Neural Networks

CMSC 422

SOHEIL FEIZI

sfeizi@cs.umd.edu

Today's topics

- Classification Methods using Neural Networks

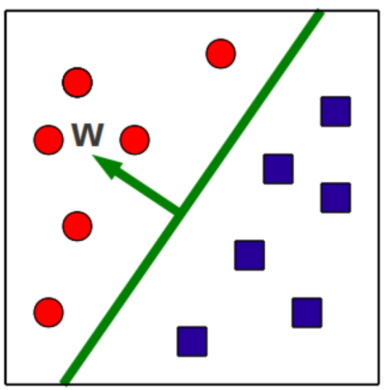
- HW4, due tonight

- Final project description, due April 2nd

What we have learned so far …

Classification Problem:

Decision trees | KNNs | Perceptron | Empirical Risk Minimization | Maximum Likelihood



Linear model ($w^t x+b$)

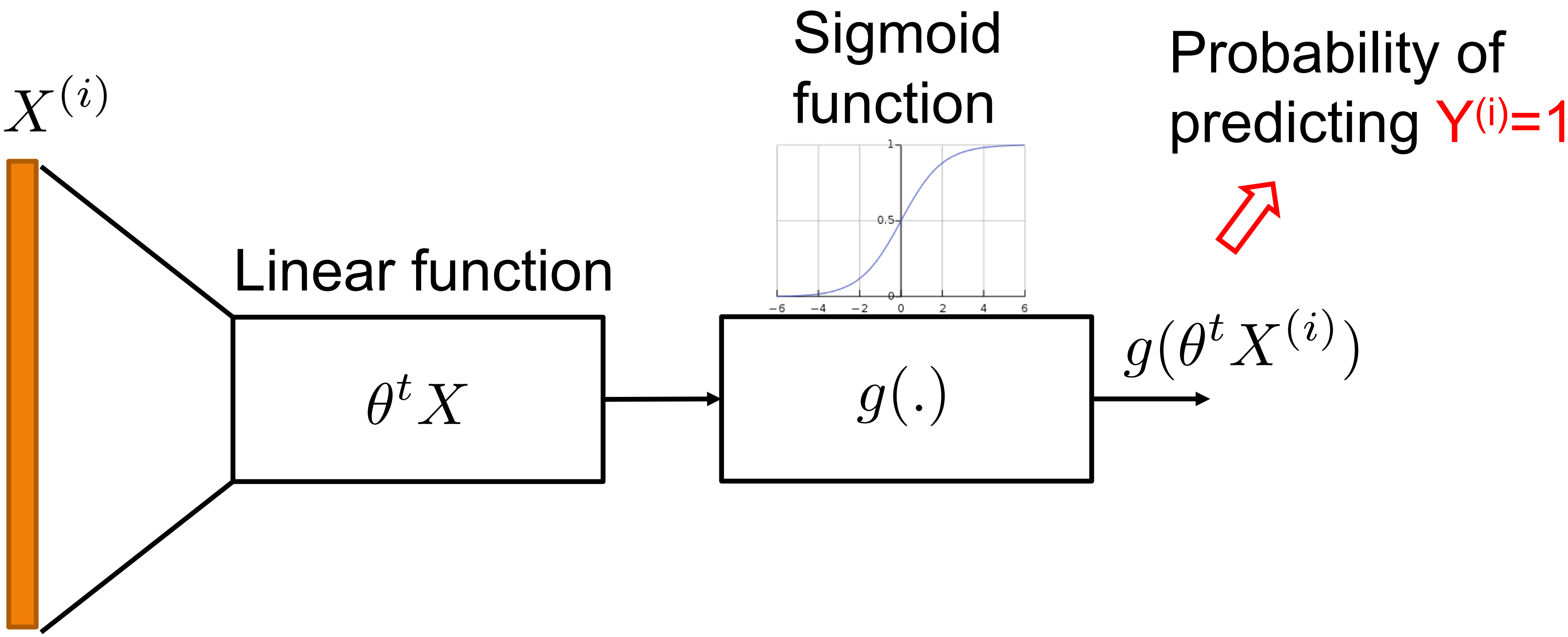
Empirical Risk Minimization: 0-1 loss → Hinge loss

Maximum Likelihood: Cross-entropy loss

Why did we restrict our models to be linear ($w^t x + b$)?

- The loss minimization is a convex opt.
- Why is this important?
- Efficient methods to find the global optimizer (e.g. Stochastic GD)
- What do we lose by restricting ourselves to linear models?

