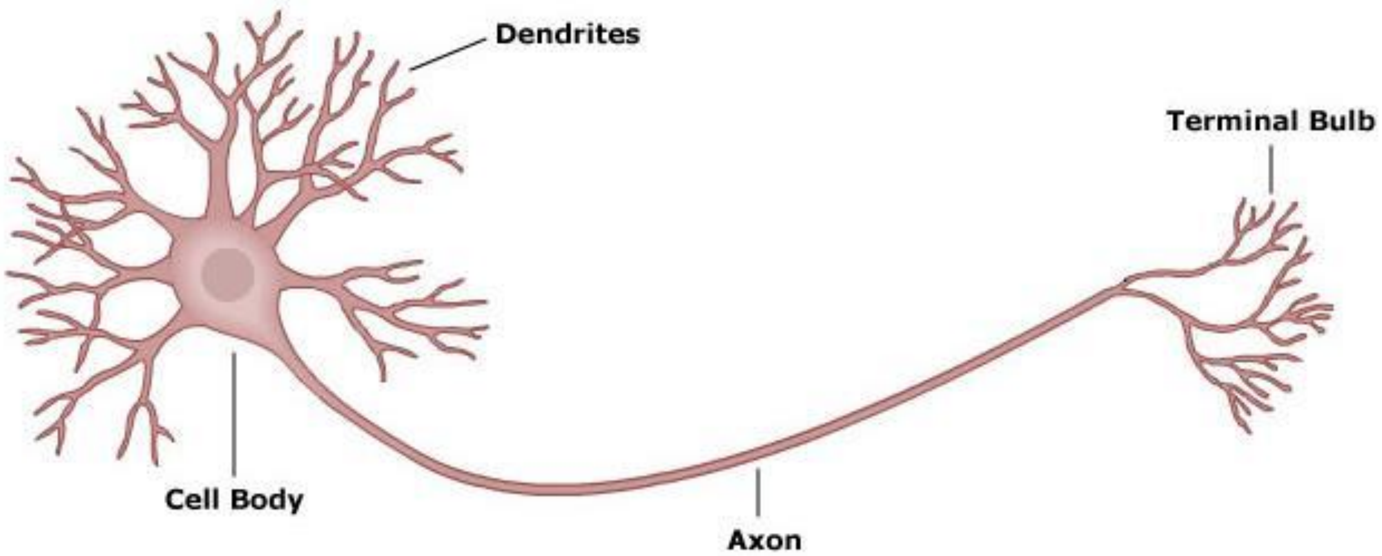
Fig. 167.—Lateral view of the head of a pigeon showing the brain, external auditory opening and semicircular canals.



Source: [Letsmaketech]

