Neural Networks II

CMSC 422

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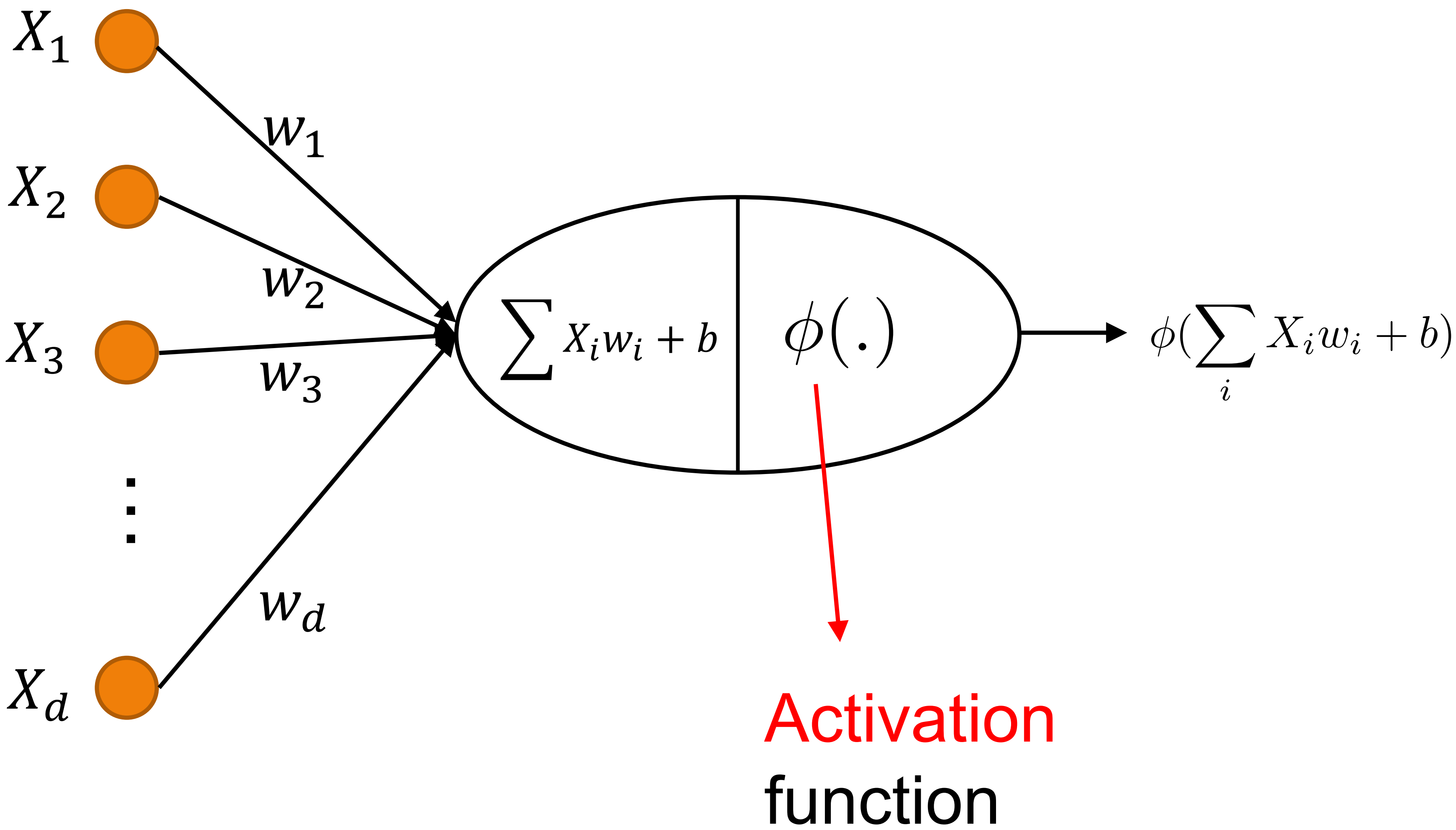
Today's topics