Recall the logistic regression

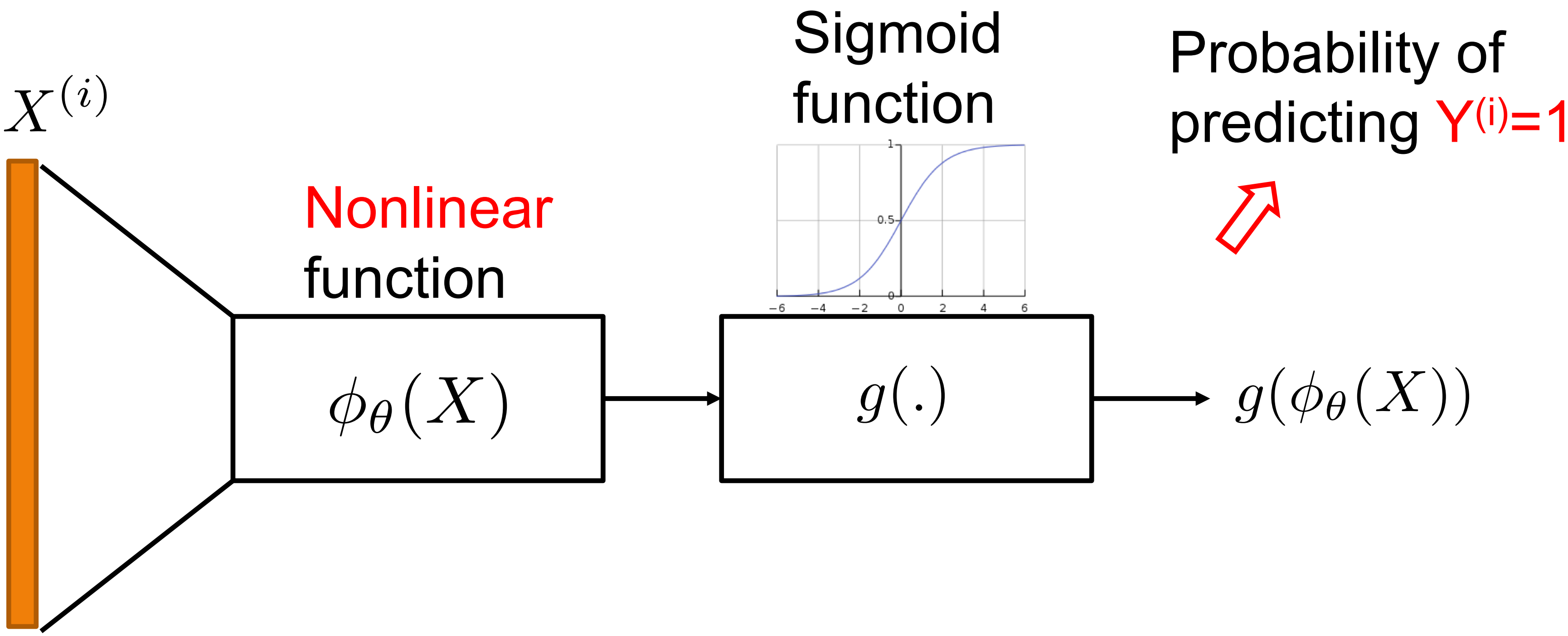


Is X->Y model linear? No!

Compute model parameters using cross-entropy loss opt:

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

Linear → Nonlinear



Is X->Y model linear? No!

Compute model parameters using cross-entropy loss opt:

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

Two Questions

- What is a “good” family of nonlinear functions to consider?

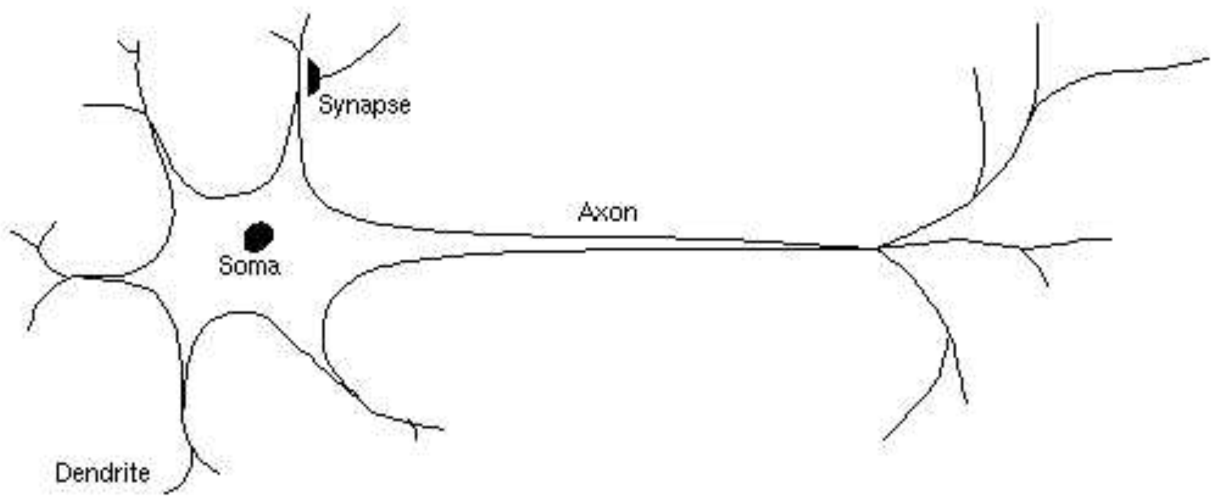
- How to solve the resulting optimization?

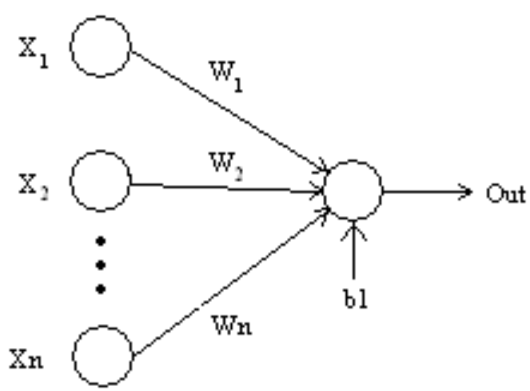
Neural Networks

- What are neural networks?

- Why are neural networks powerful?