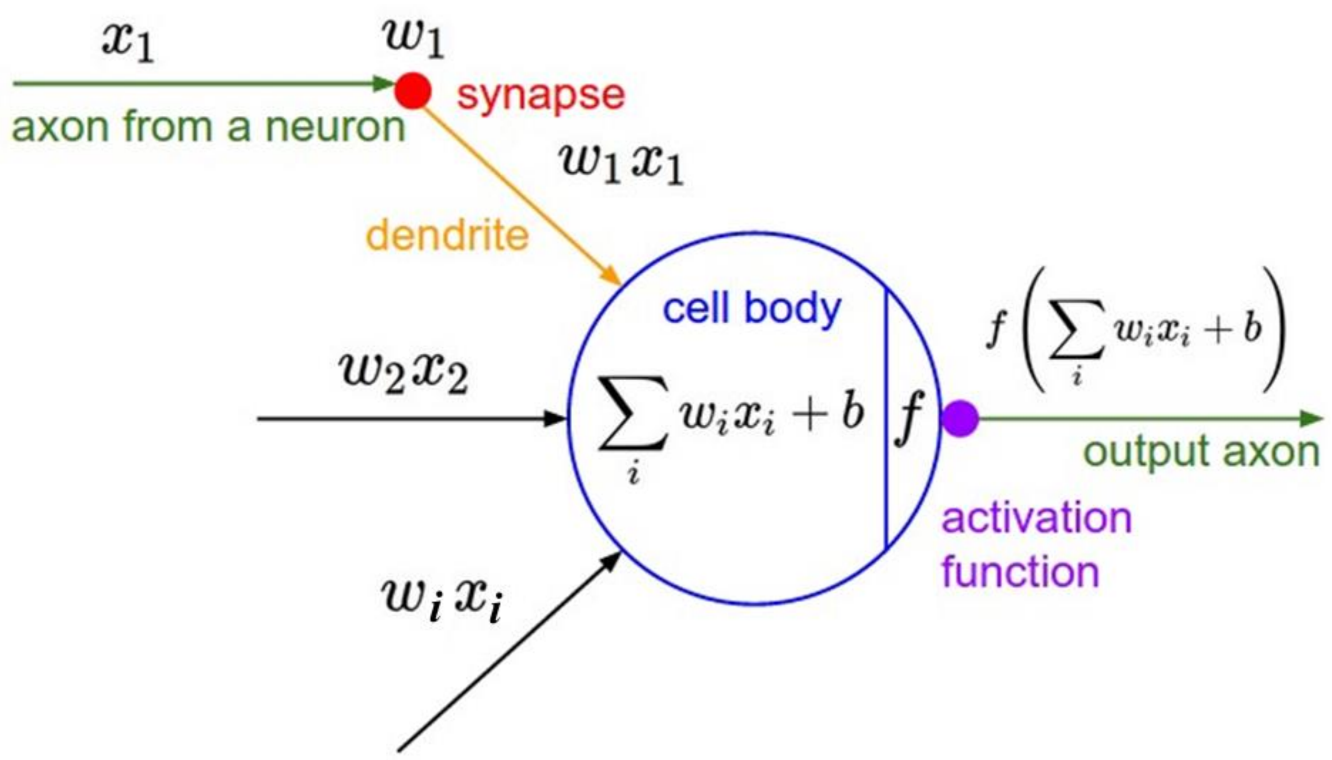
Simplified Neuron Anatomy

- **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

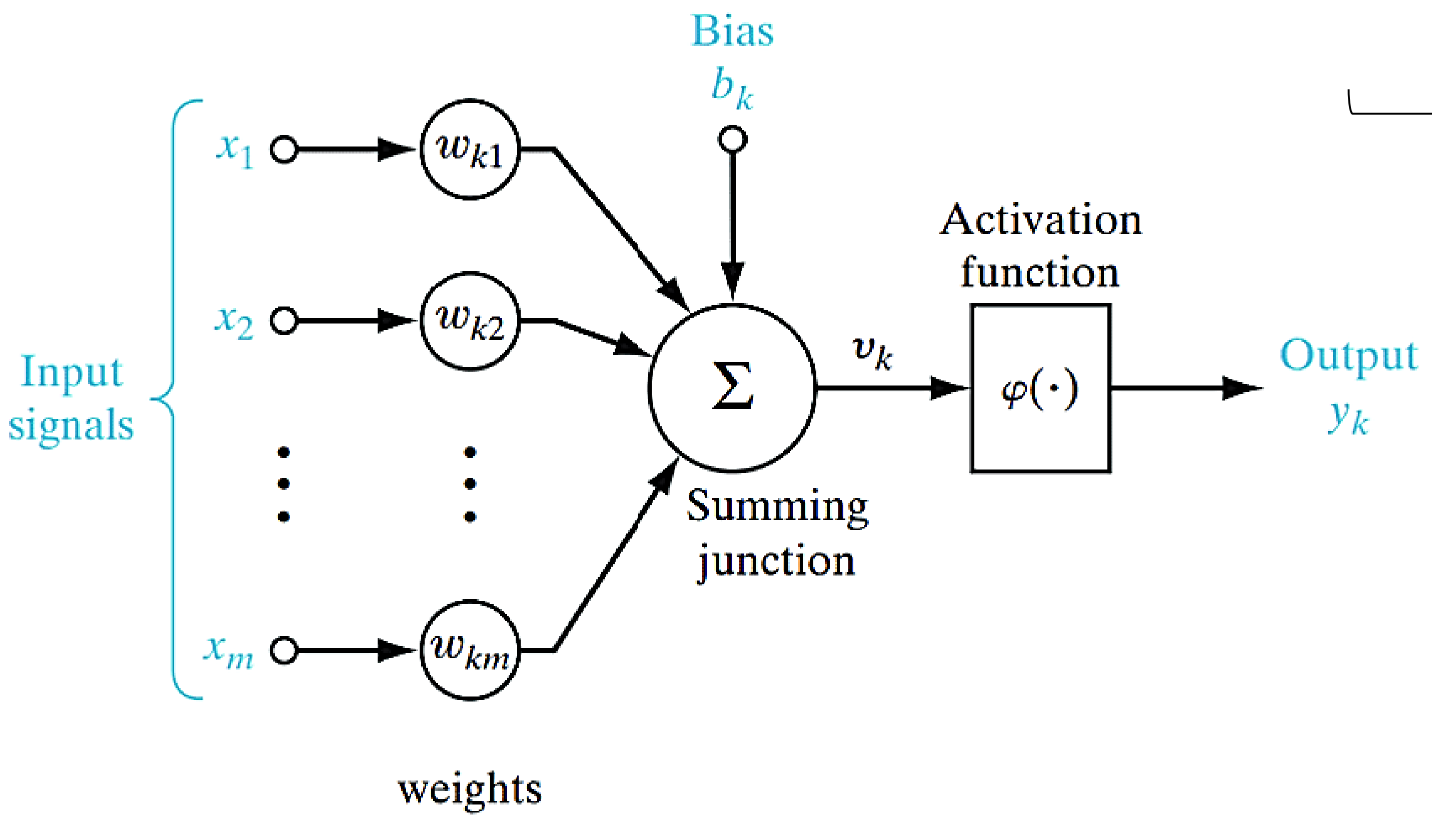
- Maybe we're note quite ready for pigeon doctors, but we can use the next best thing… an artificial pigeon (**artificial neural network)**



Artificial Neural Network

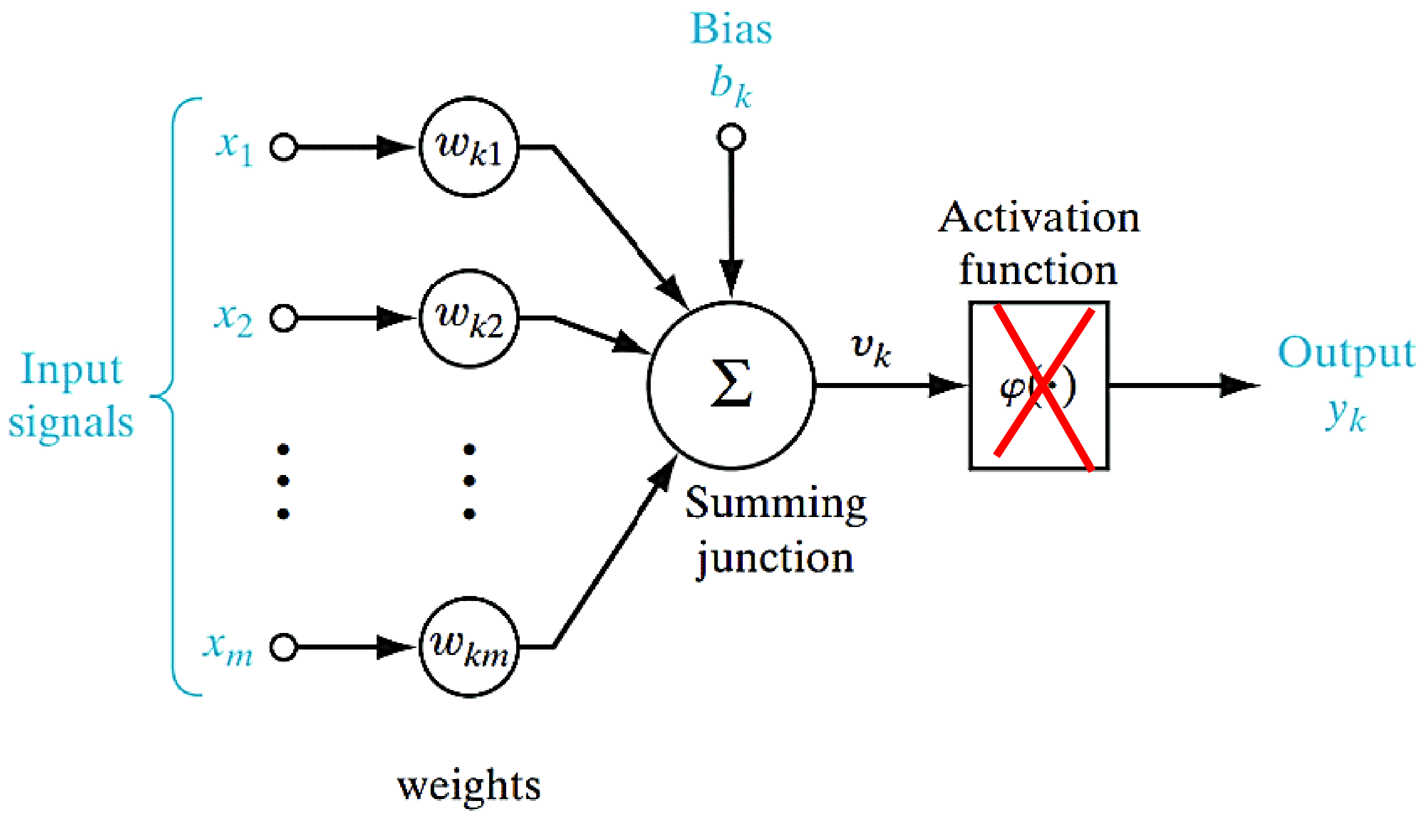
$$y = \varphi\left(\underbrace{\sum_{i=0}^{p} w_i x_i = \mathrm{w}^T \mathrm{x}}\right)$$

