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COMP 5212
Machine Learning
Lecture 18

Neural Networks, Backpropagation

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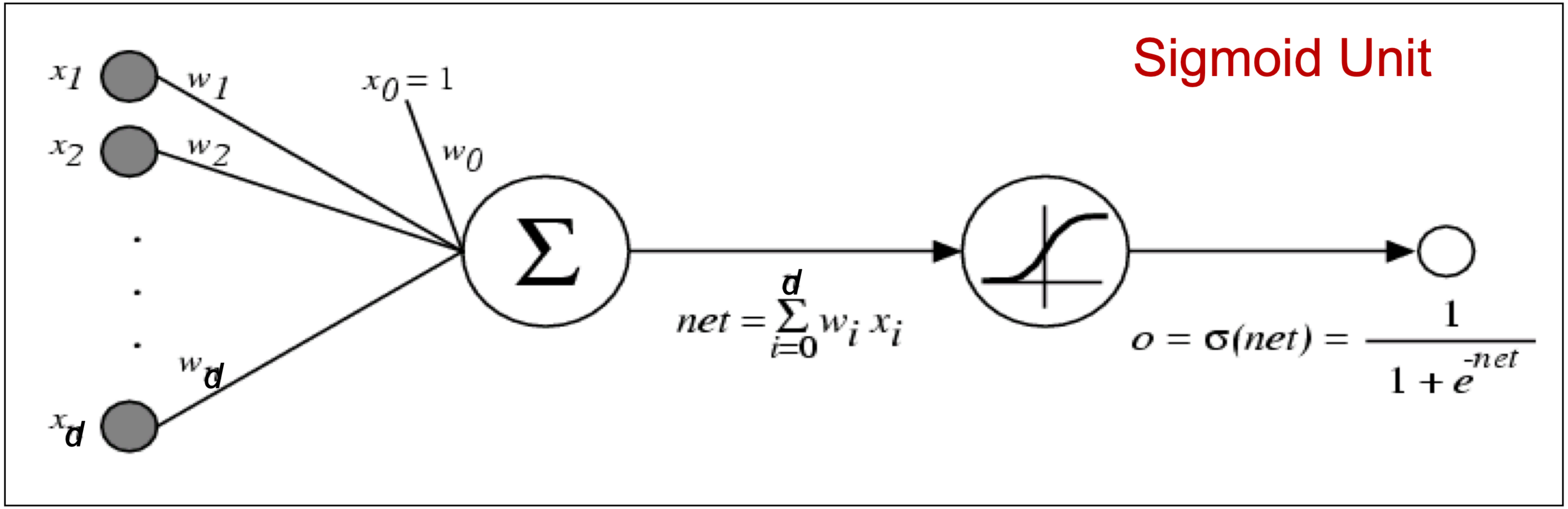
Logistic Function as a Graph

$$\text{Output, } o(\mathbf{x}) = \sigma(w_0 + \sum_i w_i X_i) = \frac{1}{1 + \exp(-(w_0 + \sum_i w_i X_i))}$$

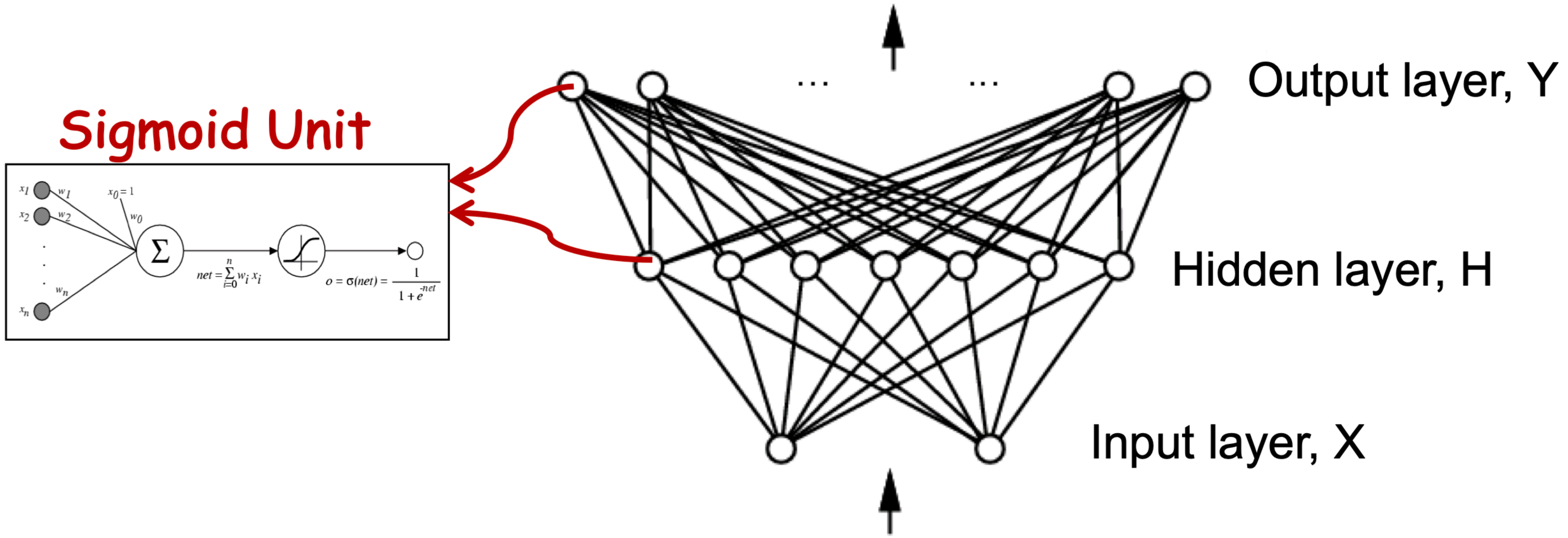


Computation Graph

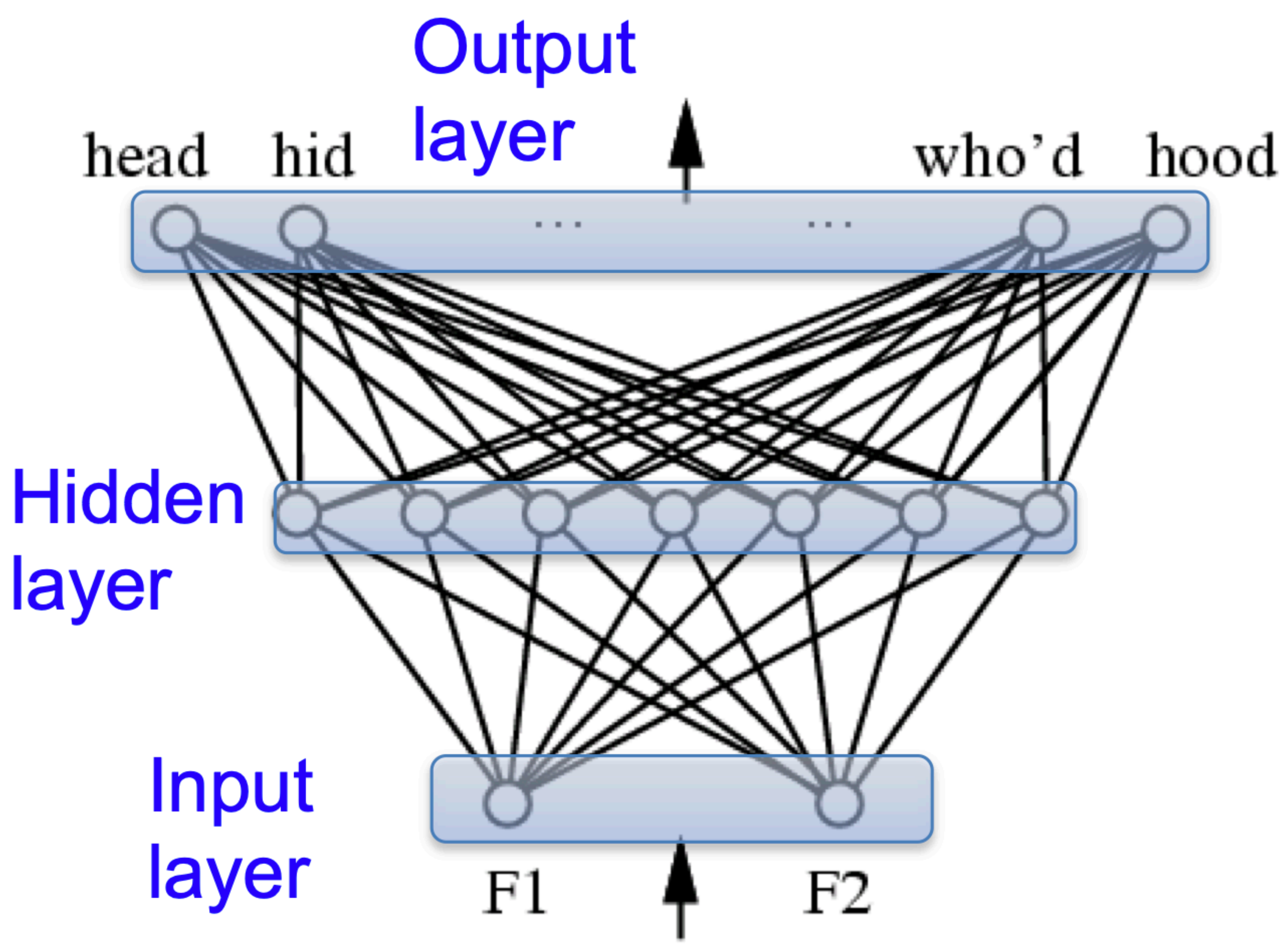
Neural Networks

- f can be a **non-linear** function
- X (vector of) continuous and/or discrete variables
- Y (**vector** of) continuous and/or discrete variables