Aside: biological inspiration





Analogy: the perceptron as a neuron

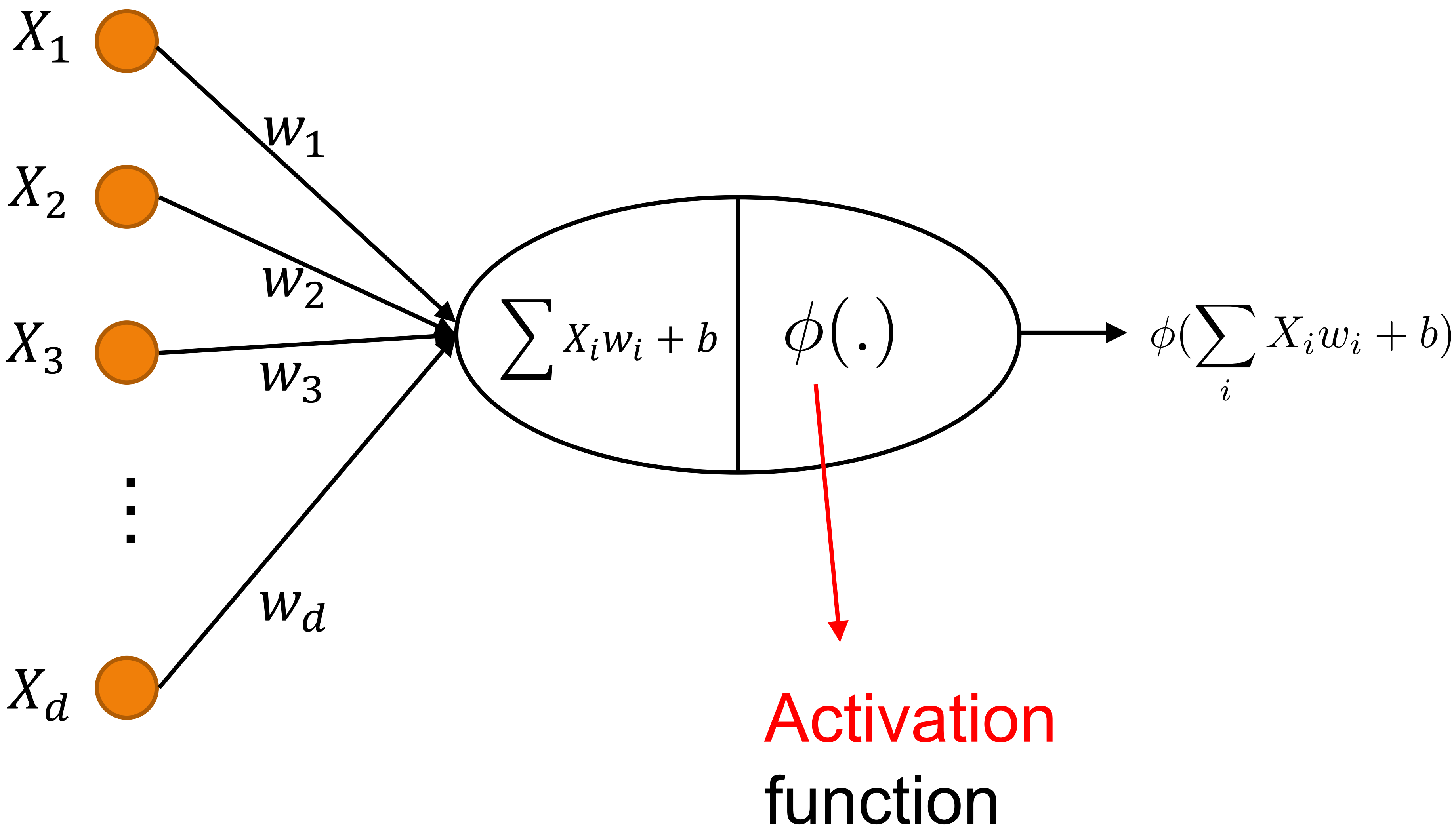
History of Neural Networks

- 1943: McCulloch and Pitts proposed a model of a neuron
- 1960s: Widrow and Hoff explored Perceptron networks (which they called “Adelines”) and the delta rule.
- 1957: Frank Rosenblatt invents the ***Perceptron***
  1962: Rosenblatt proved convergence of the perceptron training rule.
- 1969: Minsky and Papert showed that the Perceptron cannot deal with nonlinearly-separable data sets---even those that represent simple function (e.g., X-OR)
- 1970-1985: Very little research on Neural Nets
- 1986: Invention of Back Propagation [Rumelhart & McClelland; Parker; Werbos] which can learn nonlinearly-separable data sets.
- Since 1985: A lot of research in Neural Nets!
- Geoff Hinton

Neural Networks

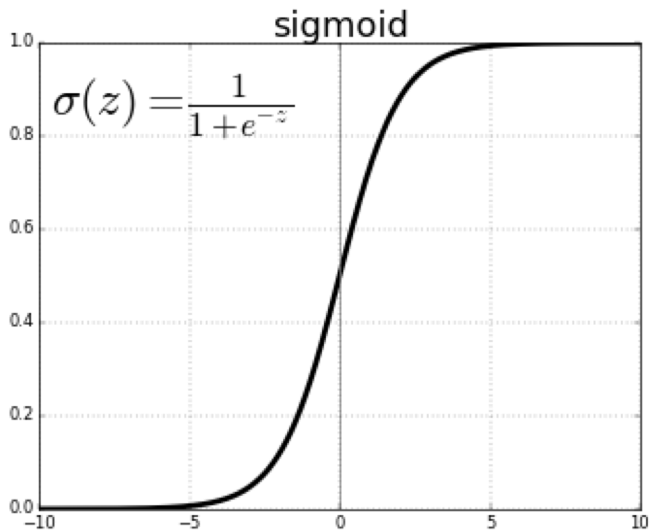
- Neural networks are made up of **nodes** or **units**, connected by **links**
- Each link has an associated **weight** and **activation level**
- Each node has an **input function** (typically summing over weighted inputs), an **activation function**, and an **output**

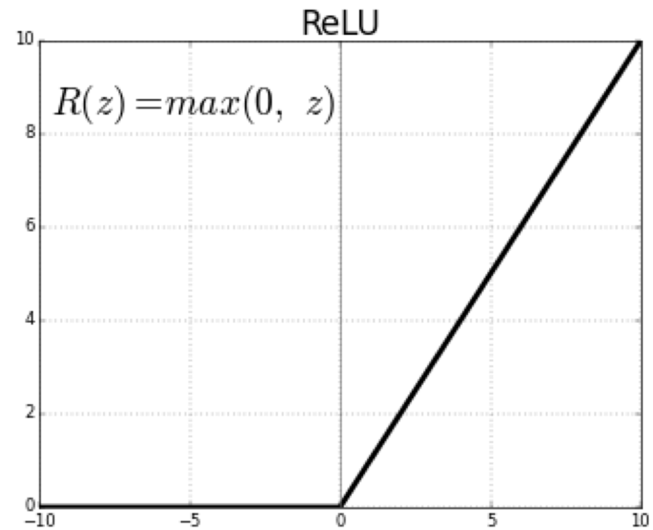
Neural Unit

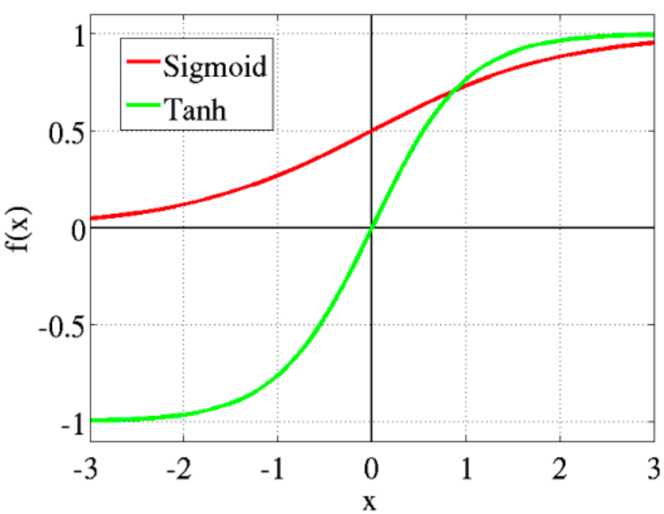


X_1
X_2
X_3
X_d
w_1
w_2
w_3
w_d
$\sum X_i w_i + b$
$\phi(.)$
$\phi(\sum_i X_i w_i + b)$
Activation
function

Popular Activation Functions

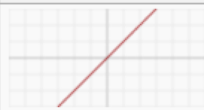
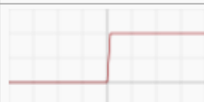
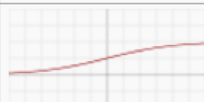
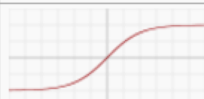
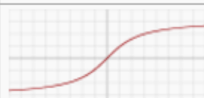
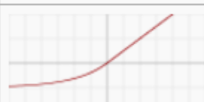
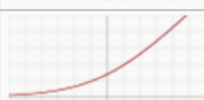