does this look familiar?



Artificial Neural Network

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



Logistic Regression!

What will we have if we exclude the activation function?

Training / Learning Parameters

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

Means Squared Error
(regression)

$$\frac{1}{2N}\sum_{n=1}^{N}\|y_n - t_n\|^2$$

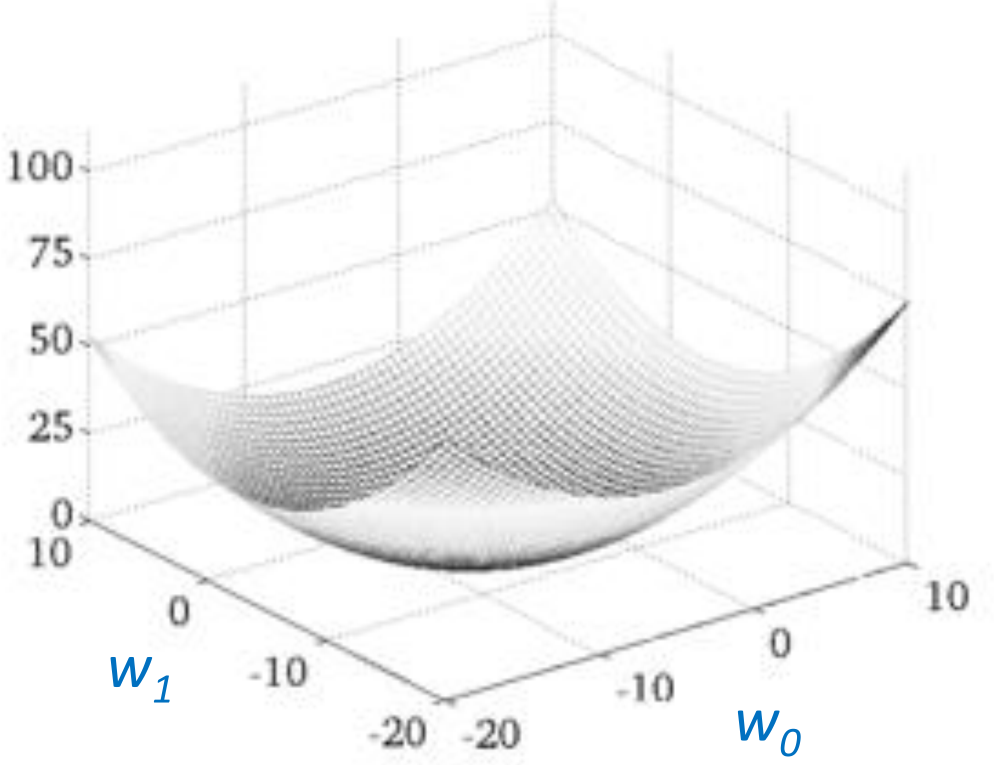
Cross-Entropy Loss
(classification)

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

implement gradient descent to learn parameters!