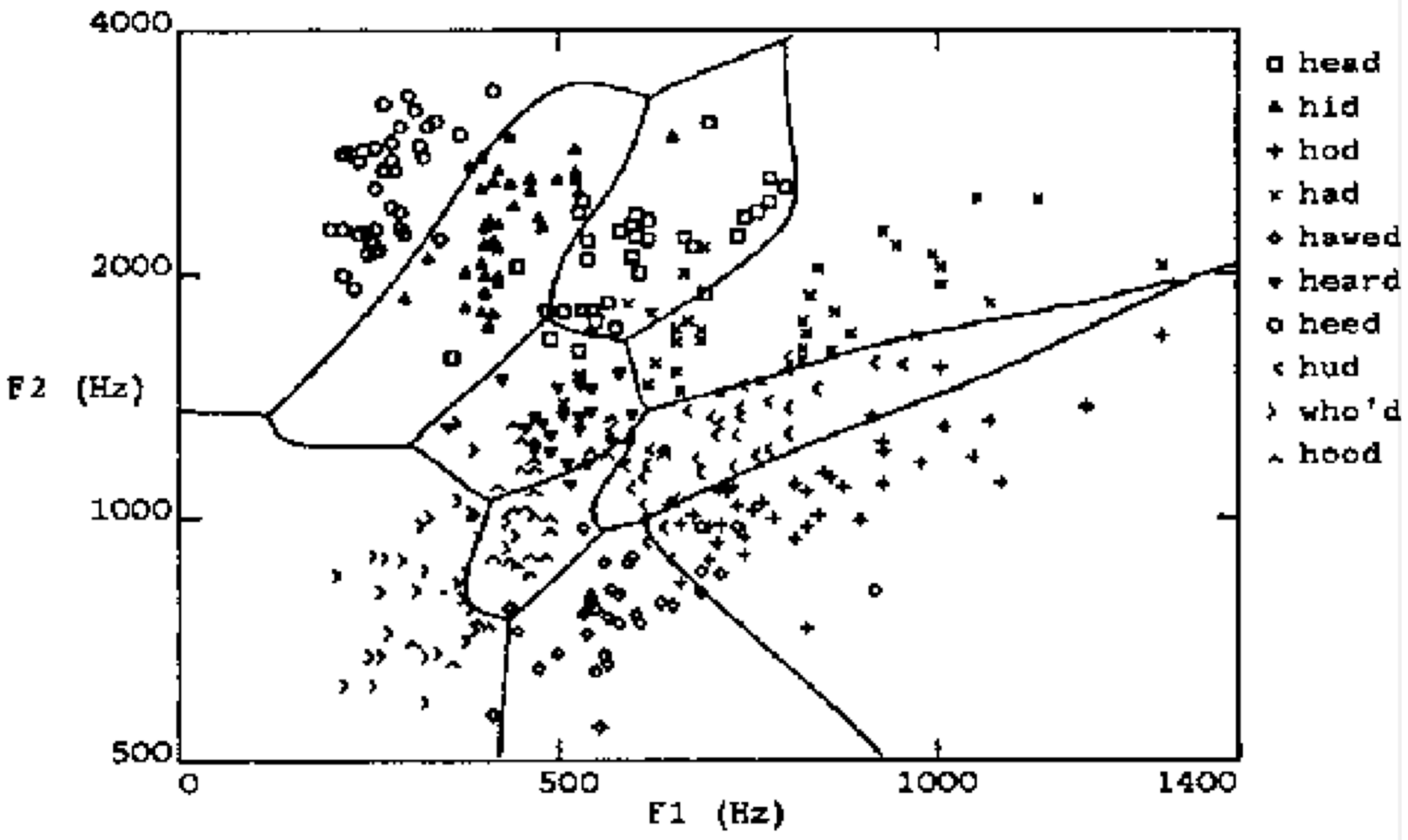
  - Neural networks - Represent f by ***network*** of sigmoid (more recently ReLU – next lecture) units :



Multilayer Networks of Sigmoid Units



Two layers of logistic units



Highly non-linear decision surface

More Applications

Neural Network trained to drive a car!

Expressive Capabilities of ANNs

Continuous functions:

- Every bounded continuous function can be approximated with arbitrarily small error, by network with one hidden layer [Cybenko 1989; Hornik et al. 1989]
- Any function can be approximated to arbitrary accuracy by a network with two hidden layers [Cybenko 1988].

Prediction using Neural Networks

Prediction – Given neural network (hidden units and weights), use it to predict the label of a test point

Forward Propagation –

Start from input layer
For each subsequent layer, compute output of sigmoid unit

Sigmoid unit:

$$o(\mathbf{x}) = \sigma(w_0 + \sum_i w_i x_i)$$

1-Hidden layer,
1 output NN:

$$o(\mathbf{x}) = \underbrace{\sigma\left(w_0 + \sum_h w_h \underbrace{\sigma(w_0^h + \sum_i w_i^h x_i)}_{o_h}\right)}_{}$$

Objective Functions for NNs

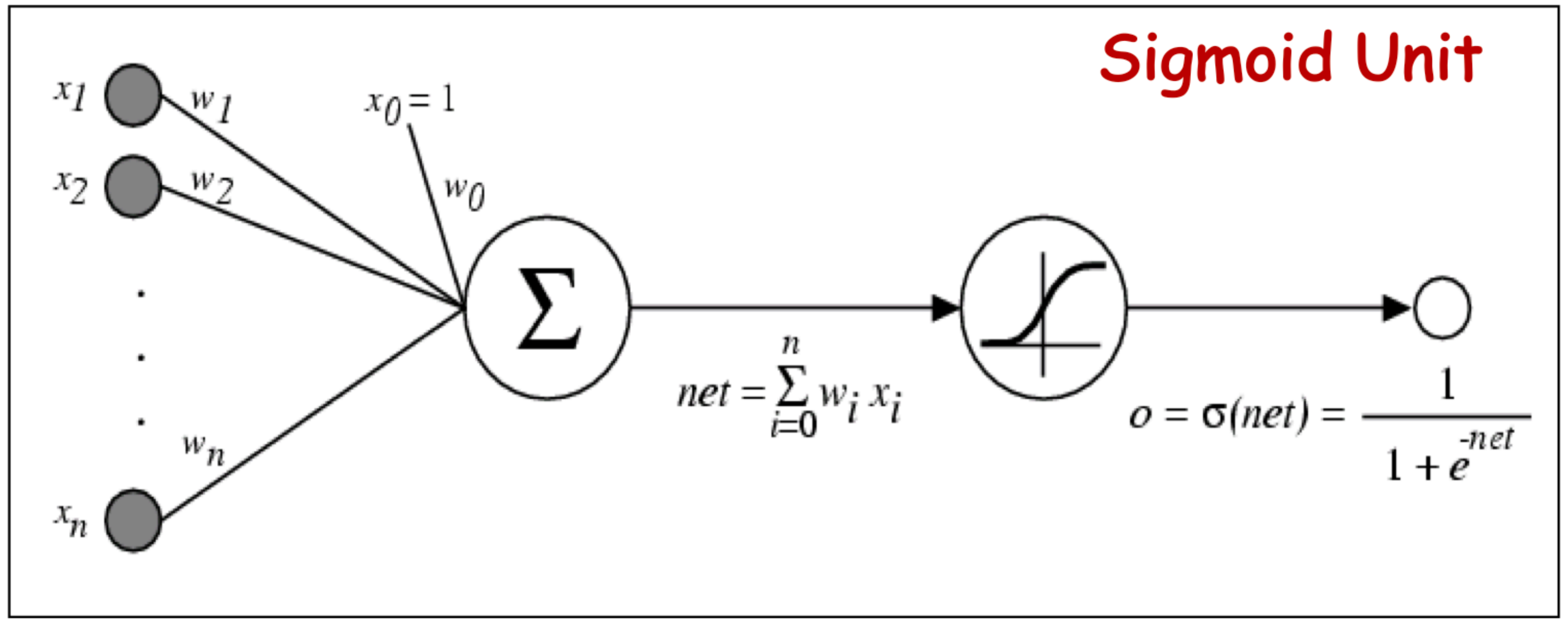
- Regression:
  - Use the same objective as Linear Regression
  - Quadratic loss (i.e. mean squared error)

- Classification:
  - Use the same objective as Logistic Regression
  - Cross-entropy (i.e. negative log likelihood)
  - This requires probabilities, so we add an additional "softmax" layer at the end of our network

Gradient descent for training NNs

$$w \leftarrow w - \alpha \cdot \frac{\partial L}{\partial w}$$

Gradient decent for 1 node:



$$\frac{\partial o}{\partial w_i} = \frac{\partial o}{\partial net} \cdot \frac{\partial net}{\partial w_i} = o(1-o)x_i$$

Chain rule

Univariate Chain Rule

- We've already been using the univariate Chain Rule.
- Recall: if $f(x)$ and $x(t)$ are univariate functions, then

$$\frac{\mathrm{d}}{\mathrm{d}t} f(x(t)) = \frac{\mathrm{d}f}{\mathrm{d}x} \frac{\mathrm{d}x}{\mathrm{d}t}.$$

Example:

$$\begin{aligned} z &= wx + b \\ y &= \sigma(z) \\ \mathcal{L} &= \frac{1}{2}(y - t)^2 \end{aligned}$$

Let's compute the loss derivatives.