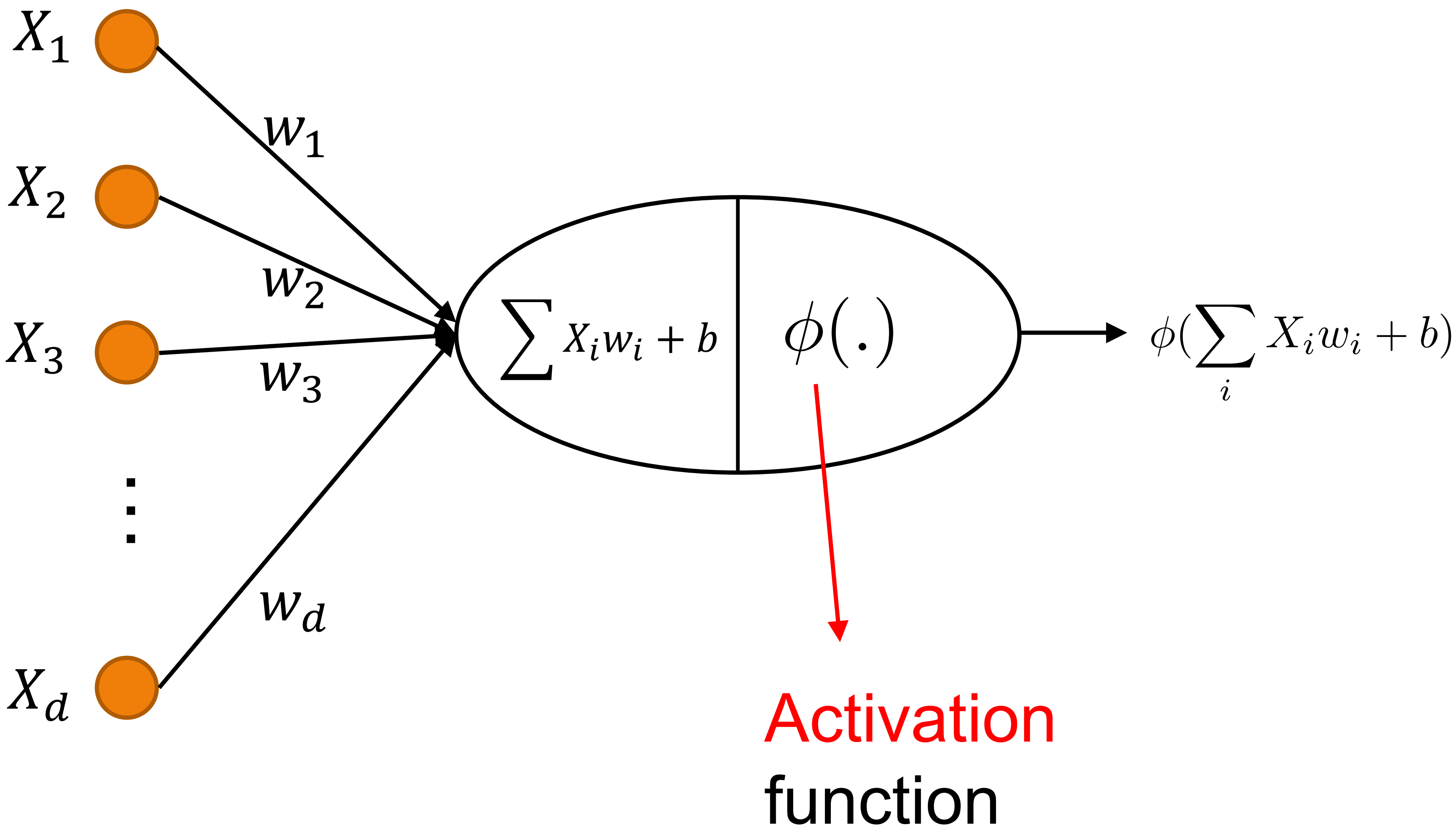


Q: how to choose a proper activation function?

So many activation functions!

Name	Plot	Equation	Derivative
Identity		$f(x) = x$	$f'(x) = 1$
Binary step		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for } x \neq 0 \\ ? & \text{for } x = 0 \end{cases}$
Logistic (a.k.a Soft step)		$f(x) = \frac{1}{1 + e^{-x}}$	$f'(x) = f(x)(1 - f(x))$
TanH		$f(x) = \tanh(x) = \frac{2}{1 + e^{-2x}} - 1$	$f'(x) = 1 - f(x)^2$
ArcTan		$f(x) = \tan^{-1}(x)$	$f'(x) = \frac{1}{x^2 + 1}$
Rectified Linear Unit (ReLU)		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
Parameteric Rectified Linear Unit (PReLU)[2]		$f(x) = \begin{cases} \alpha x & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} \alpha & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
Exponential Linear Unit (ELU)[3]		$f(x) = \begin{cases} \alpha(e^x - 1) & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} f(x) + \alpha & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
SoftPlus		$f(x) = \log_e(1 + e^x)$	$f'(x) = \frac{1}{1 + e^{-x}}$