Gradients

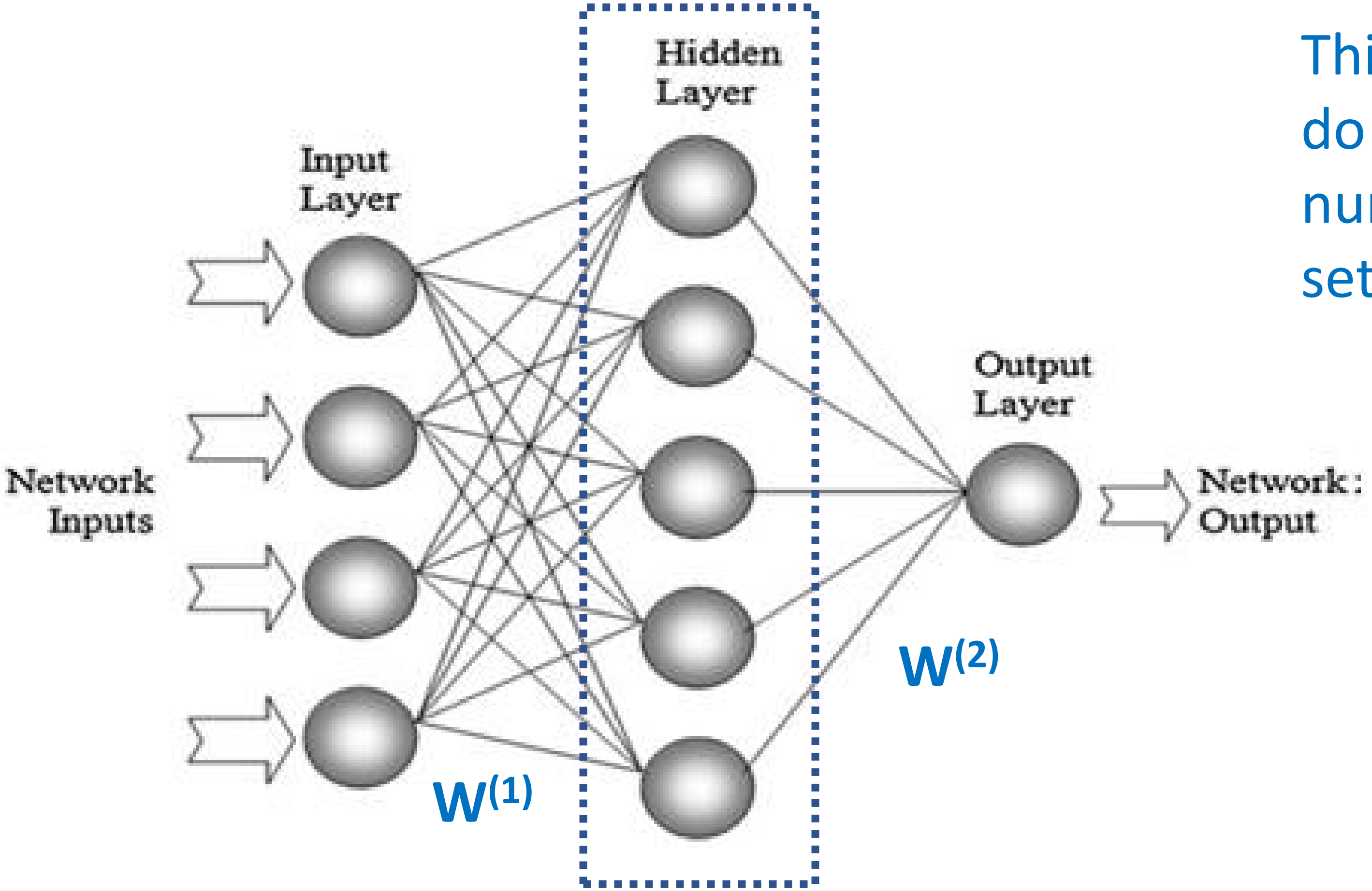
- For this simple version of neural networks all the gradient calculations are the same as we've seen earlier…
- It probably wouldn't be a surprise to find out that to train this simple ANN is a convex problem (not true for all ANNs).



parameters (w) can be multidimensional

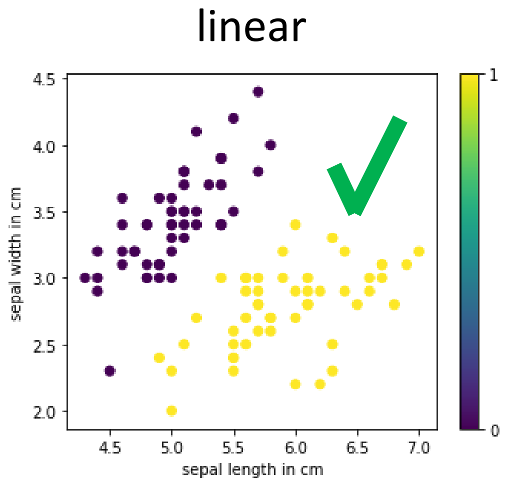
Achieving Nonlinearity

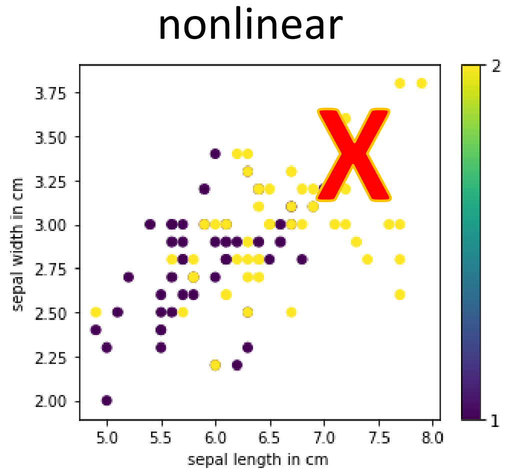
Add More Neurons?