- Neural Networks for the regression problem

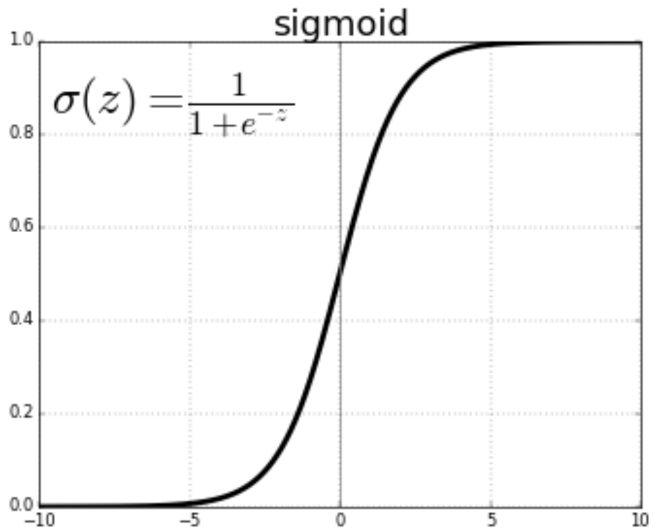
- Back Propagation: SGD+ Chain rule

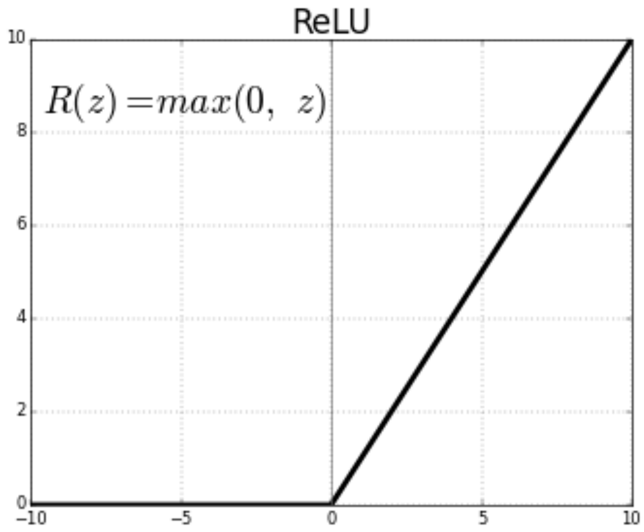
Neural Unit

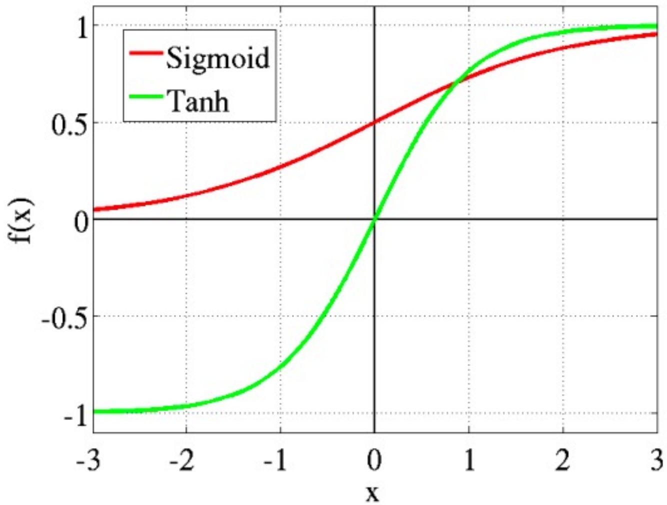


X_1
X_2
X_3
X_d
w_1
w_2
w_3
w_d
$\sum X_i w_i + b$
$\phi(.)$
$\phi(\sum_i X_i w_i + b)$
Activation
function