Lets make the picture more concise



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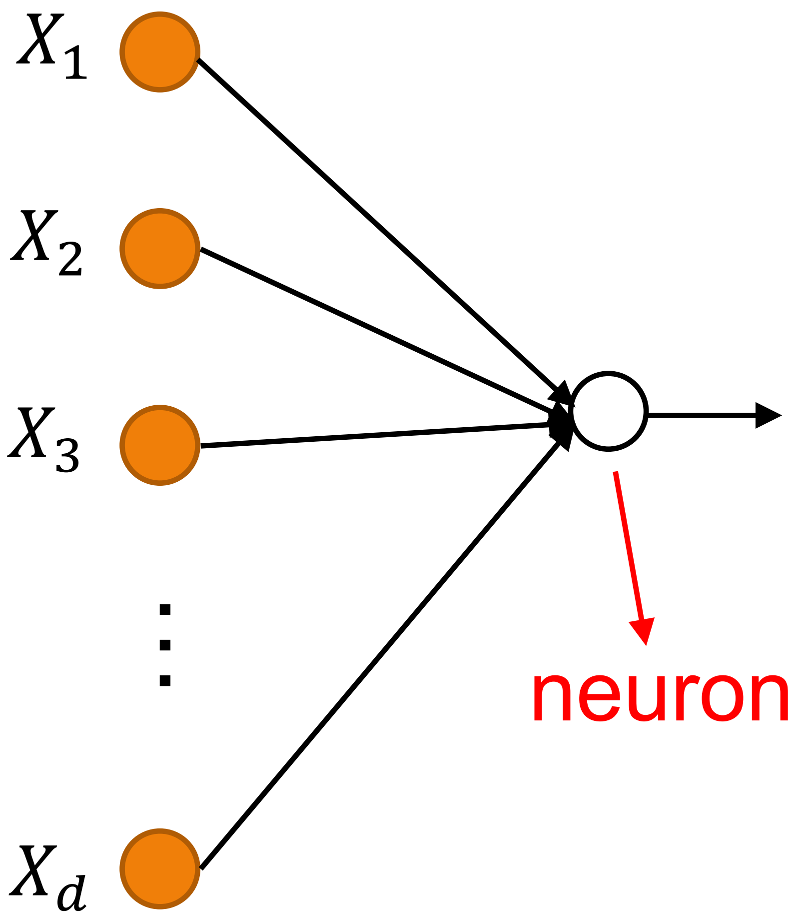
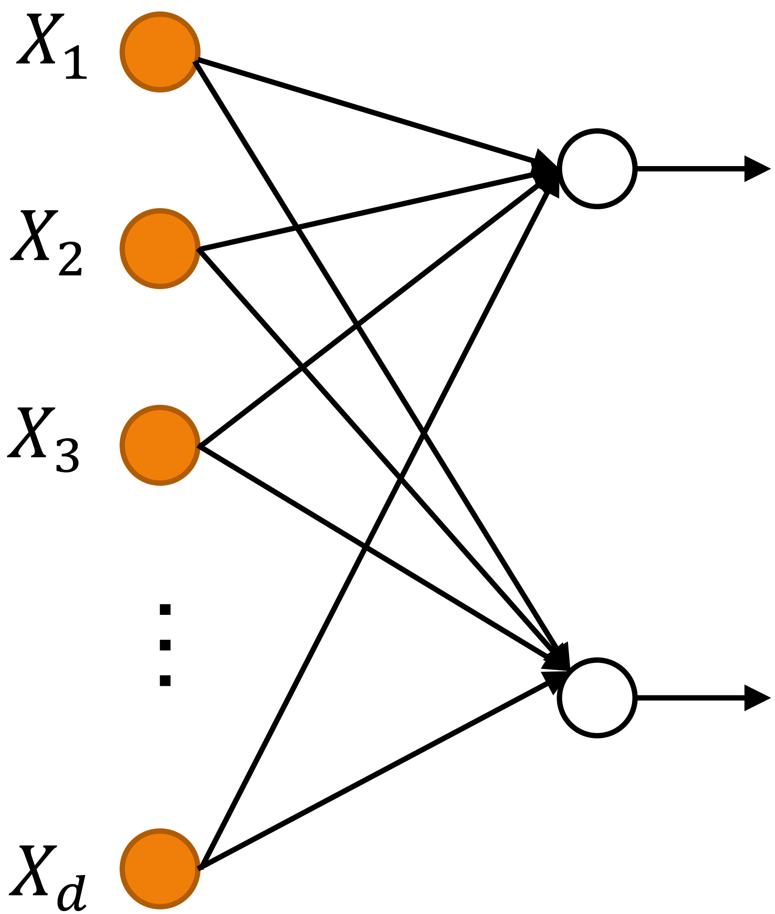


Implicitly we assume

- Edges have weights
- Neurons have activations

Q: can we make the function more complex (i.e. higher representation power)?

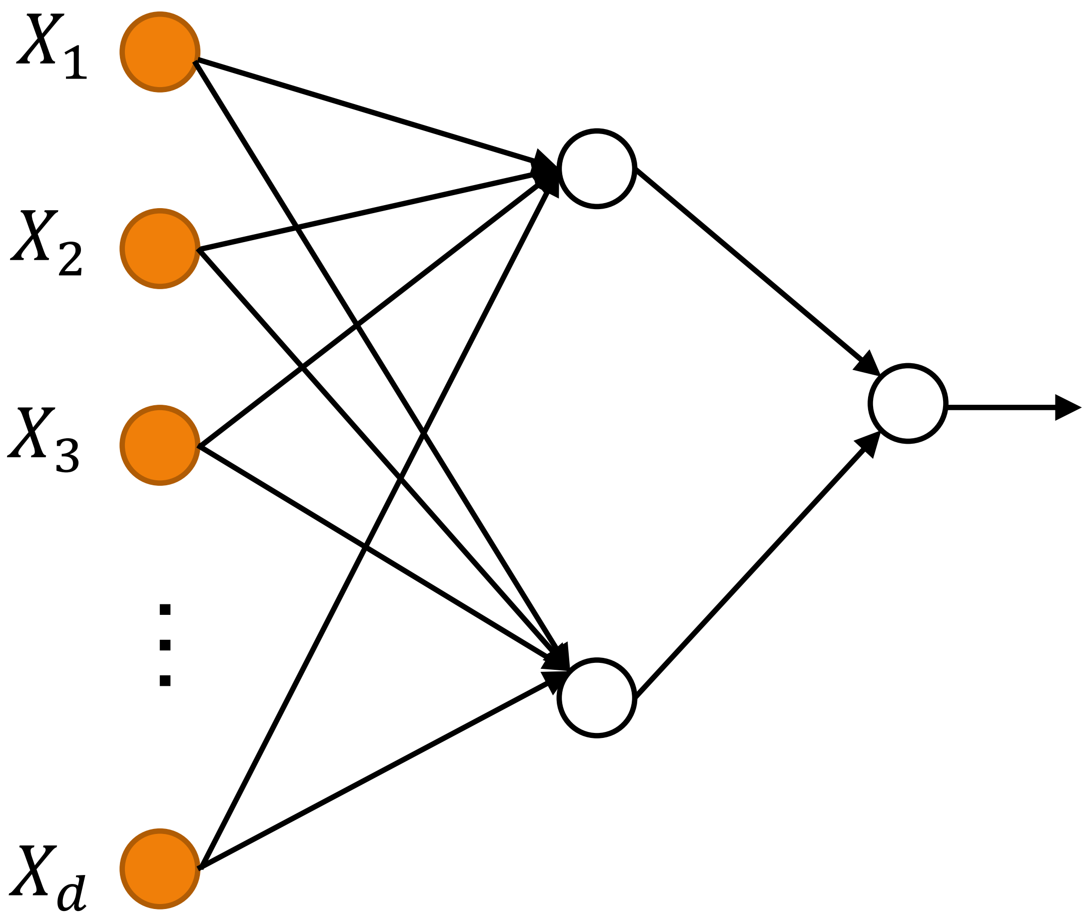
Lets add one more neuron



But my desired function is from d-dimension to one dimension.

How can I resolve this?