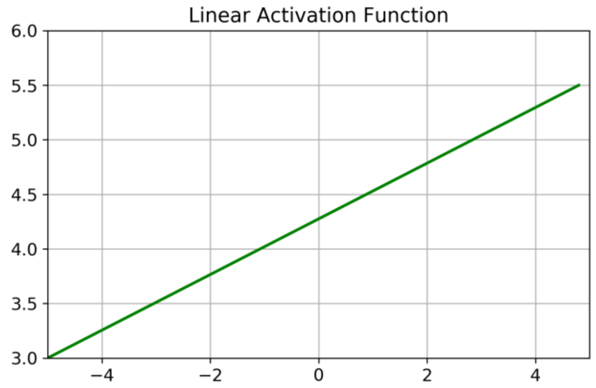


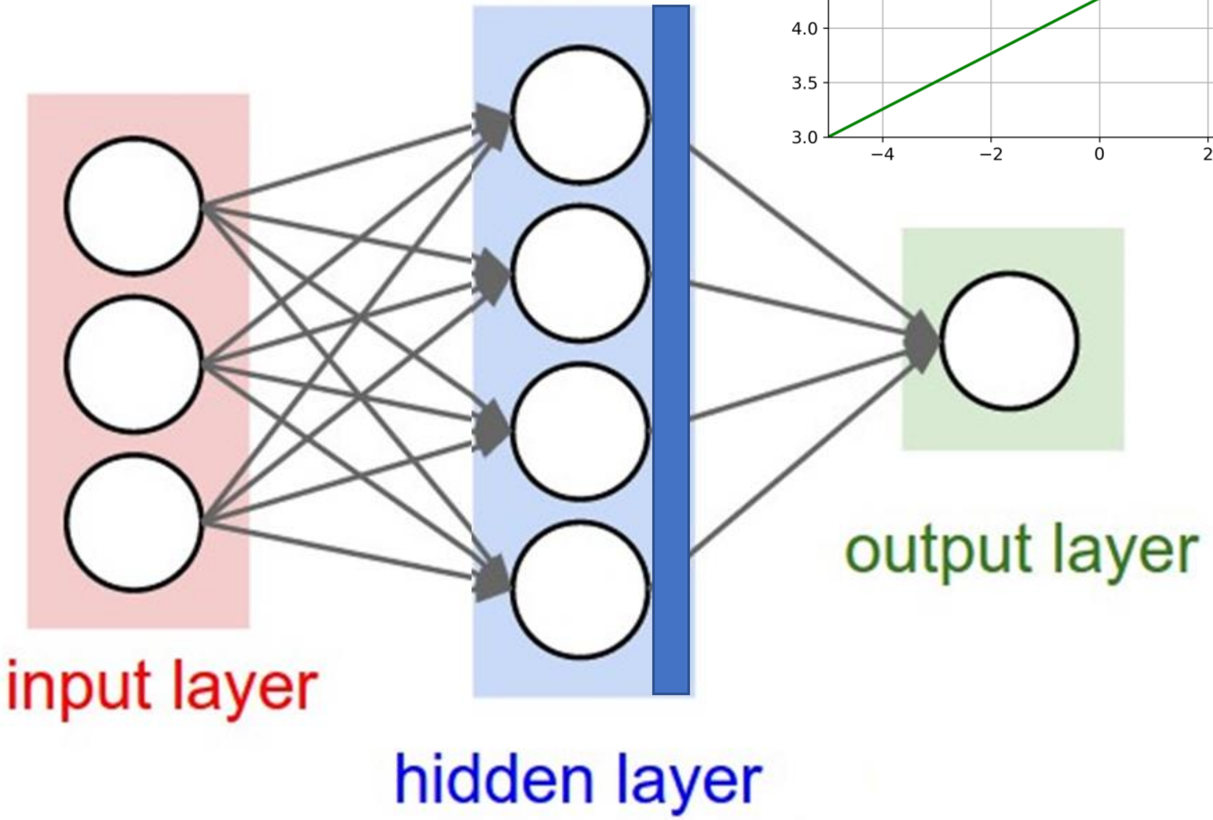
This is a 2-layer neural network. We do not count the input layer, so the number of layers equal number of sets of weights and biases.

2-layer ANN with Linear Activation









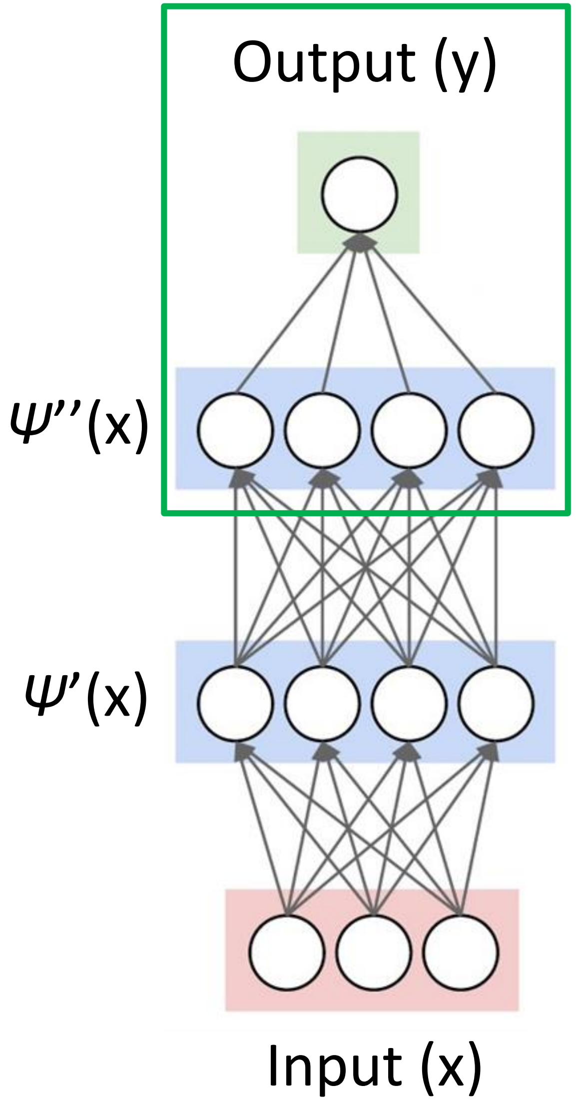
Expressive Power

- 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.

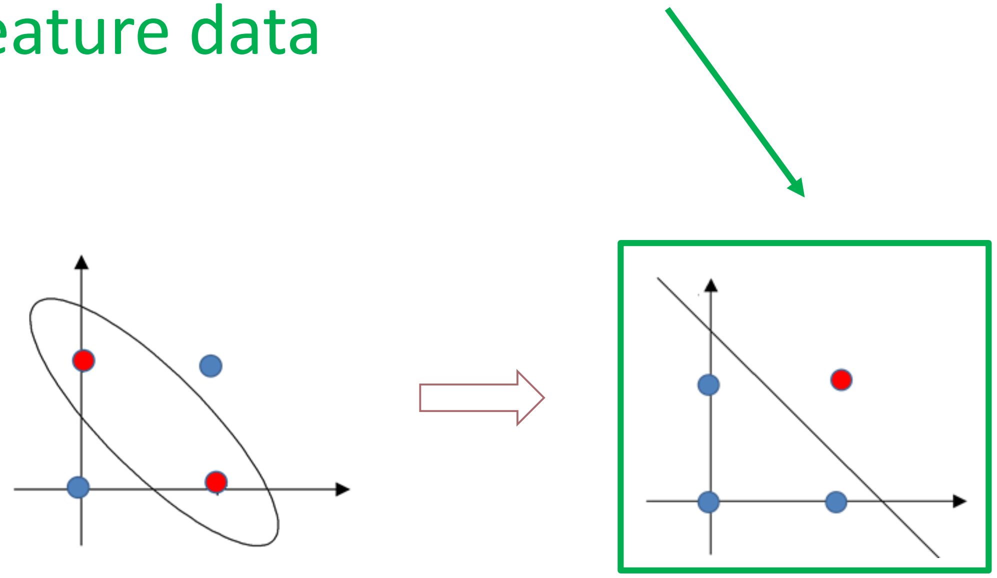
$$\hat{\mathbf{y}} = \underbrace{\mathbf{W}^{(1)}\mathbf{W}^{(2)}\mathbf{W}^{(3)}}_{\mathbf{W}'}\mathbf{x}$$