Example of Chain Rule

$$
\begin{aligned}
\mathcal{L} &= \frac{1}{2}(\sigma(wx+b)-t)^2 \\
\frac{\partial \mathcal{L}}{\partial w} &= \frac{\partial}{\partial w}\left[\frac{1}{2}(\sigma(wx+b)-t)^2\right] \\
&= \frac{1}{2}\frac{\partial}{\partial w}(\sigma(wx+b)-t)^2 \\
&= (\sigma(wx+b)-t)\frac{\partial}{\partial w}(\sigma(wx+b)-t) \\
&= (\sigma(wx+b)-t)\sigma'(wx+b)\frac{\partial}{\partial w}(wx+b) \\
&= (\sigma(wx+b)-t)\sigma'(wx+b)x
\end{aligned}
$$

Using Chain Rules

Computing the loss:

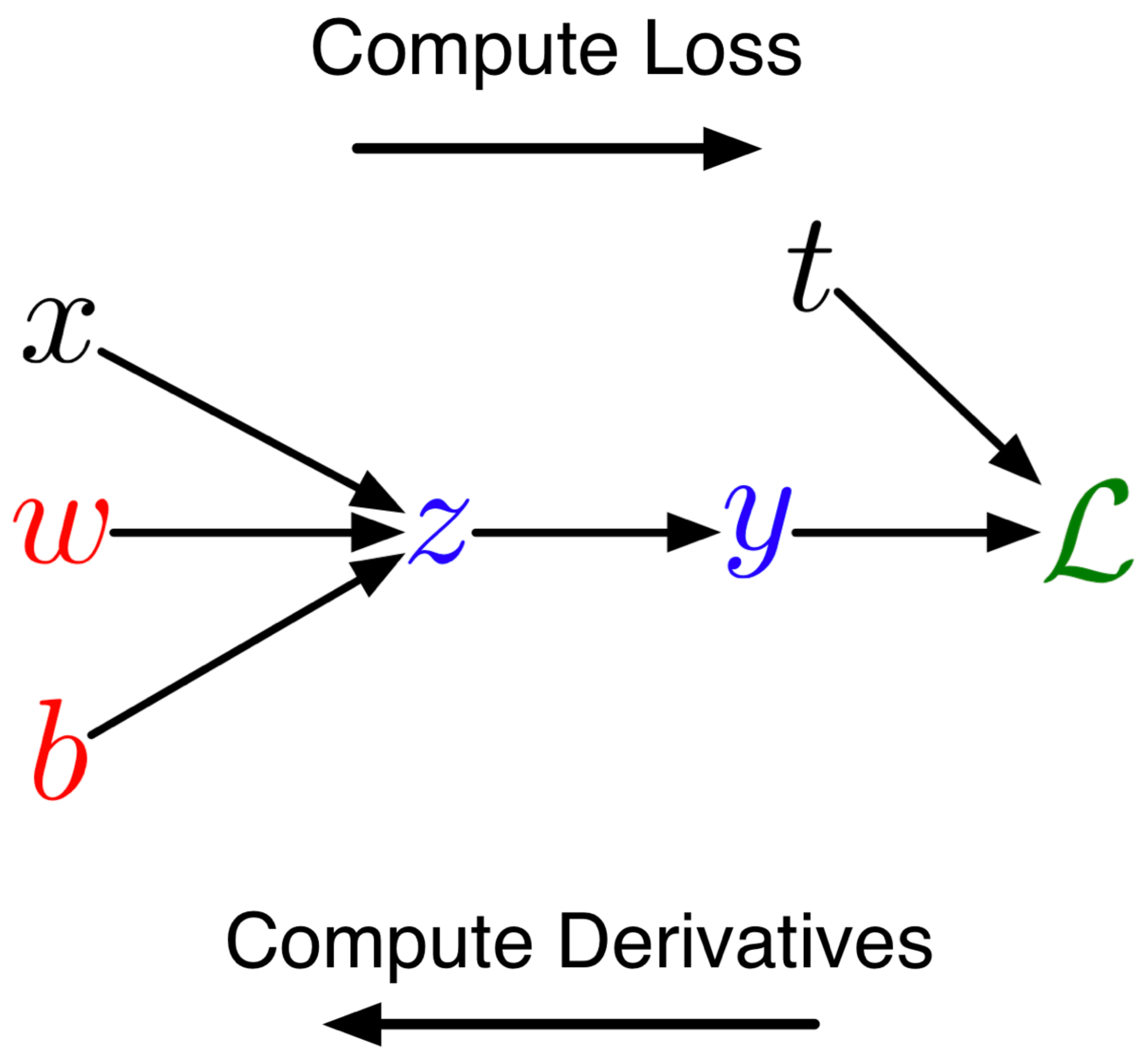
$$z = wx + b$$
$$y = \sigma(z)$$
$$\mathcal{L} = \frac{1}{2}(y - t)^2$$

Computing the derivatives:

$$\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}y} = y - t$$
$$\frac{\mathrm{d}\mathcal{L}}{\mathrm{d}z} = \frac{\mathrm{d}\mathcal{L}}{\mathrm{d}y}\,\sigma'(z)$$
$$\frac{\partial\mathcal{L}}{\partial w} = \frac{\mathrm{d}\mathcal{L}}{\mathrm{d}z}\,x$$
$$\frac{\partial\mathcal{L}}{\partial b} = \frac{\mathrm{d}\mathcal{L}}{\mathrm{d}z}$$

The goal isn’t to obtain closed-form solutions, but to be able to write a program that efficiently computes the derivatives

Univariate Chain Rule



A Slightly More Convenient Notation

Use $\overline{y}$ to denote the derivative $\mathrm{d}\mathcal{L}/\mathrm{d}y$, sometimes called the error signal

Computing the loss:

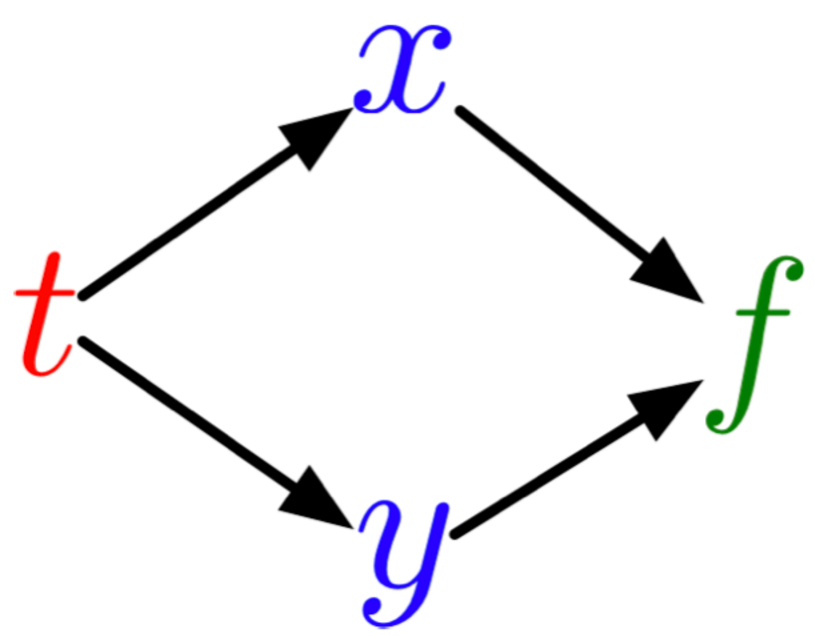
$$
\begin{aligned}
z &= wx + b \\
y &= \sigma(z) \\
\mathcal{L} &= \frac{1}{2}(y - t)^2
\end{aligned}
$$

Computing the derivatives:

$$
\begin{aligned}
\overline{y} &= y - t \\
\overline{z} &= \overline{y}\,\sigma'(z) \\
\overline{w} &= \overline{z}\,x \\
\overline{b} &= \overline{z}
\end{aligned}
$$

Multivariate Chain Rule

Problem: what if the computation graph has fan-out > 1?
This requires the multivariate Chain Rule!



$$\frac{\mathrm{d}}{\mathrm{d}t} f(x(t), y(t)) = \frac{\partial f}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}t} + \frac{\partial f}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}t}$$

Example:

$$f(x, y) = y + e^{xy}$$
$$x(t) = \cos t$$
$$y(t) = t^2$$

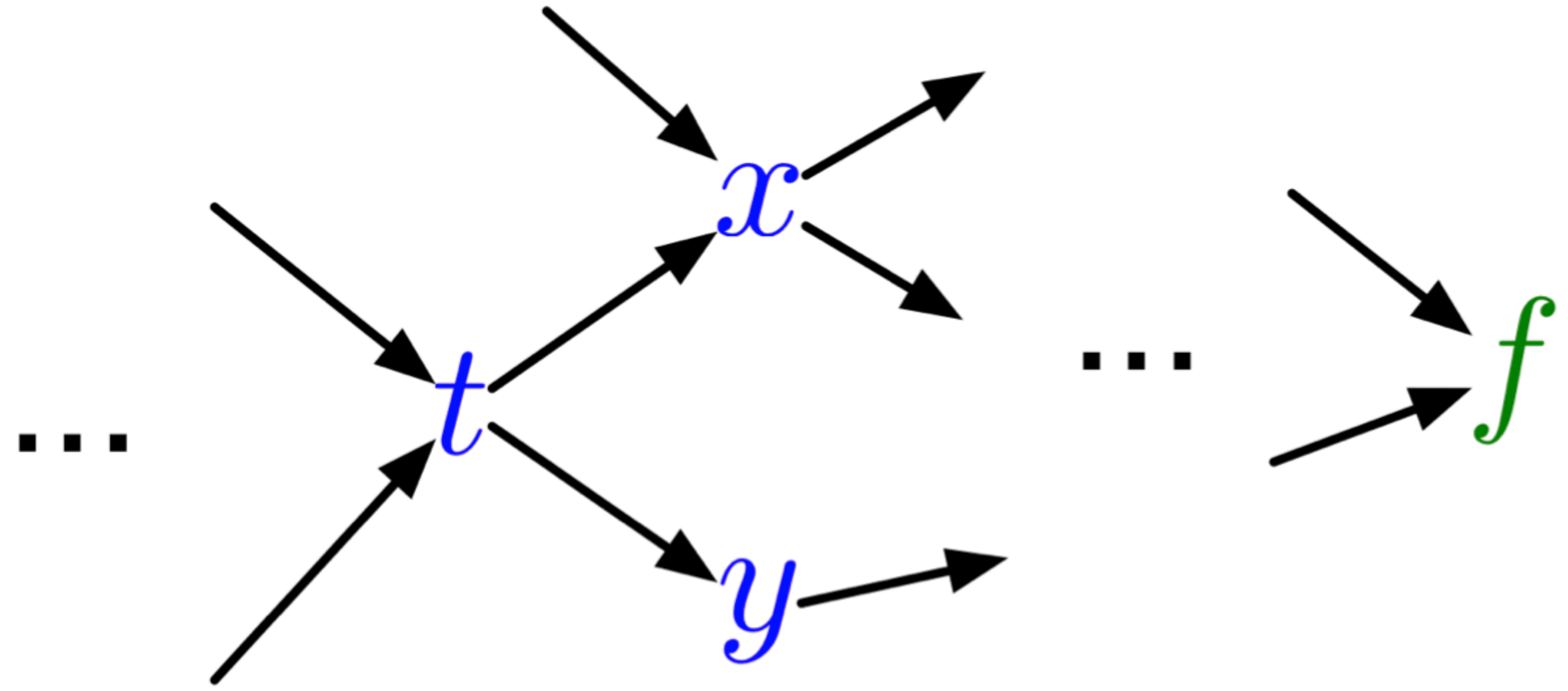
$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}t} + \frac{\partial f}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}t}$$
$$= (ye^{xy}) \cdot (-\sin t) + (1 + xe^{xy}) \cdot 2t$$