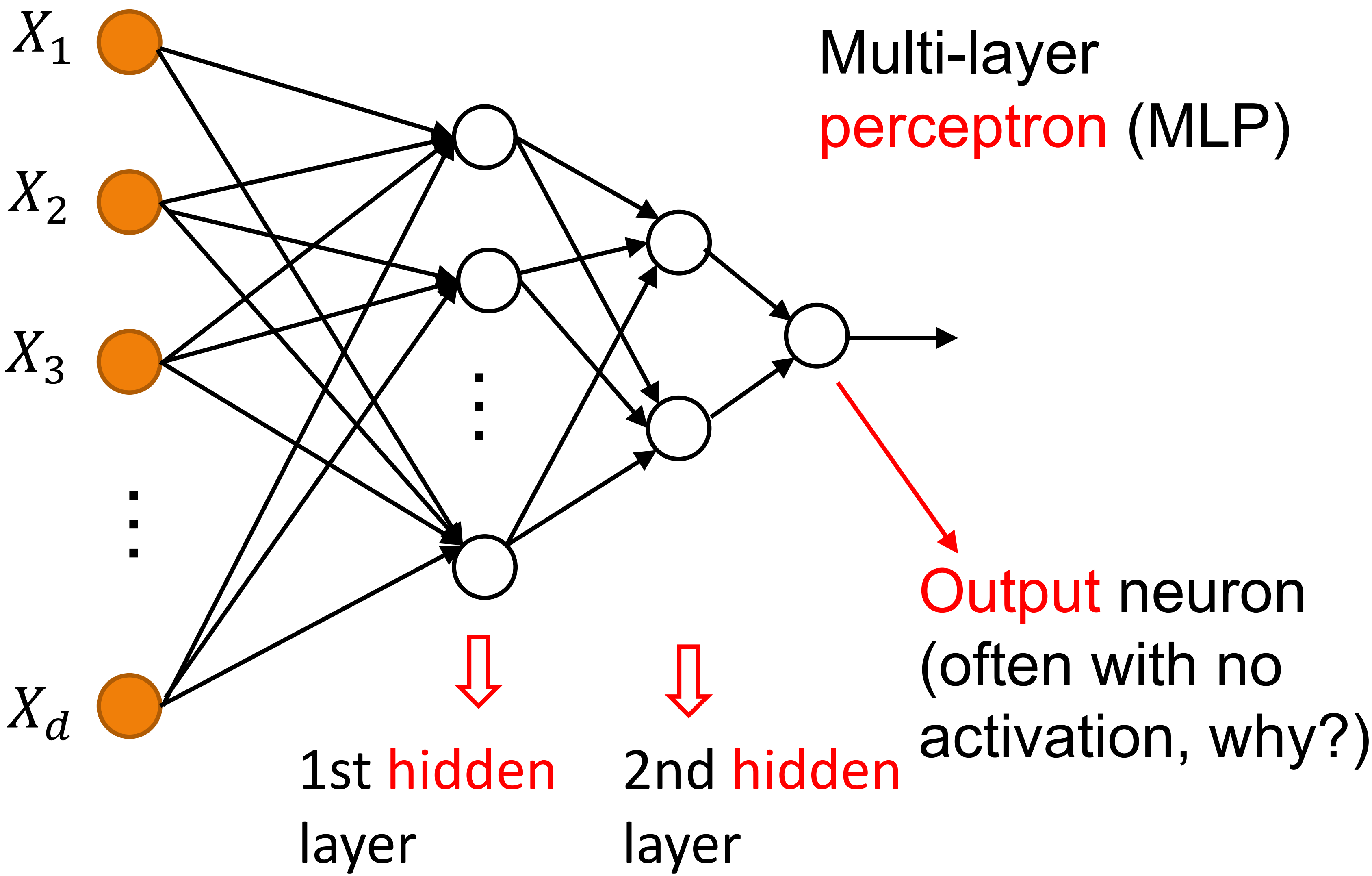
Lets add one more neuron!



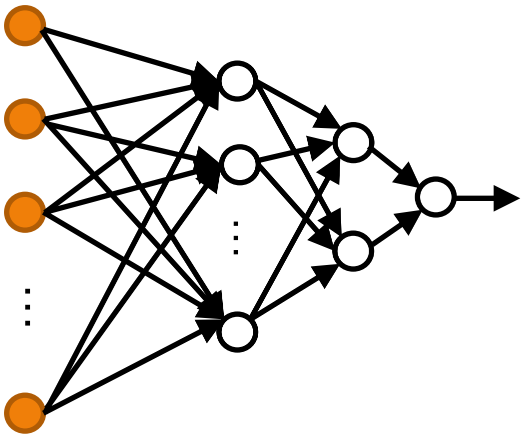
Can we add even more neurons?

Yes, we can!

Multi-Layer Neural Network



Neural Networks



- What are neural networks?

- Why are neural networks powerful?

Two-Layer Networks are Universal Function Approximators

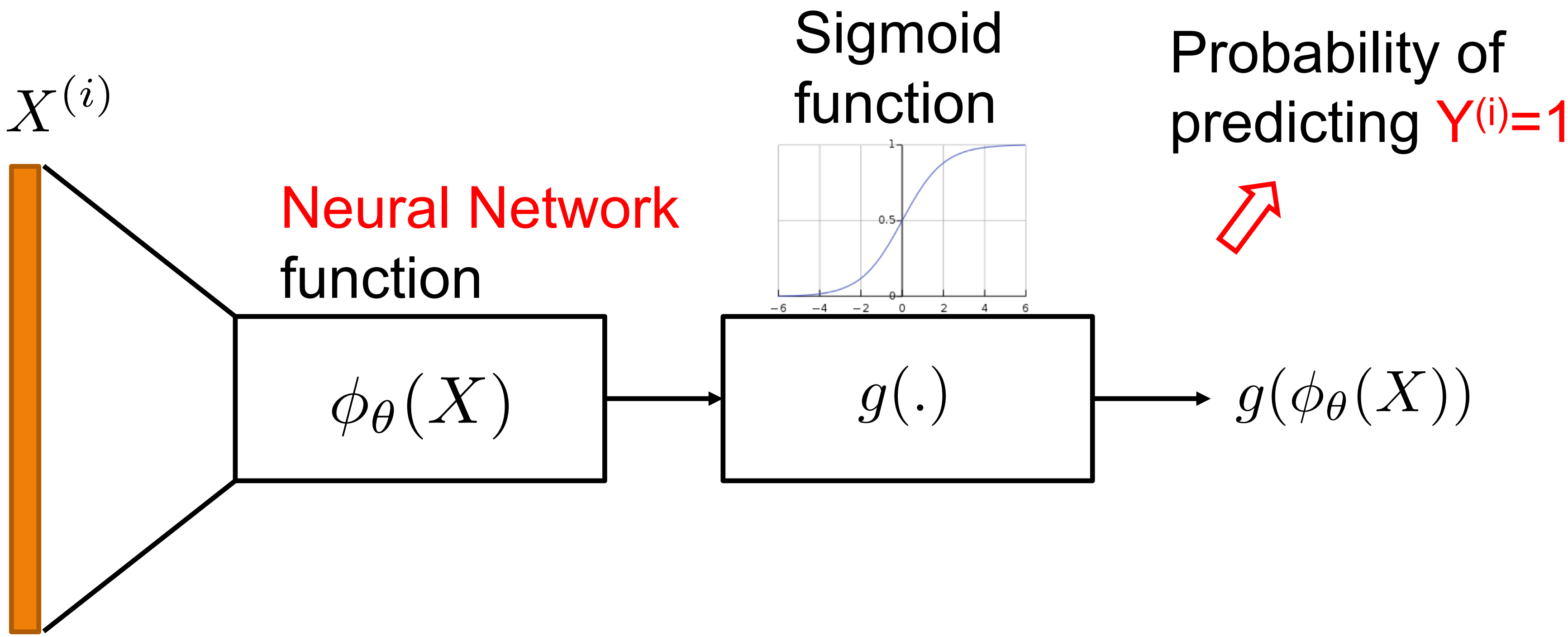
Theorem (Th 9 in CIML):