- Deep linear networks are no more expressive than **linear regression!**

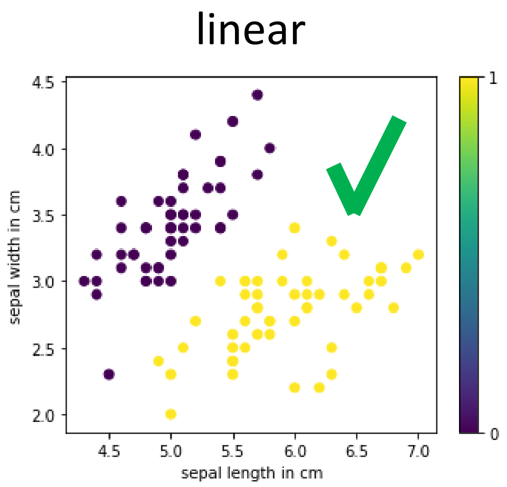
Need an Activation Function

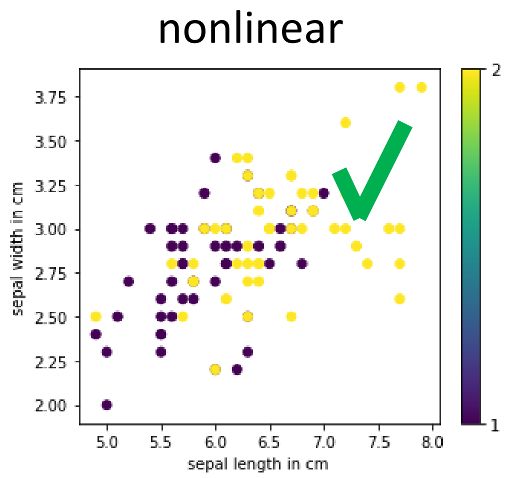


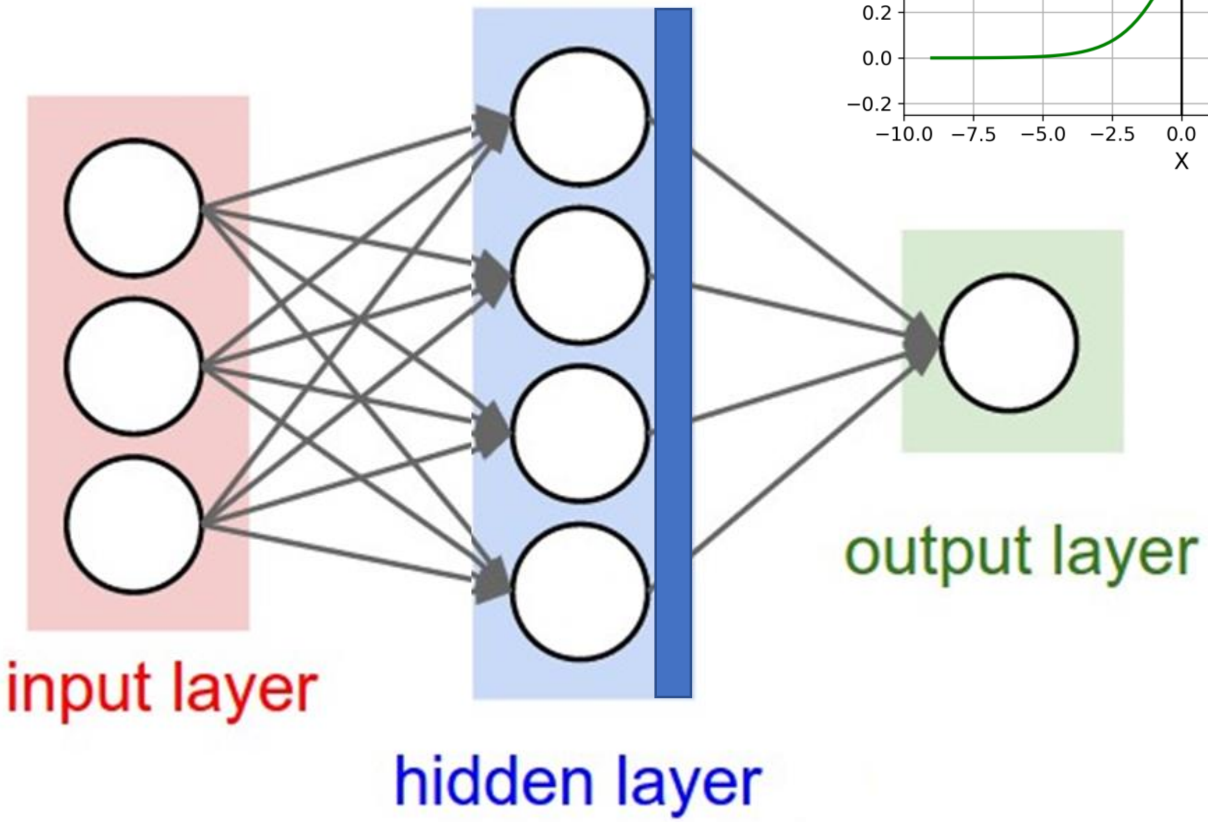
- Neural Networks can be viewed as a **way of learning features**
- The goal being that the final layer is presented with linearly separable feature data