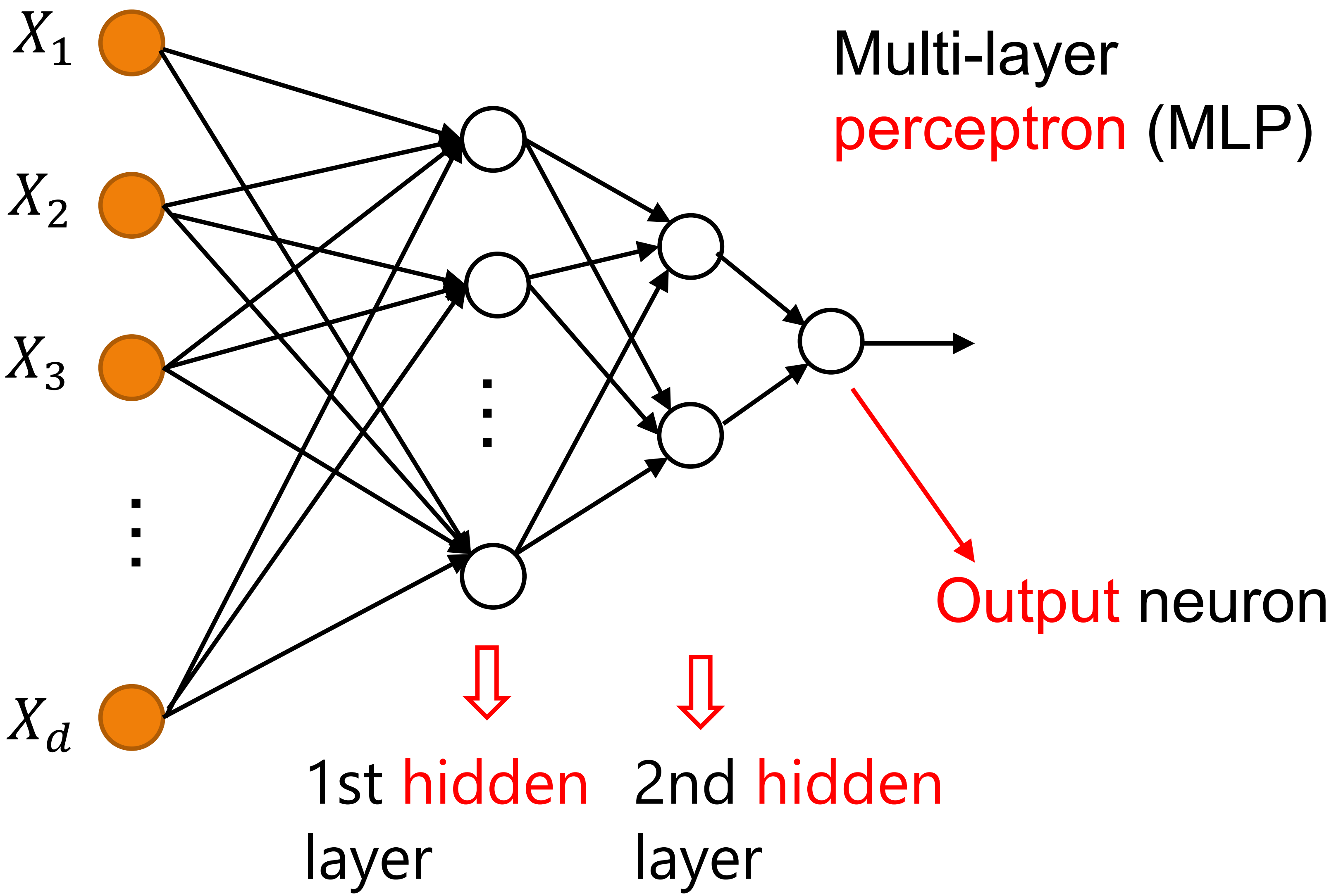
Popular Activation Functions



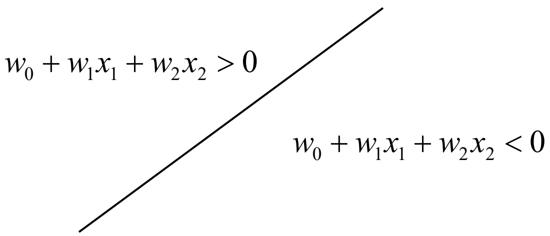


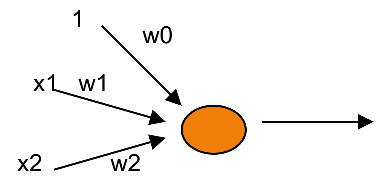


Multi-Layer Neural Network

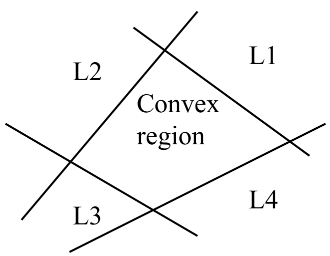


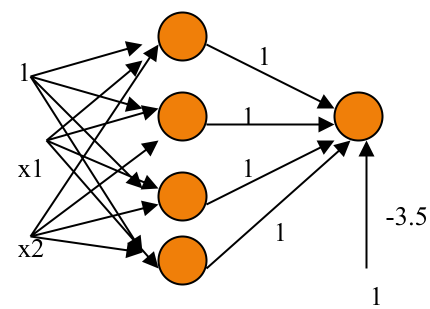
Types of decision regions



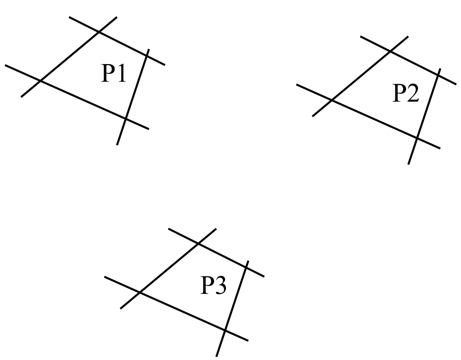


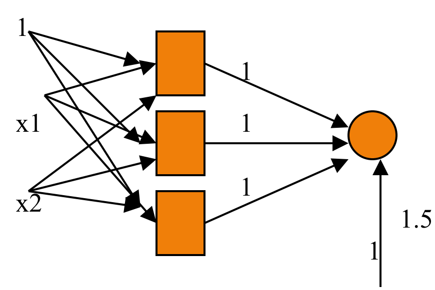
Network with a single node





One-hidden layer network that realizes the convex region: each hidden node realizes one of the lines bounding the convex region





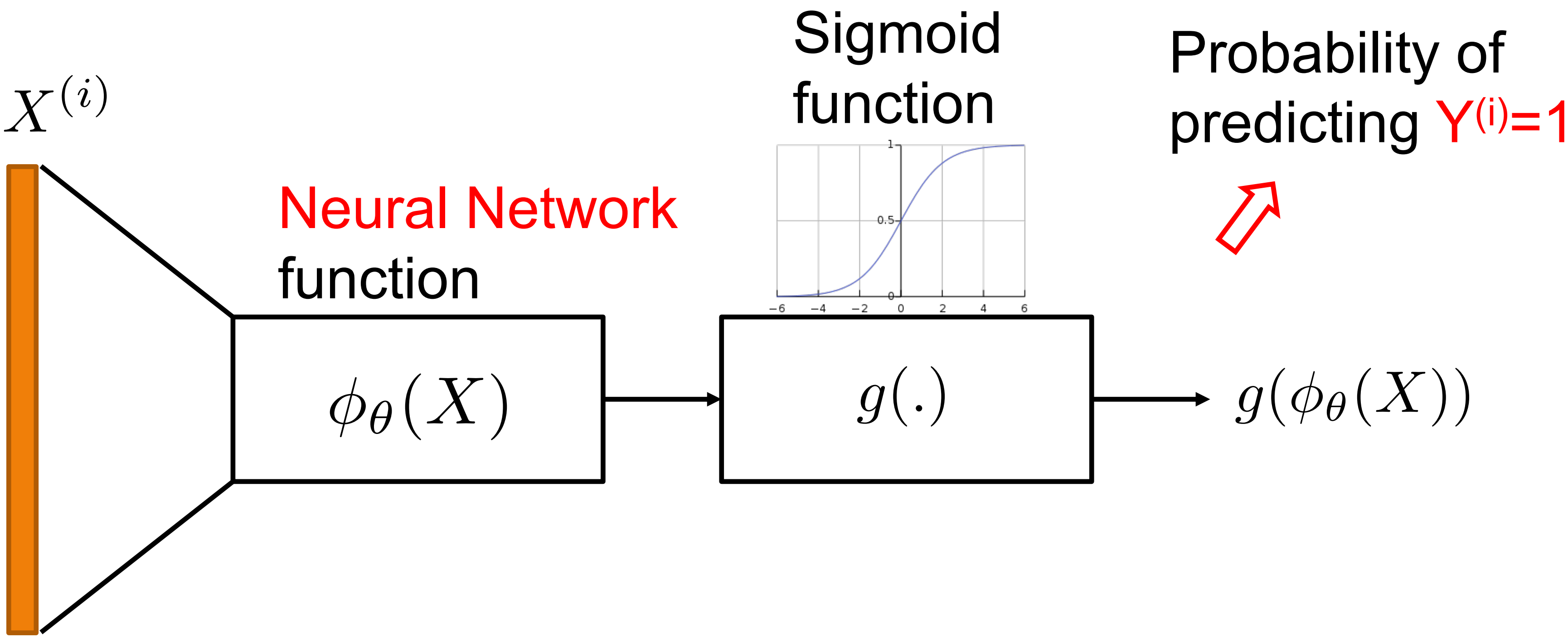
two-hidden layer network that realizes the union of three convex regions: each box represents a one hidden layer network realizing one convex region