Let F be a continuous function on a bounded subset of D-dimensional space. Then there exists a two-layer neural network $\hat{F}$ with a finite number of hidden units that approximates F *arbitrarily well*.

Namely, for all x in the domain of F,

$$\left|F(\boldsymbol{x}) - \hat{F}(\boldsymbol{x})\right| < \epsilon$$

Classification using Neural Network



What is θ ?

Compute model parameters using cross-entropy loss opt:

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

Two Questions

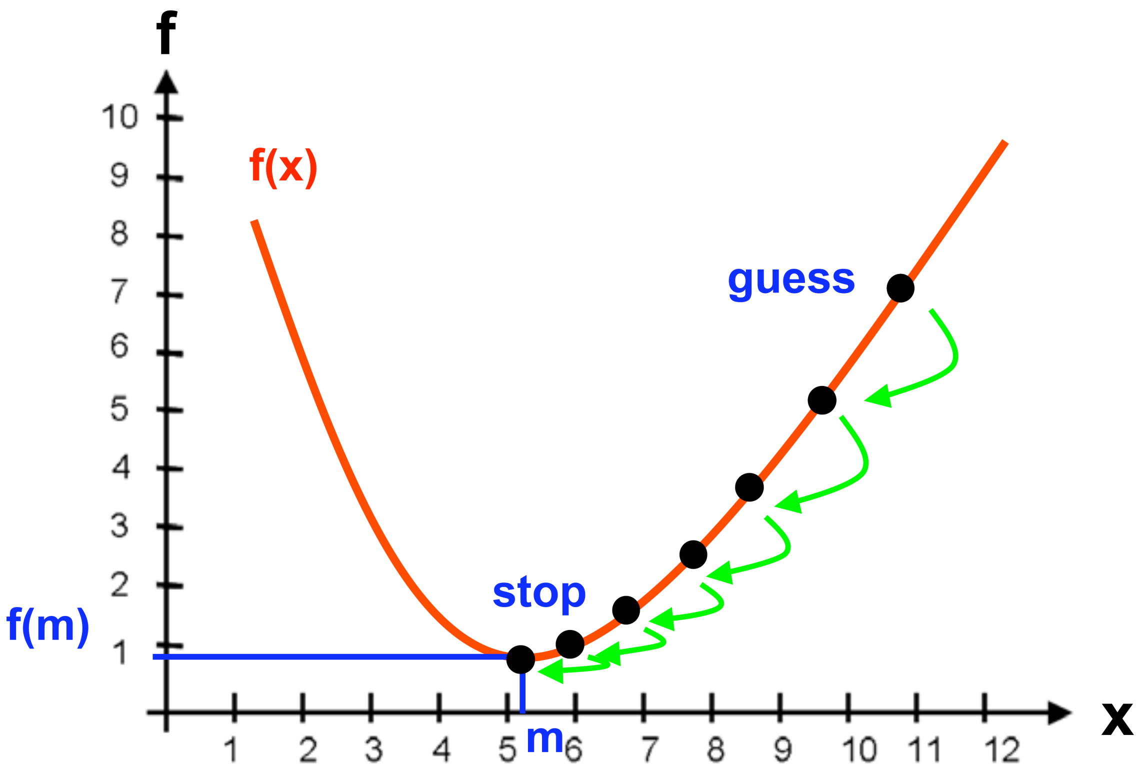
- What is a “good” family of nonlinear functions to consider? Neural Networks

- How to solve the resulting optimization?

Can we still use stochastic GD?

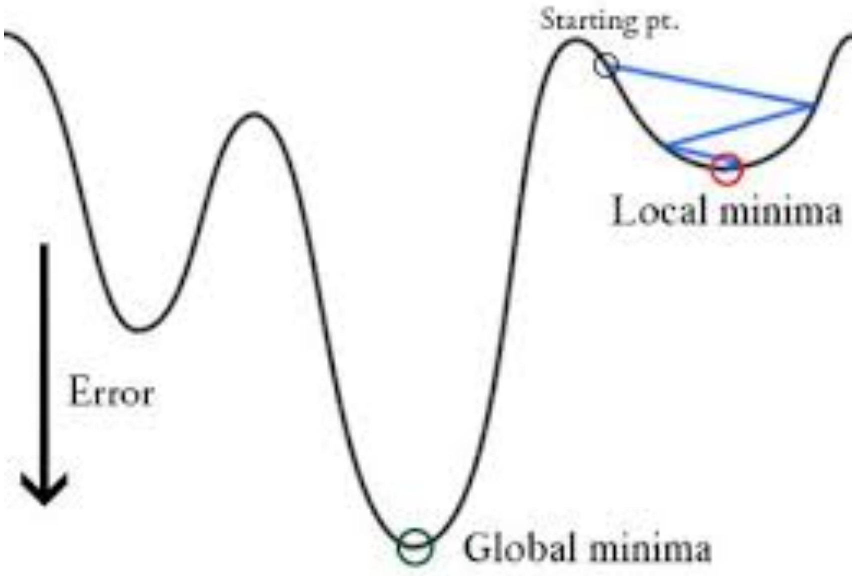
Stochastic Gradient Descent

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?

Two Questions

- What is a “good” family of nonlinear functions to consider? Neural Networks

- How to solve the resulting optimization? Can we still use stochastic GD? Yes!