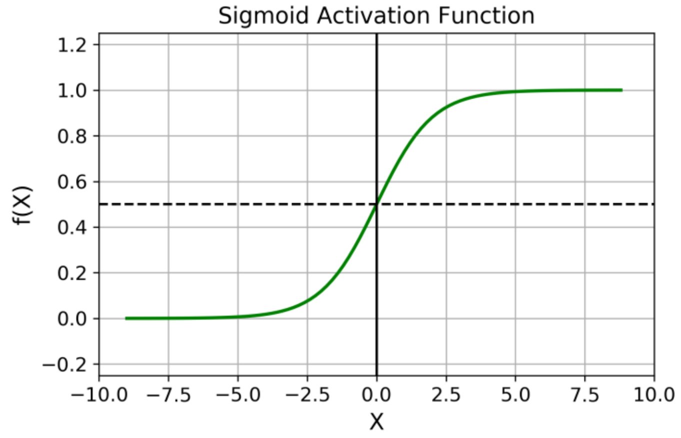


2-layer ANN with Nonlinear Activation







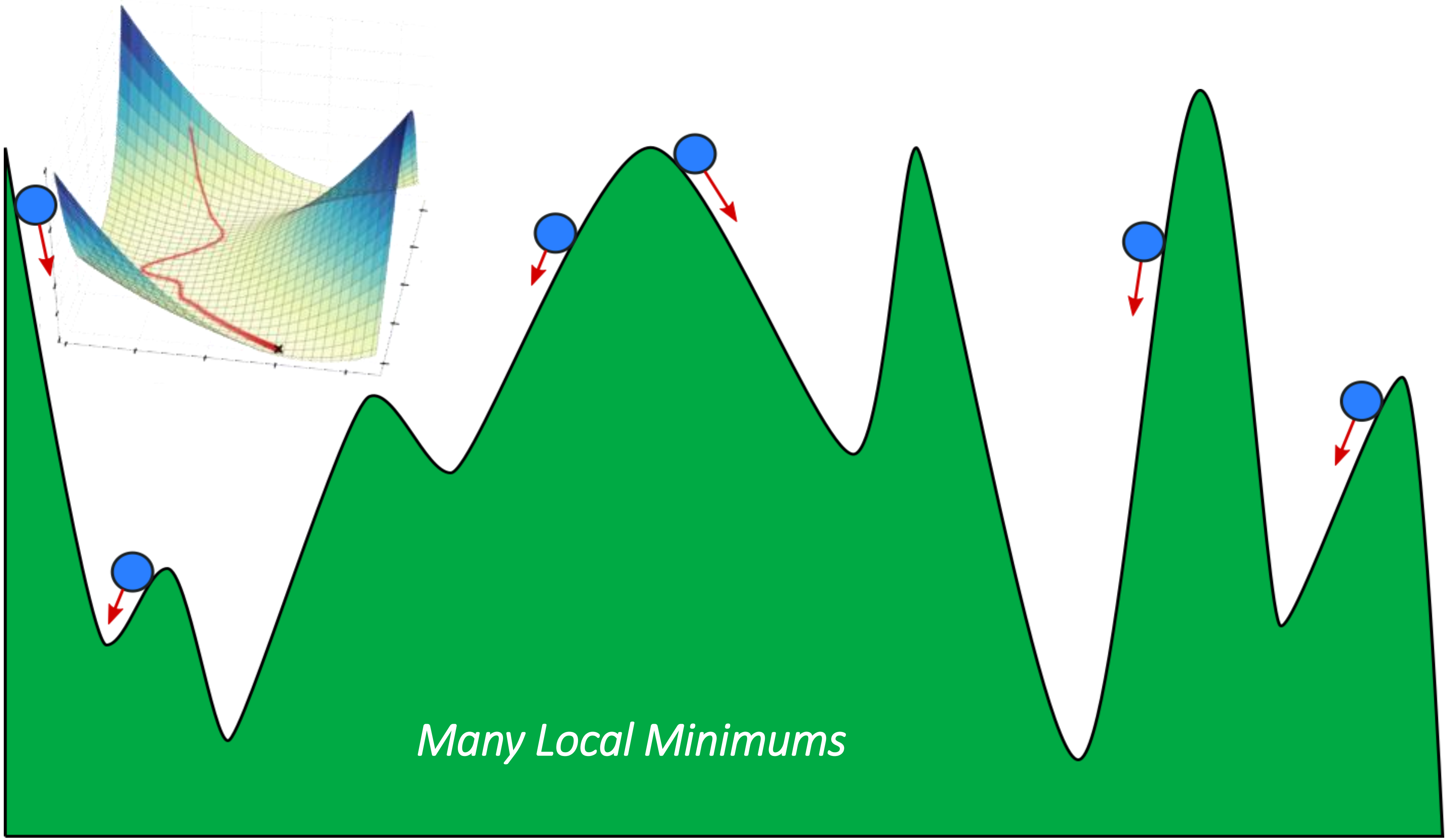


Expressive Power

- 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!