Discussion

- 2-layer perceptron lets us
  - Discover more complex decision boundaries than perceptron
  - Learn combinations of features that are useful for classification

- Key design question: How many hidden units?
  - More hidden units yield more complex functions
  - Fewer hidden units requires fewer examples to train

Classification using Neural Network



What is θ ?

Compute model parameters using cross-entropy loss opt:

$$\max_{\theta} \quad \sum_{i=1}^{N} Y^{(i)} \log g(\phi_\theta(X^{(i)})) + (1 - Y^{(i)}) \log(1 - g(\phi_\theta(X^{(i)})))$$

Regression Problem

- Learning a functional relationship about a real-valued number, i.e., when y is tomorrow's temperature.

- Training data: $\{(X^{(i)}, Y^{(i)})\}$

$$Y^{(i)} \in \mathbb{R}$$

Regression examples

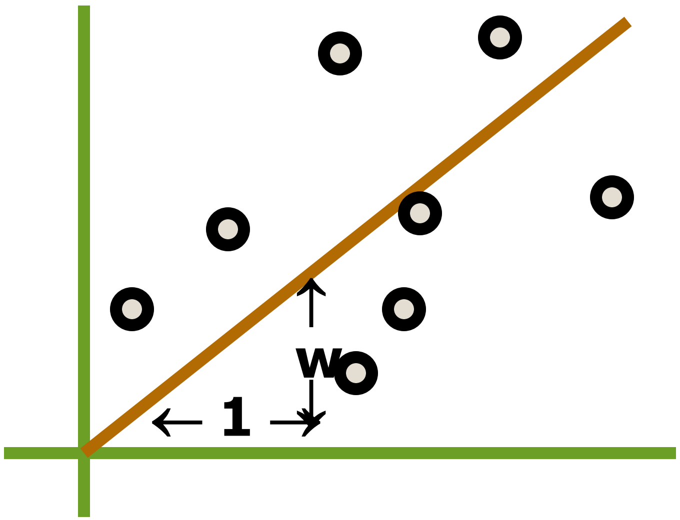
Stock market

Weather prediction

Temperature
72° F

Predict the temperature at any given location

Linear Regression



DATASET

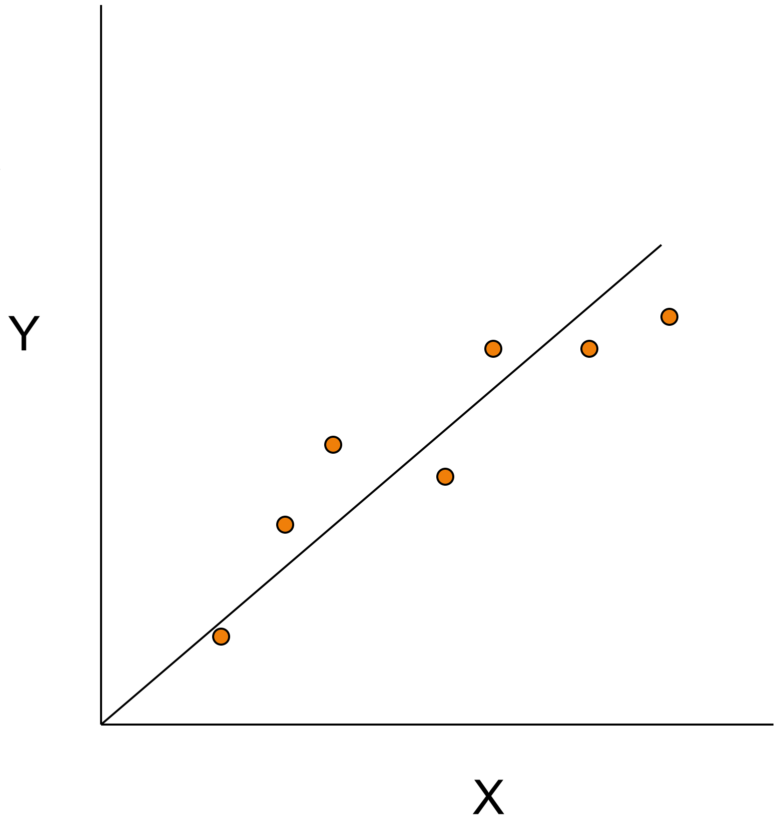
inputs	outputs
$x_1 = 1$	$y_1 = 1$
$x_2 = 3$	$y_2 = 2.2$
$x_3 = 2$	$y_3 = 2$
$x_4 = 1.5$	$y_4 = 1.9$
$x_5 = 4$	$y_5 = 3.1$

Simplest case: Out(x) = w^t x+ b for some unknown w,b.