Stochastic Gradient Descent

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

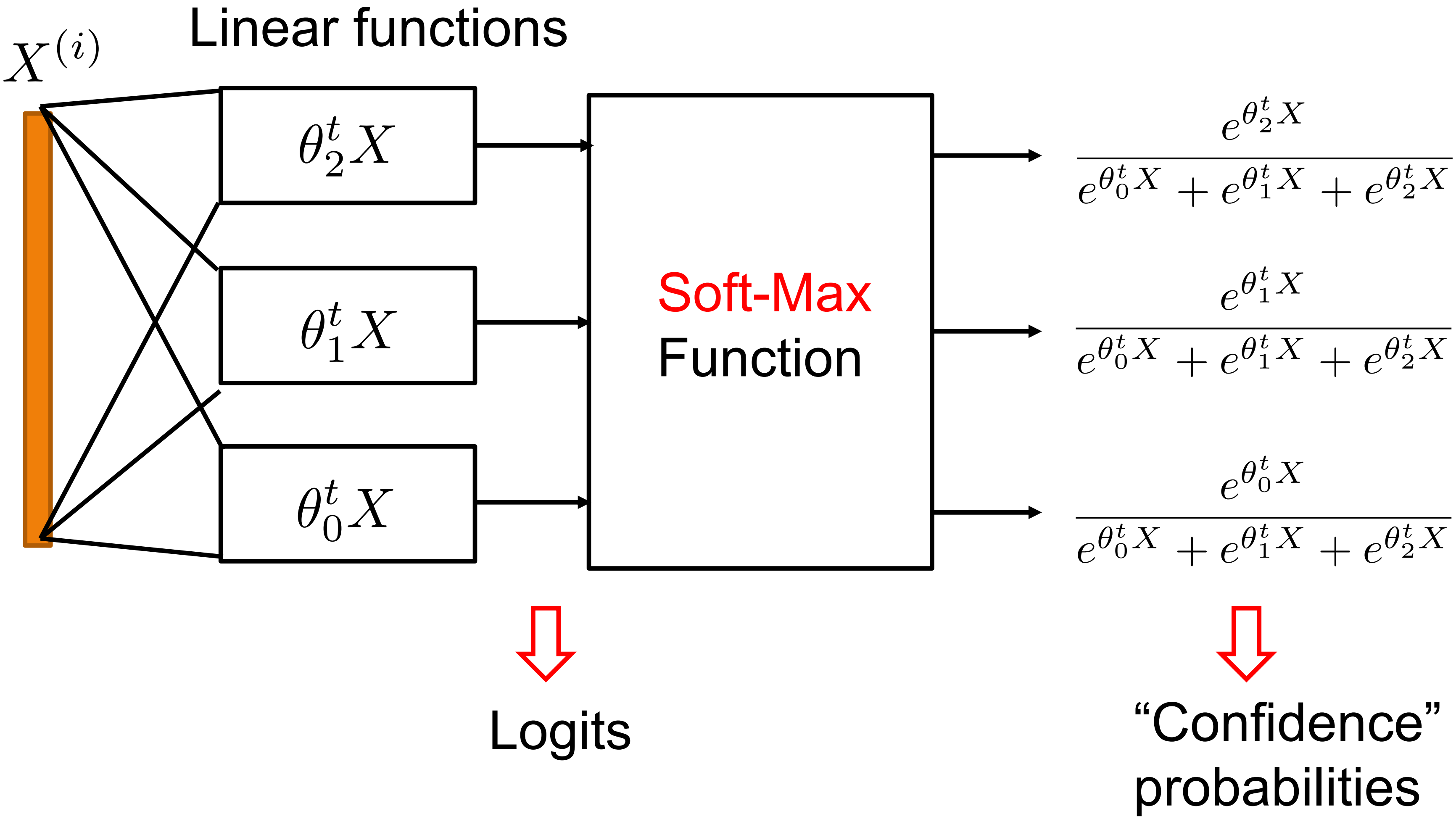
Computation of the gradient of the loss function with respect to model parameters

Next lecture, an efficient algorithm for this task!

For the next lecture

Think about how to extend our method for multi-label classification

Recall: Multi-Label Classification, Logistic Regression



Training a Neural Network

The Backpropagation Algorithm

=

Gradient descent + Chain rule

Recall: THE CHAIN RULE

If $y = f(x)$ and $x = g(t)$,
where f and g are differentiable functions, then y is indirectly a differentiable function of t, and

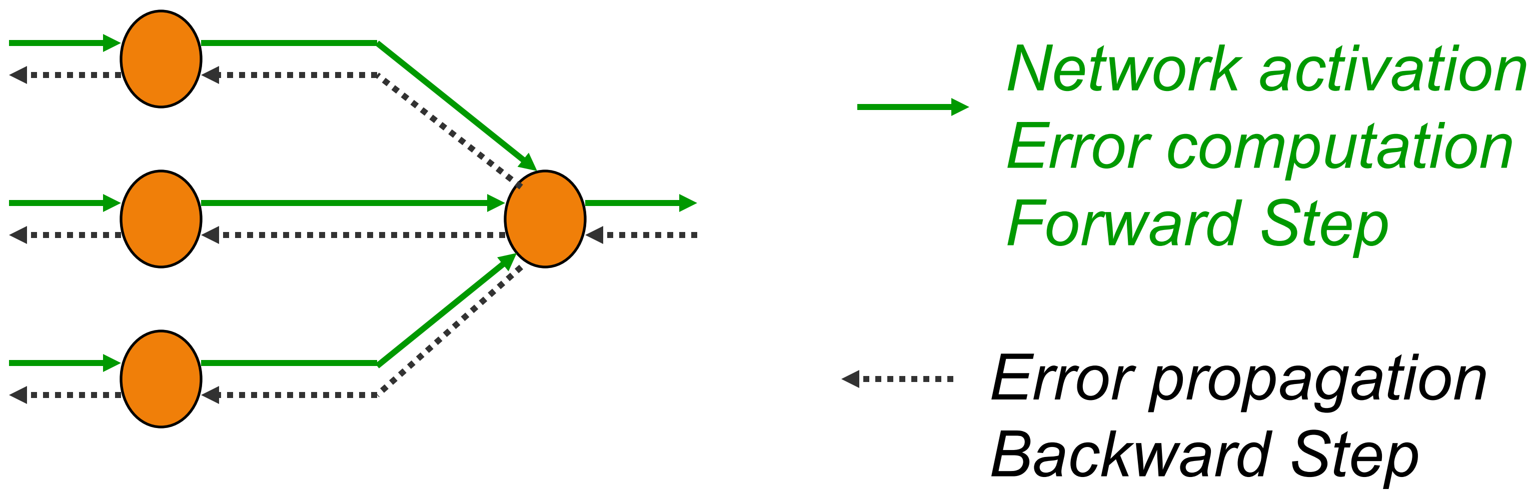
$$\frac{dy}{dt} = \frac{dy}{dx}\frac{dx}{dt}$$

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.