Multivariate Chain Rule

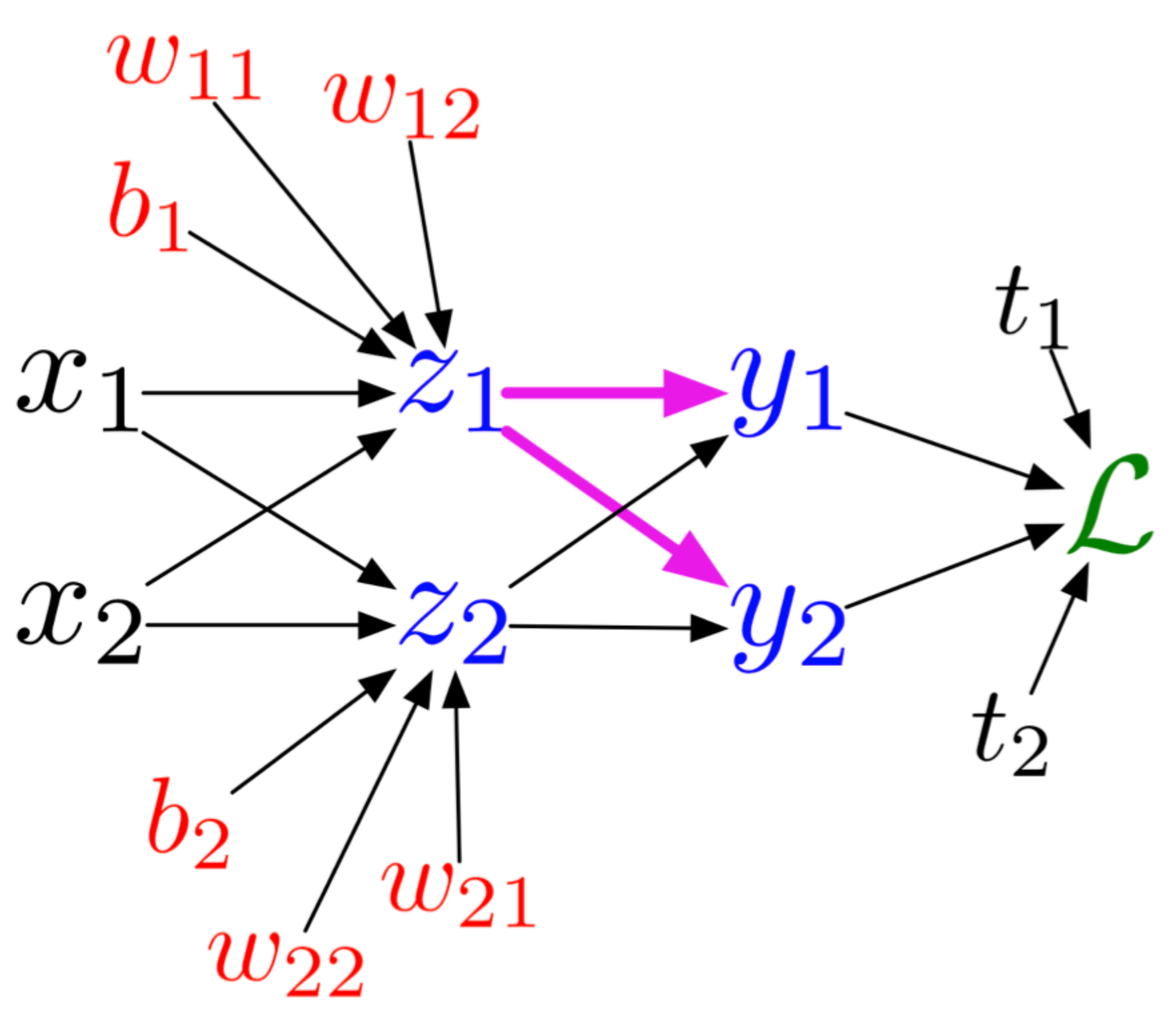
Mathematical expressions
to be evaluated

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}t} + \frac{\partial f}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}t}$$

Values already computed
by our program



Another Example



$$z_\ell = \sum_j w_{\ell j} x_j + b_\ell$$

$$y_k = \frac{e^{z_k}}{\sum_\ell e^{z_\ell}}$$

$$\mathcal{L} = -\sum t_k \log y_k$$

Backpropagation

Let $v_1, \ldots, v_N$ be a topological ordering of the computation graph (i.e. parents come before children.)

v_N denotes the variable we're trying to compute derivatives of (e.g. loss).

forward pass

$$\text{For } i = 1, \ldots, N$$
$$\quad \text{Compute } v_i \text{ as a function of } \mathrm{Pa}(v_i)$$

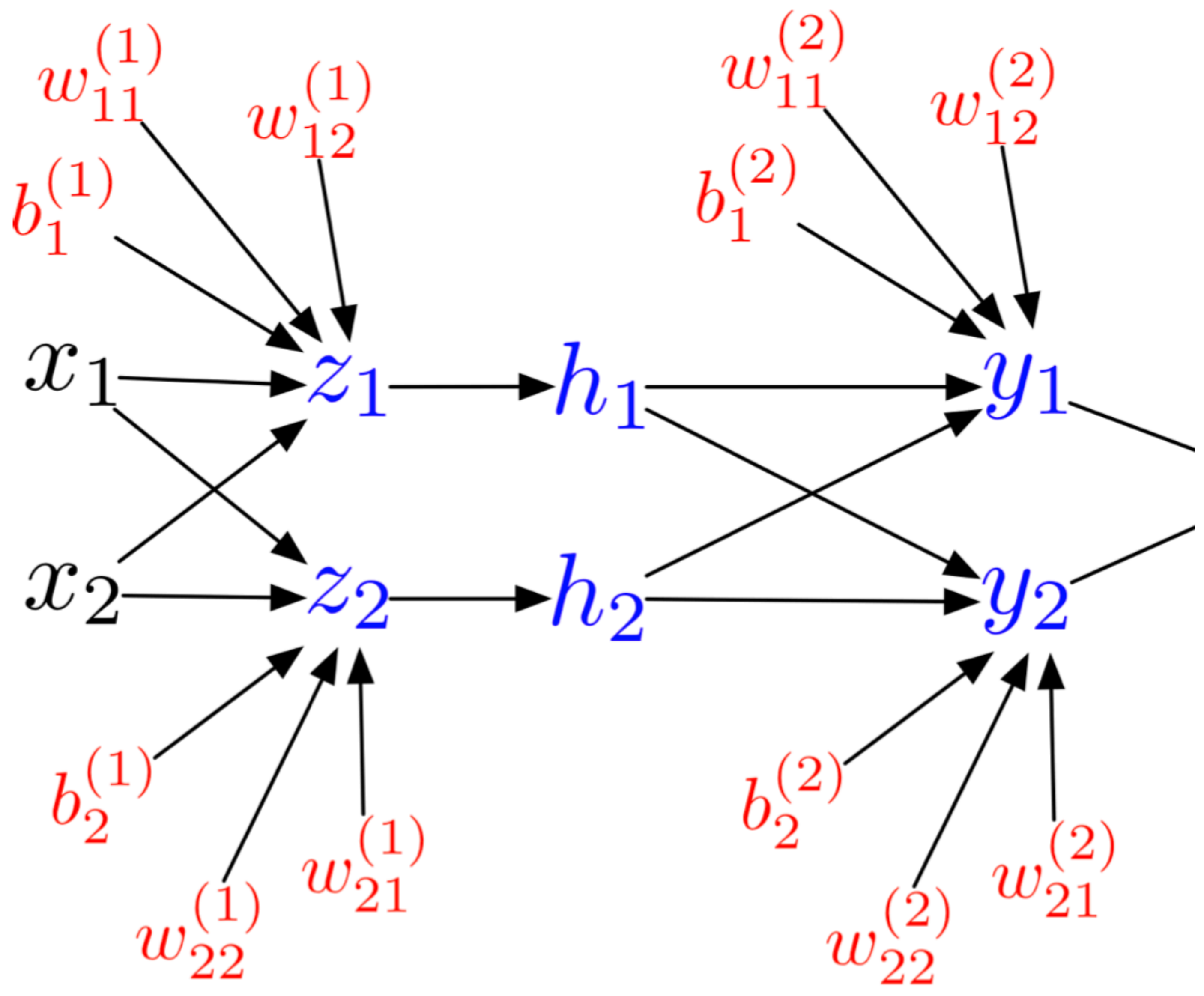
backward pass

$$\overline{v_N} = 1$$
$$\text{For } i = N-1, \ldots, 1$$
$$\quad \overline{v_i} = \sum_{j \in \mathrm{Ch}(v_i)} \overline{v_j} \frac{\partial v_j}{\partial v_i}$$