Given the data, we can estimate w,b.

Linear regression

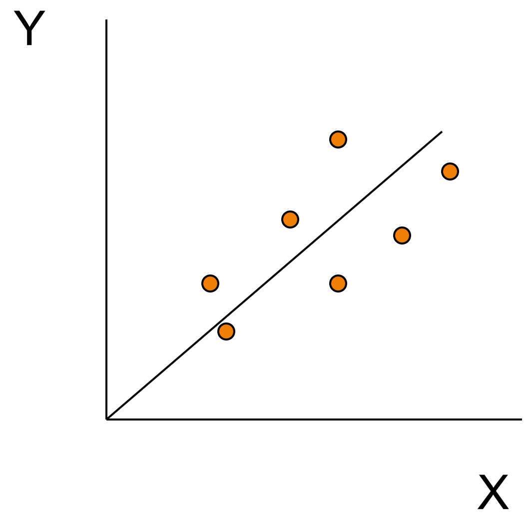
- Given an input x we would like to compute an output y
- For example:
  - Predict height from age
  - Predict Google's price from Apple's price
  - Predict distance from wall from sensors
  - BMI based on height and weight
  - Papers published based on age



Linear regression

Our goal is to estimate *w,b* from a training dataset

Optimization: minimize squared error (least squares)

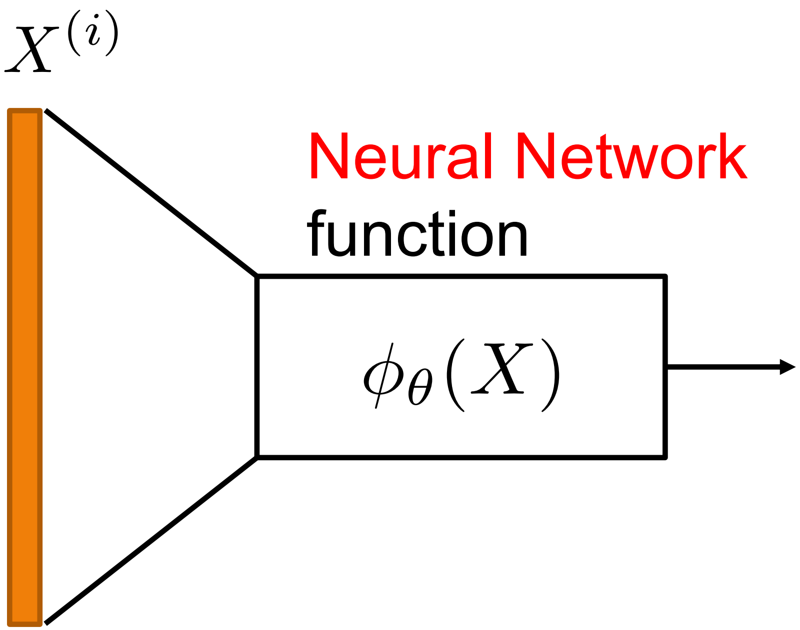


$$\min_{w,b} \sum_{i=1}^{N} (y^{(i)} - \hat{y}^{(i)})^2$$

$$\hat{y}^{(i)} = w^t X^{(i)} + b$$

Why quadratic?

Nonlinear Regression using Neural Network



$$\hat{y}^{(i)} = \phi_\theta(X^{(i)})$$

What is θ ?

Compute model parameters using quadratic loss opt:

$$\min_\theta \sum_{i=1}^{N} (y^{(i)} - \phi_\theta(X^{(i)}))^2$$

Loss functions

Classification Problem

- Hinge loss
- Cross entropy loss

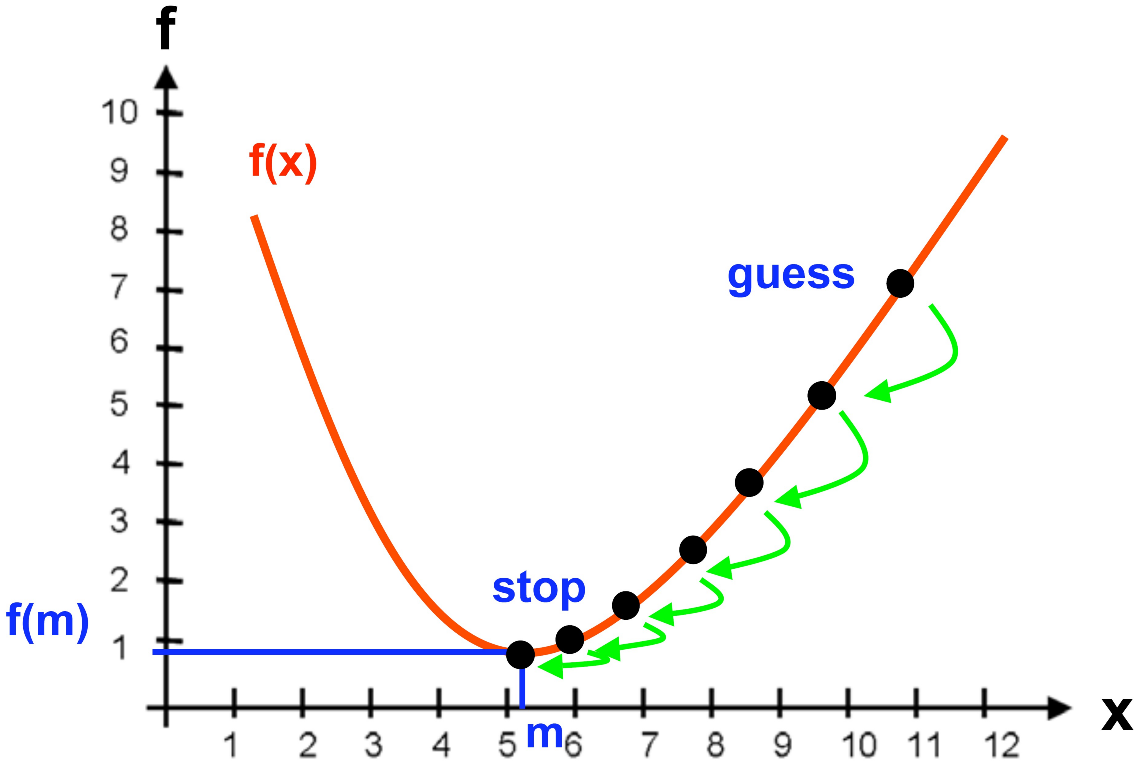
Regression Problem

- Quadratic loss

How to find optimal model parameters?

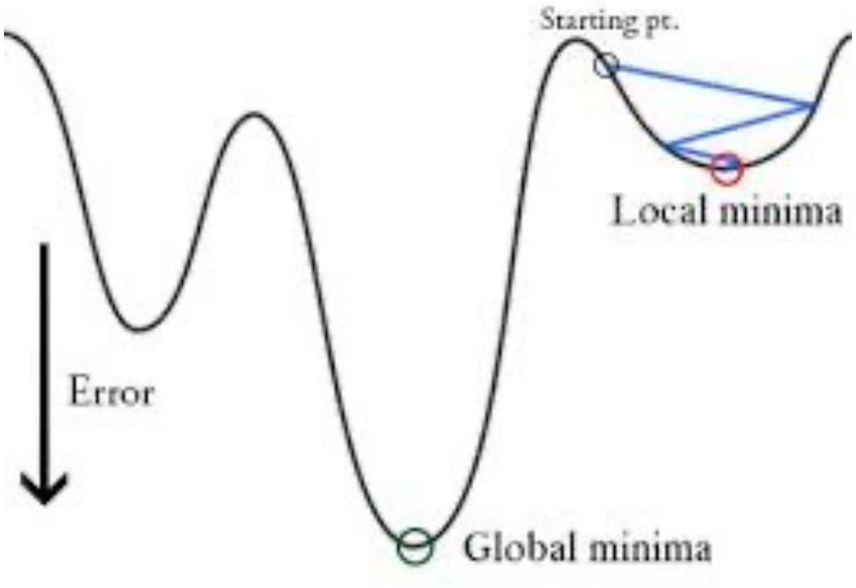
Stochastic Gradient Descent

If the objective of optimization is convex



Stochastic Gradient Descent

If the objective of optimization is non-convex



In practice, SGD still performs well. Why?

Stochastic Gradient Descent

What do we need to be able to use SGD in deep learning?

Computation of the gradient of the loss function with respect to model parameters

Training a Neural Network

The Backpropagation Algorithm

=

Gradient descent + Chain rule

Review of Chain Rule

X,Y,Z in R
Y=g(X)
Z=f(Y)

$$\frac{dZ}{dX} = \frac{dZ}{dY}\frac{dY}{dX}$$

Practice:
Y=X^2 and Z=2Y+1

compute

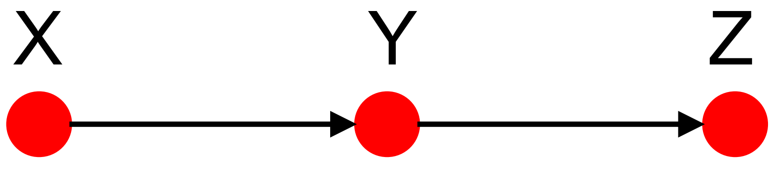
$$\frac{dZ}{dX} = ?$$

Review of Chain Rule

X,Y,Z in R
Y=g(X)
Z=f(Y)

$$\frac{dZ}{dX} = \frac{dZ}{dY}\frac{dY}{dX}$$

Graph representation:



This is NOT a neural network

Review of Chain Rule

$X \in \mathbb{R}^n, Y \in \mathbb{R}^m, Z \in \mathbb{R}$

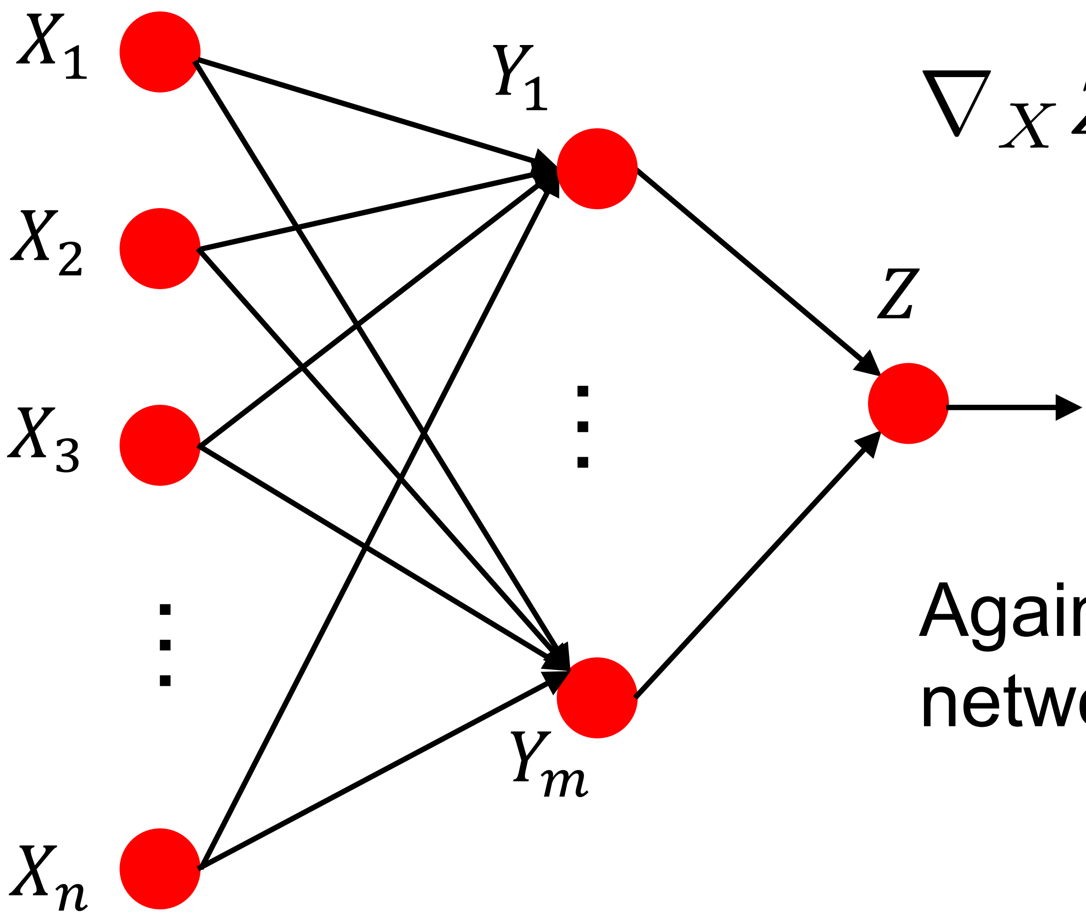
Y=g(X), Z=f(Y)

$$\nabla_X Z = (\underbrace{\frac{dY}{dX}}_{\text{Jacobian matrix}})\nabla_Y Z = \sum_{j=1}^{m}(\nabla_X Y_j)\frac{dZ}{dY_j}$$

Practice: $Y_1=X_1+X_2$^2, $Y_2=X_2+X_3$^2, $Z=Y_1$^2+Y_2^2

Compute $\nabla_X Z$

Graph Representation



$$\nabla_X Z = \sum_{j=1}^{m} (\nabla_X Y_j) \frac{dZ}{dY_j}$$

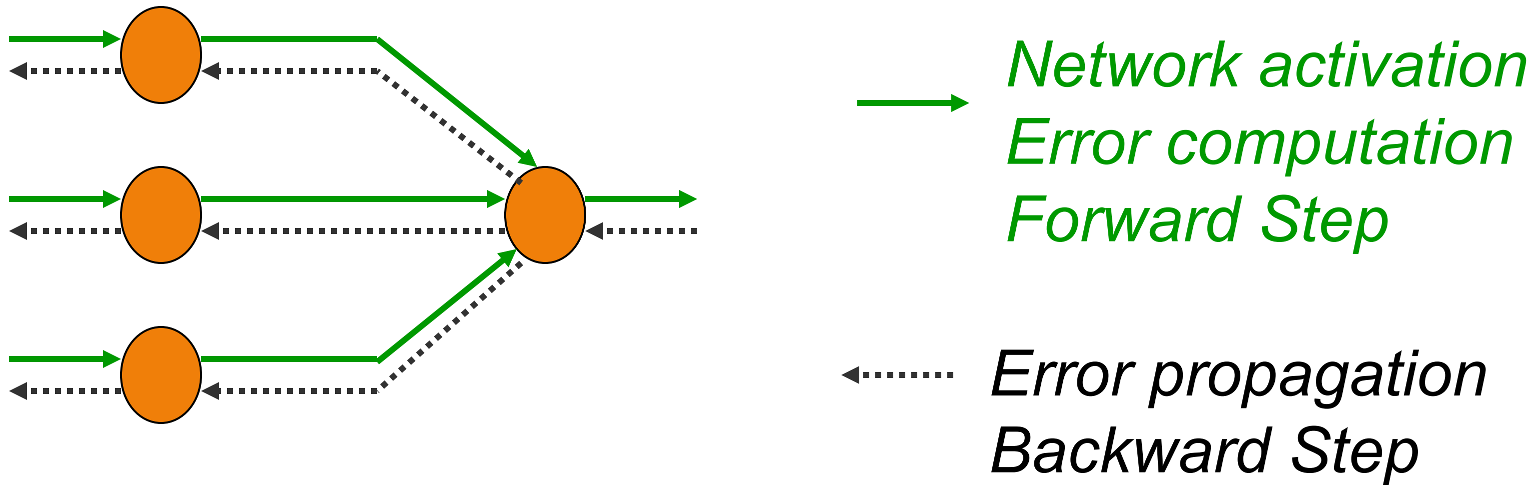
Again, this is NOT a neural network!