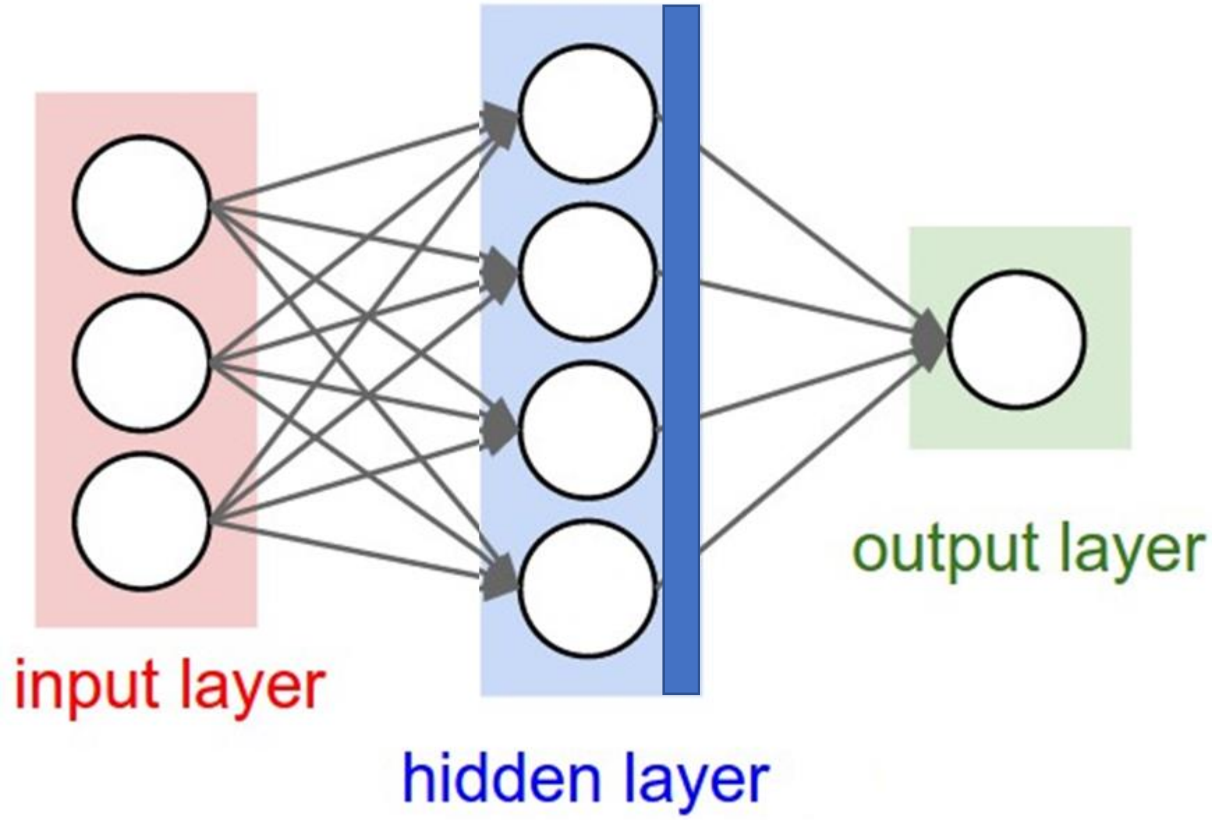
Tuning Neural Networks

Changing ANN Architecture:

- Number of hidden units
- Weights
- Activation Functions

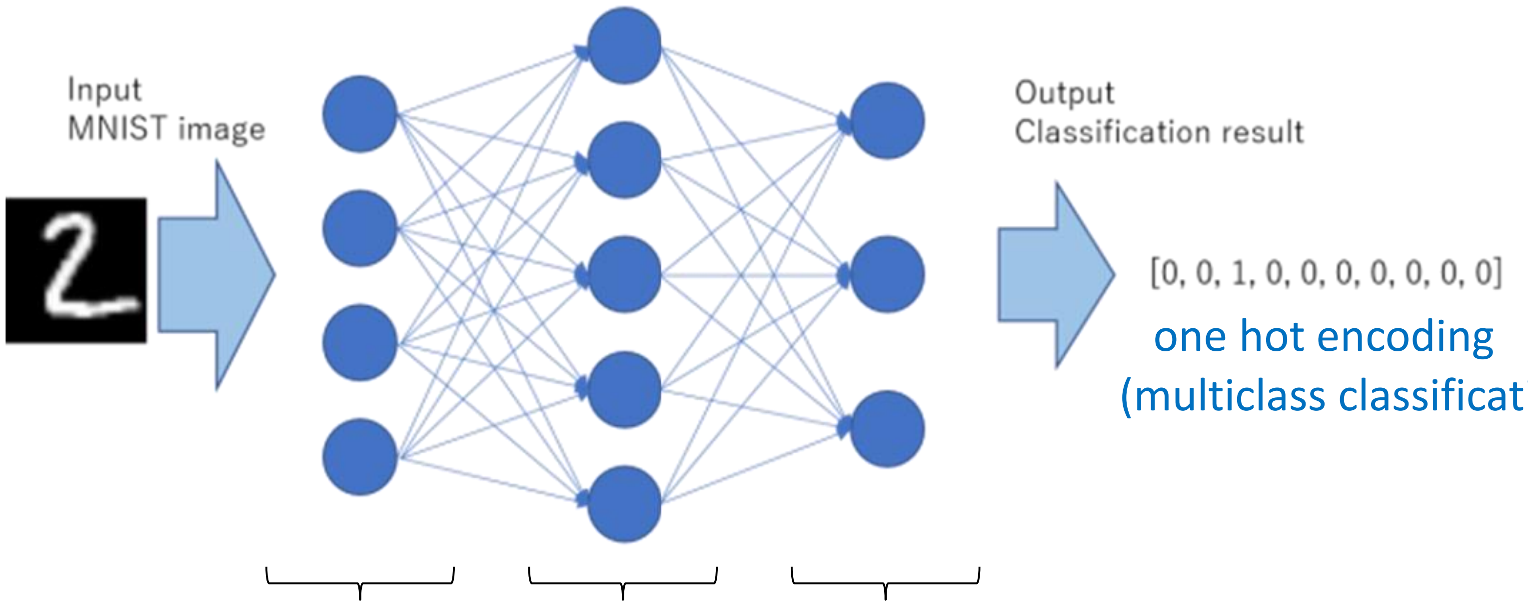
Applying Different Training Techniques:

- Number of iterations
- Learning rate and adaptive learning rate
- Momentum
- Batching of Data
- Regularization
- Dropout
- Feature Augmentation
- Many more…



Take Home Exercise

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 squared error loss.



one hot encoding
(multiclass classification)

Input Layer   Hidden Layer   Output Layer

Next Time

- Week 10 Support Session
  - Project 4 – Linear Regression due April 1 at 11pm

- Week 11 Lecture – Deep Learning (and More)
  - Monte Carlo Methods
  - Sampling Methods
  - **Neural Network Architectures**
  - **Automatic Differentiation**
  - Discrete Optimization