[1] David Rumelhart, Geoffrey Hinton, Ronald Williams. Learning representations by back-propagating errors. Nature. 1986

Backpropagation

Multilayer Perceptron (multiple outputs):



Forward pass:

$$z_i = \sum_j w^{(1)}_{ij} x_j + b^{(1)}_i$$

$$h_i = \sigma(z_i)$$

$$y_k = \sum_i w^{(2)}_{ki} h_i + b^{(2)}_k$$

$$\mathcal{L} = \frac{1}{2} \sum_k (y_k - t_k)^2$$

Backward pass:

$$\overline{\mathcal{L}} = 1$$

$$\overline{y_k} = \overline{\mathcal{L}}\,(y_k - t_k)$$

$$\overline{w^{(2)}_{ki}} = \overline{y_k}\, h_i$$

$$\overline{b^{(2)}_k} = \overline{y_k}$$

$$\overline{h_i} = \sum_k \overline{y_k} w^{(2)}_{ki}$$

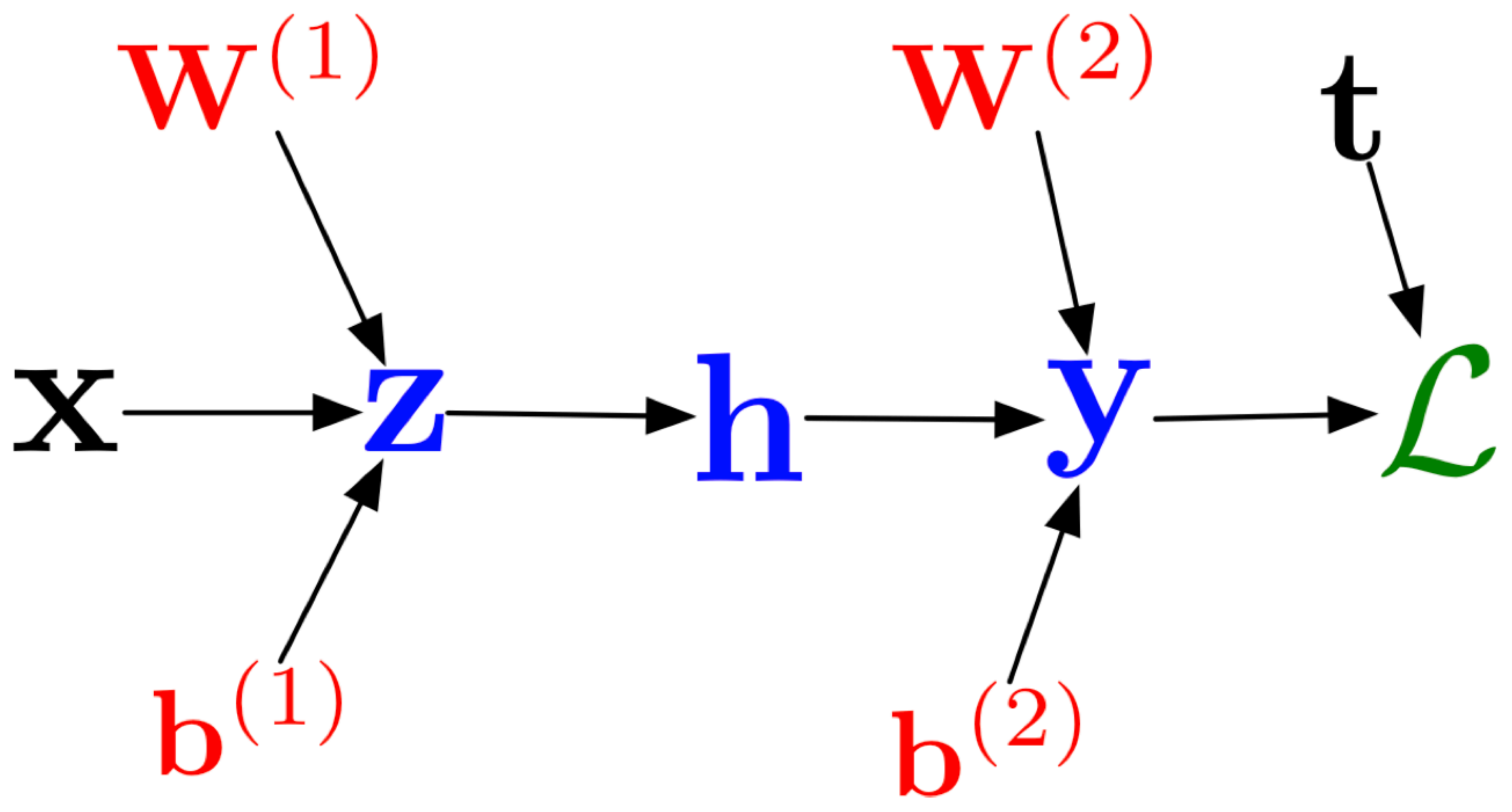
$$\overline{z_i} = \overline{h_i}\, \sigma'(z_i)$$

$$\overline{w^{(1)}_{ij}} = \overline{z_i}\, x_j$$

$$\overline{b^{(1)}_i} = \overline{z_i}$$

Backpropagation

In vectorized form:



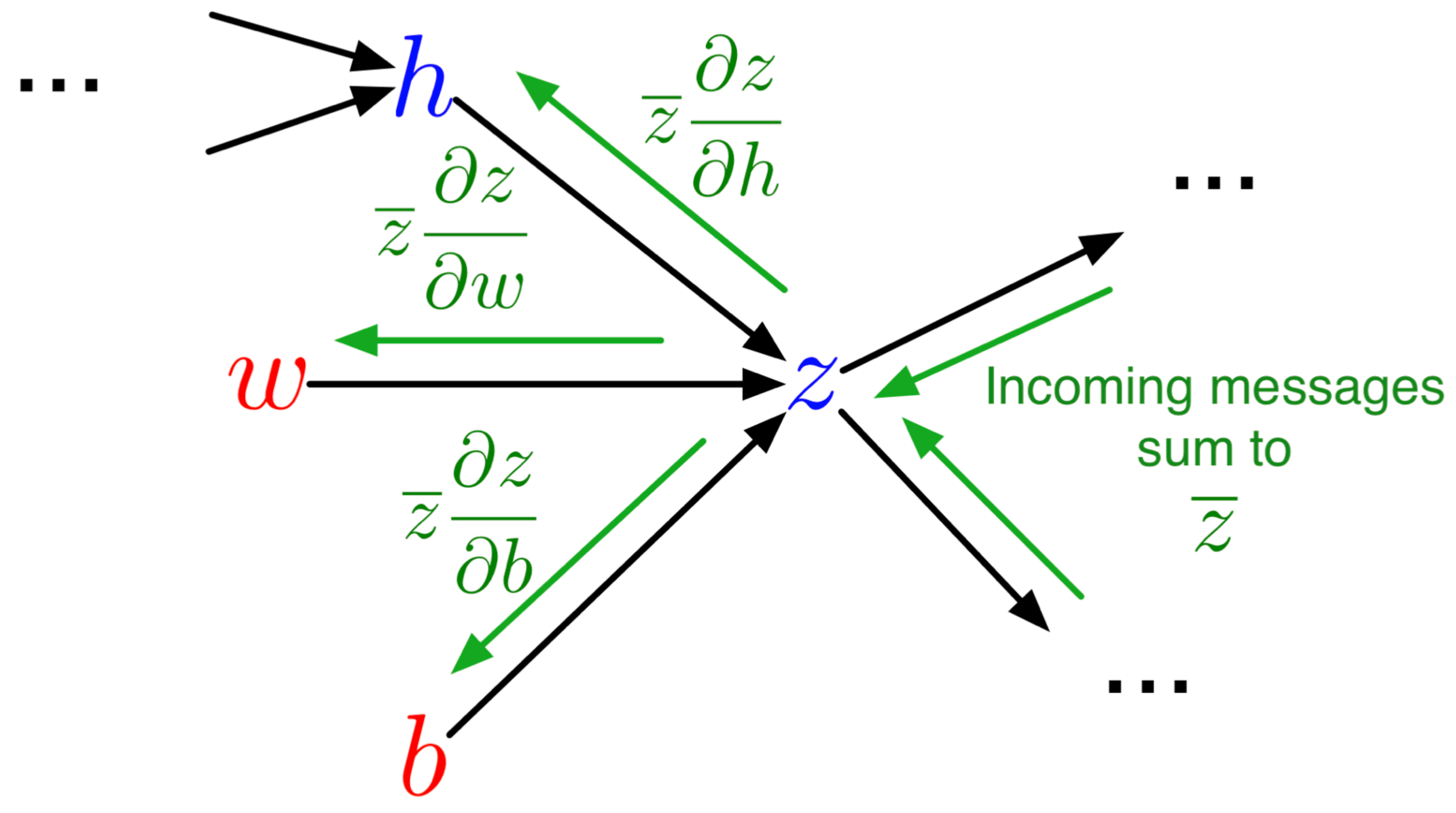
Forward pass:

$$\begin{aligned}
\mathbf{z} &= \mathbf{W}^{(1)}\mathbf{x} + \mathbf{b}^{(1)} \\
\mathbf{h} &= \sigma(\mathbf{z}) \\
\mathbf{y} &= \mathbf{W}^{(2)}\mathbf{h} + \mathbf{b}^{(2)} \\
\mathcal{L} &= \frac{1}{2}\|\mathbf{t} - \mathbf{y}\|^2
\end{aligned}$$

Backward pass:

$$\begin{aligned}
\overline{\mathcal{L}} &= 1 \\
\overline{\mathbf{y}} &= \overline{\mathcal{L}}\,(\mathbf{y} - \mathbf{t}) \\
\overline{\mathbf{W}^{(2)}} &= \overline{\mathbf{y}}\mathbf{h}^\top \\
\overline{\mathbf{b}^{(2)}} &= \overline{\mathbf{y}} \\
\overline{\mathbf{h}} &= \mathbf{W}^{(2)\top}\overline{\mathbf{y}} \\
\overline{\mathbf{z}} &= \overline{\mathbf{h}} \circ \sigma'(\mathbf{z}) \\
\overline{\mathbf{W}^{(1)}} &= \overline{\mathbf{z}}\mathbf{x}^\top \\
\overline{\mathbf{b}^{(1)}} &= \overline{\mathbf{z}}
\end{aligned}$$

Backpropagation as Message Passing



- Each node receives a bunch of messages from its children, which it aggregates to get its error signal. It then passes messages to its parents.