Training: Backpropogation Algorithm

- Searches for weight values that **minimize the total error of the network** over the set of training examples.
- **Repeated** procedures of the following two passes:
  - **Forward pass**: Compute the **outputs** of all units in the network, and the **error** of the output layers.
  - **Backward pass**: The network error is used for updating the weights.
    - Starting at the output layer, **the error is propagated backwards through the network, layer by layer**. This is done by recursively computing the local gradient of each neuron.

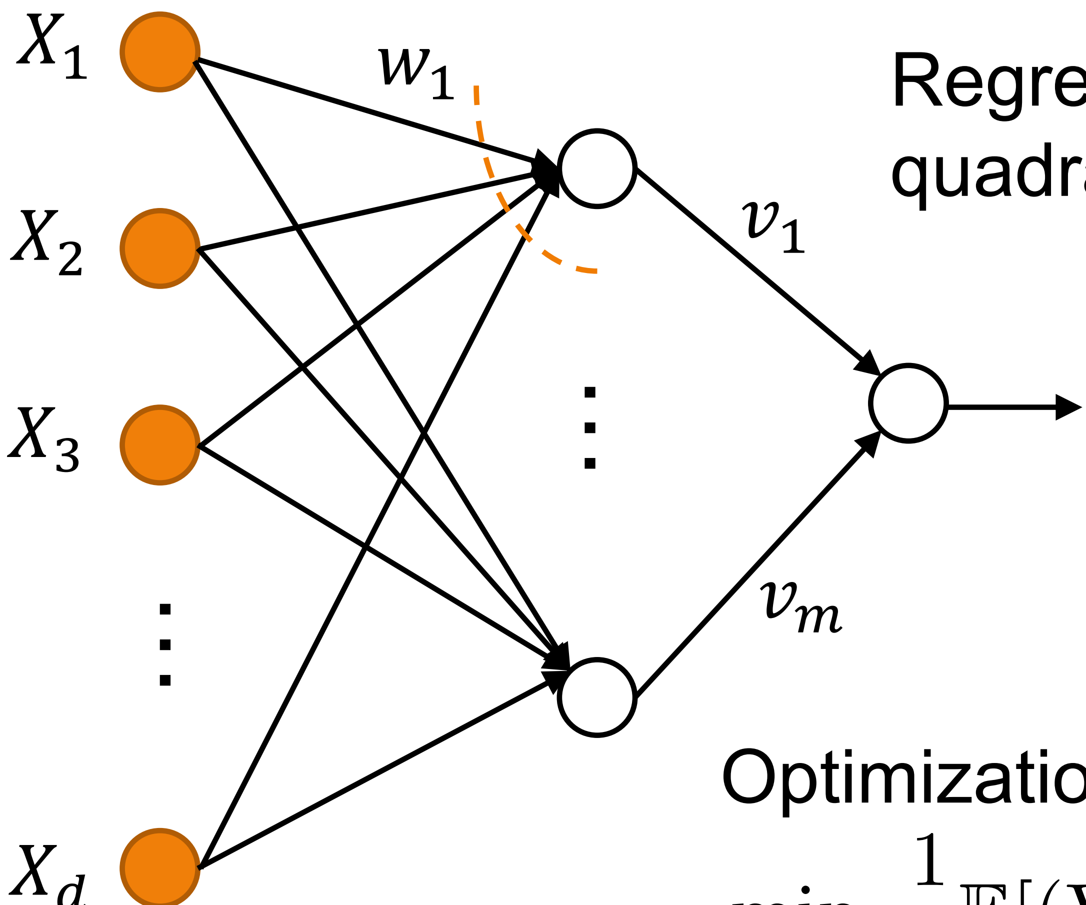
The Backpropogation Algorithm

Back-propagation training algorithm, illustrated:



Backprop adjusts the weights of the NN in order to minimize the network total mean squared error.

Example: two layer NN



Regression problem with quadratic loss function

Optimization:

$$\min_{W,v} \frac{1}{2}\mathbb{E}[(Y - \sum_{i=1}^{m} v_i \underbrace{\phi(w_i^t X)}_{\phi_i})^2]$$

Gradient of objective w.r.t. output layer weights v

$$\nabla_{v_i} L = \mathbb{E}\left[(Y - \sum_{i=1}^{m} v_i \phi(w_i^t X)) \phi(w_i^t X) \right]$$

Error term: $Y - \hat{Y}$

activation of hidden unit i

Gradient of objective w.r.t. hidden unit weights $\boldsymbol{w_i}$

$$\nabla_L w_1 = (\frac{dL}{d\phi_1})\nabla_{w_1}\phi_1$$

$$= -\mathbb{E}\left[(Y - \sum_{i=1}^{m} v_i\phi(w_i^t X))v_1\right]$$

$$= \mathbb{E}\left[\phi'(w_1^t X)X\right]$$

Multi-Label Classification

Q: how to extend our method for multi-label classification?

Recall: Multi-Label Classification, Logistic Regression