Each node only has to know how to compute derivatives with respect to its arguments, and doesn't have to know anything about the rest of the graph

Computational Cost

- Computational cost of forward pass: one add-multiply operation per weight

$$z_i = \sum_j w_{ij}^{(1)} x_j + b_i^{(1)}$$

- Computational cost of backward pass: two add-multiply operations per weight

$$\overline{w_{ki}^{(2)}} = \overline{y_k}\, h_i$$
$$\overline{h_i} = \sum_k \overline{y_k} w_{ki}^{(2)}$$

The backward pass is about as expensive as two forward passes

For a multilayer perceptron, this means the cost is linear in the number of layers, quadratic in the number of units per layer

Backpropagation

- Backprop is used to train the overwhelming majority of neural nets today.
  - Even optimization algorithms much fancier than gradient descent (e.g. second-order methods) use backprop to compute the gradients.

- Despite its practical success, backprop is believed to be neurally implausible.
  - No evidence for biological signals analogous to error derivatives.
  - All the biologically plausible alternatives we know about learn much more slowly (on computers).
  - So how on earth does the brain learn?

Backpropagation

- By now, we've seen three different ways of looking at gradients:
  - **Geometric:** visualization of gradient in weight space
  - **Algebraic:** mechanics of computing the derivatives
  - **Implementational:** efficient implementation on the computer

Stochastic Gradient Descent

Vanilla backpropagation training is slow with lot of data and lot of weights

Denote the loss of a single data example x_i as $l(x_i)$, the training loss L is:

$$L = \mathbb{E}_{x \sim p_{data}} l(x) \approx \frac{1}{N} \sum_{i=1}^{N} l(x_i)$$

N is the size of the entire training dataset

This is slow on the entire training dataset, thus we use MCMC to approximate:

$$\nabla L = \nabla \mathbb{E}_{x \sim p_{data}} l(x) \approx \nabla \frac{1}{n} \sum_{i=1}^{n} l(x_i)$$

n is the size of a random minibatch (batch size)

n can be as small as one

Background

A Recipe for Machine Learning

1. Given training data:

$$\{\boldsymbol{x}_i, \boldsymbol{y}_i\}_{i=1}^N$$

2. Choose each of these:

- Decision function

$$\hat{\boldsymbol{y}} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

- Loss function

$$\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}_i) \in \mathbb{R}$$

3. Define goal:

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^N \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

4. Train with SGD:

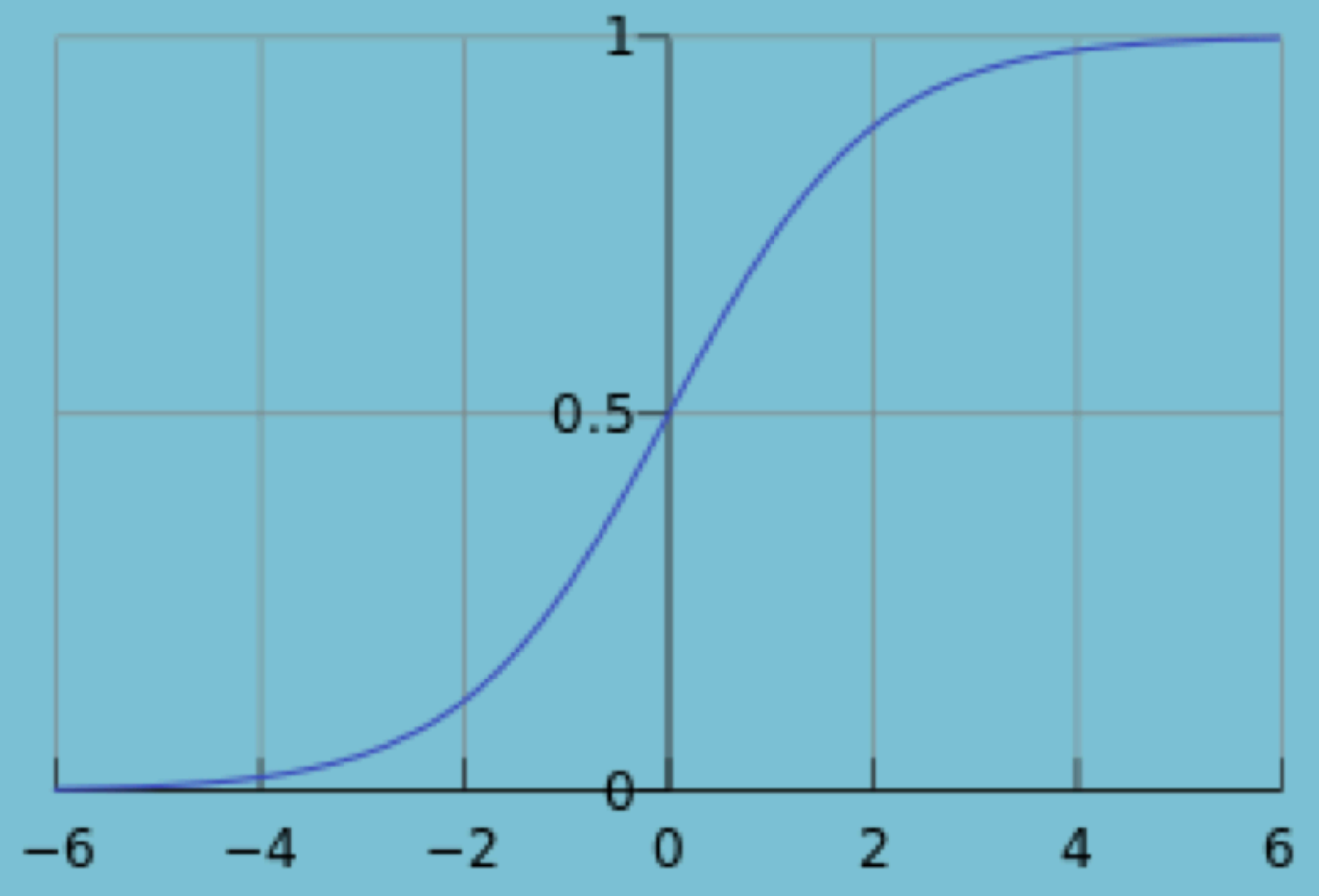
(take small steps opposite the gradient)

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \eta_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

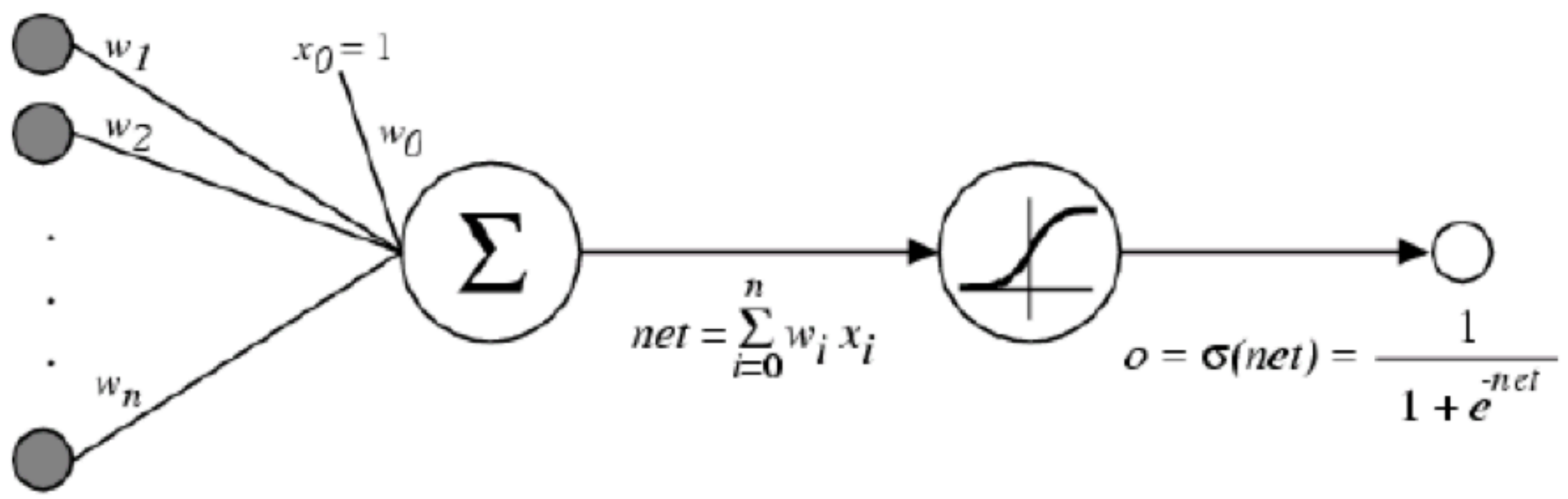
Activation Functions

Sigmoid / Logistic Function

$$\text{logistic}(u) \equiv \frac{1}{1+e^{-u}}$$

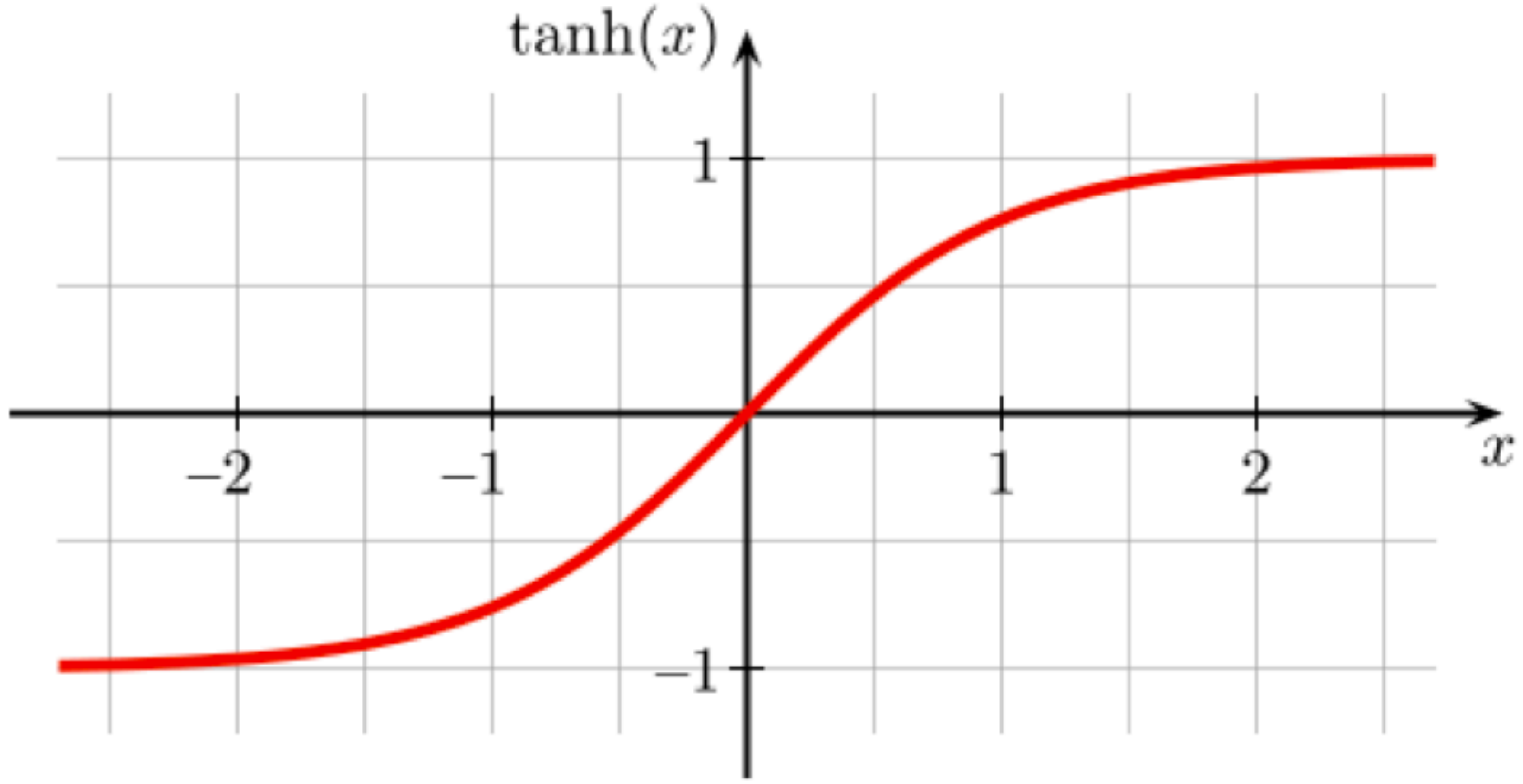


So far, we've assumed that the activation function (nonlinearity) is always the sigmoid function…



Tanh

- A new change: modifying the nonlinearity
  - The logistic is not widely used in modern ANNs



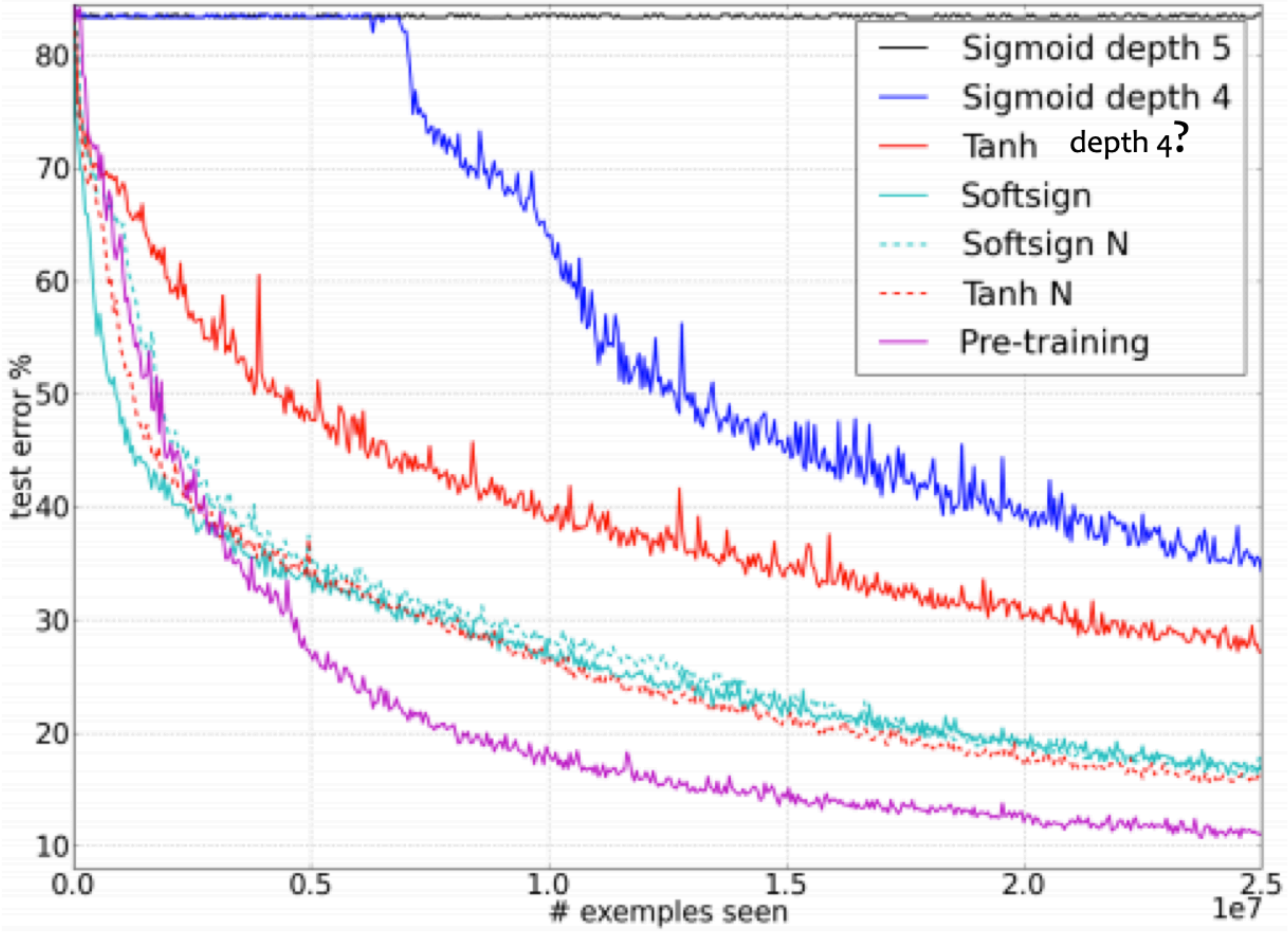
Alternate 1: tanh

Like logistic function but shifted to range [-1, +1]

Activation Function

Understanding the difficulty of training deep feedforward neural networks

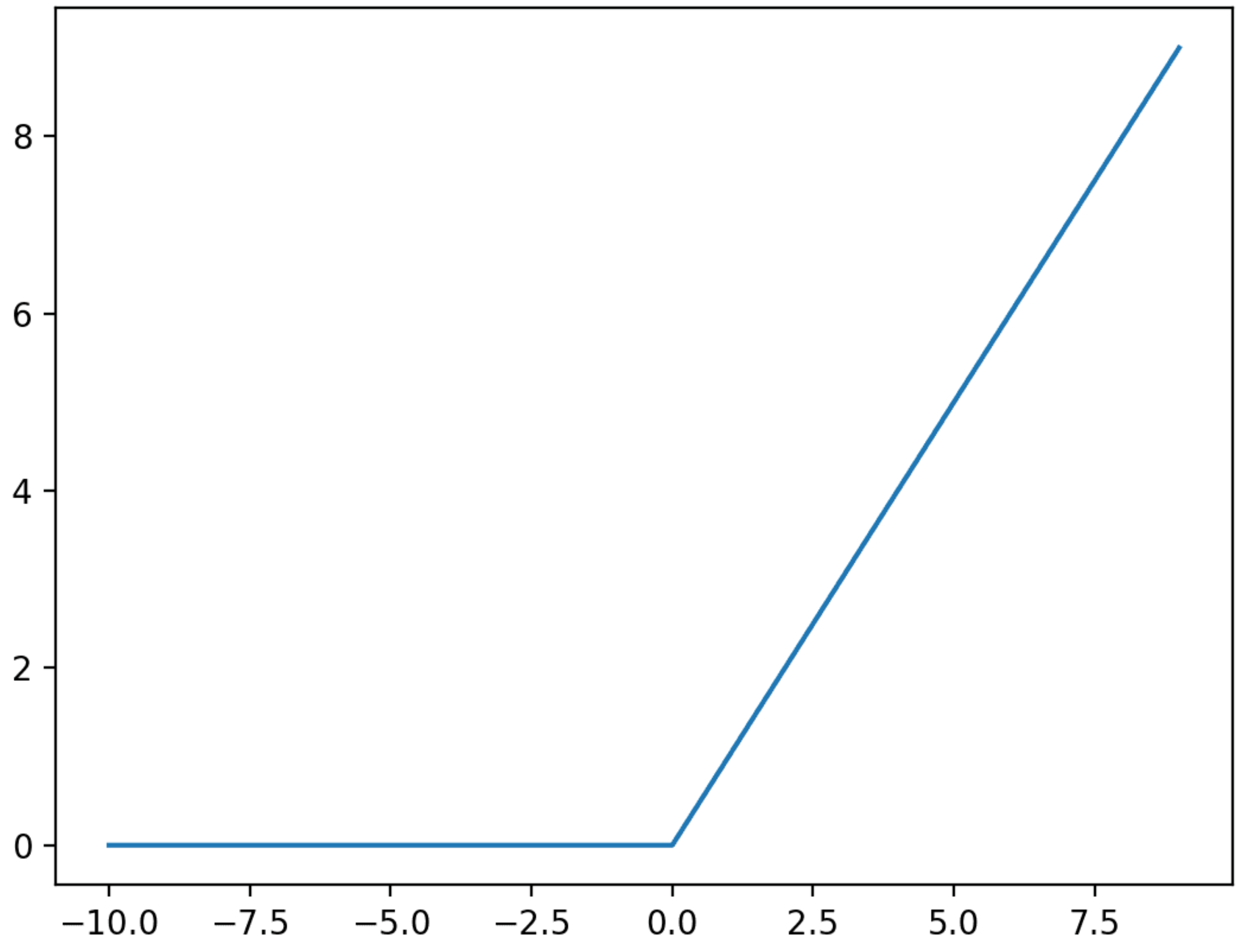
AI Stats 2010



sigmoid
vs.
tanh

Figure from Glorot & Bentio (2010)

ReLU



Other Activation Functions

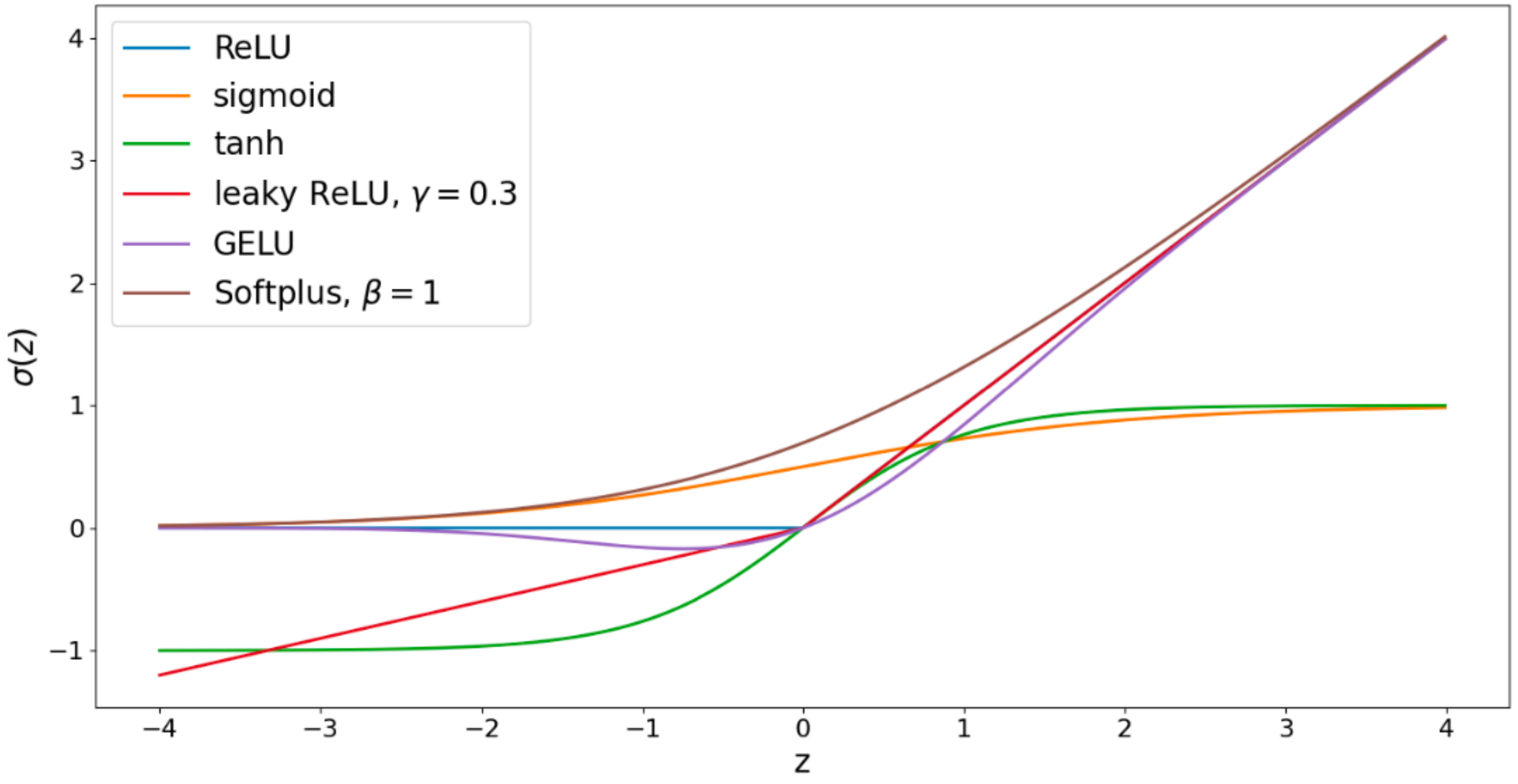
$$\sigma(z) = \frac{1}{1+e^{-z}} \qquad \text{(sigmoid)}$$

$$\sigma(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}} \qquad \text{(tanh)}$$

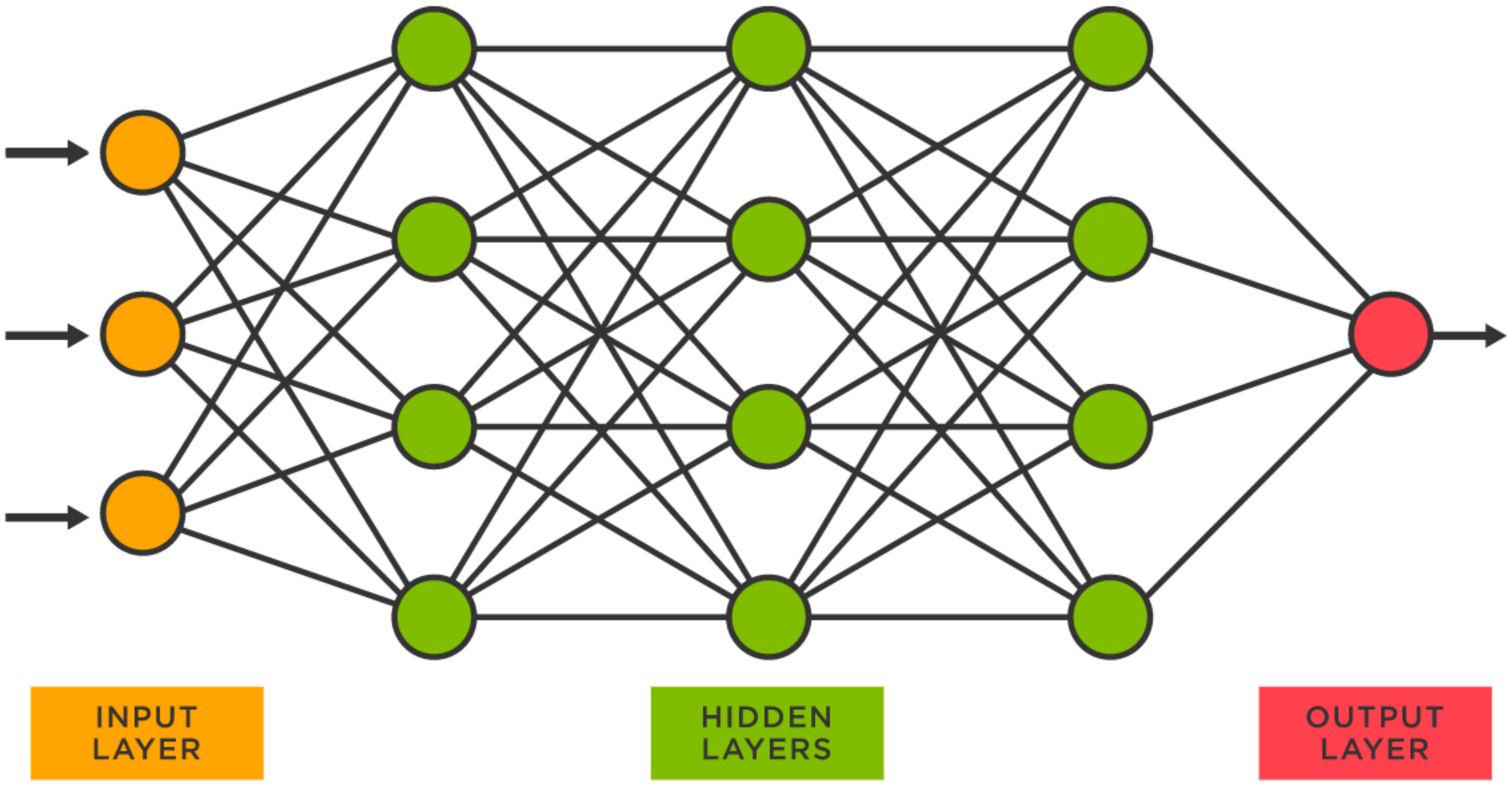
$$\sigma(z) = \max\{z, \gamma z\}, \gamma \in (0,1) \qquad \text{(leaky ReLU)}$$

$$\sigma(z) = \frac{z}{2}\left[1 + \text{erf}\left(\frac{z}{\sqrt{2}}\right)\right] \qquad \text{(GELU)}$$

$$\sigma(z) = \frac{1}{\beta}\log(1+\exp(\beta z)), \beta > 0 \qquad \text{(Softplus)}$$



Multilayer Perceptron Neural Networks (MLP)



Thank You!