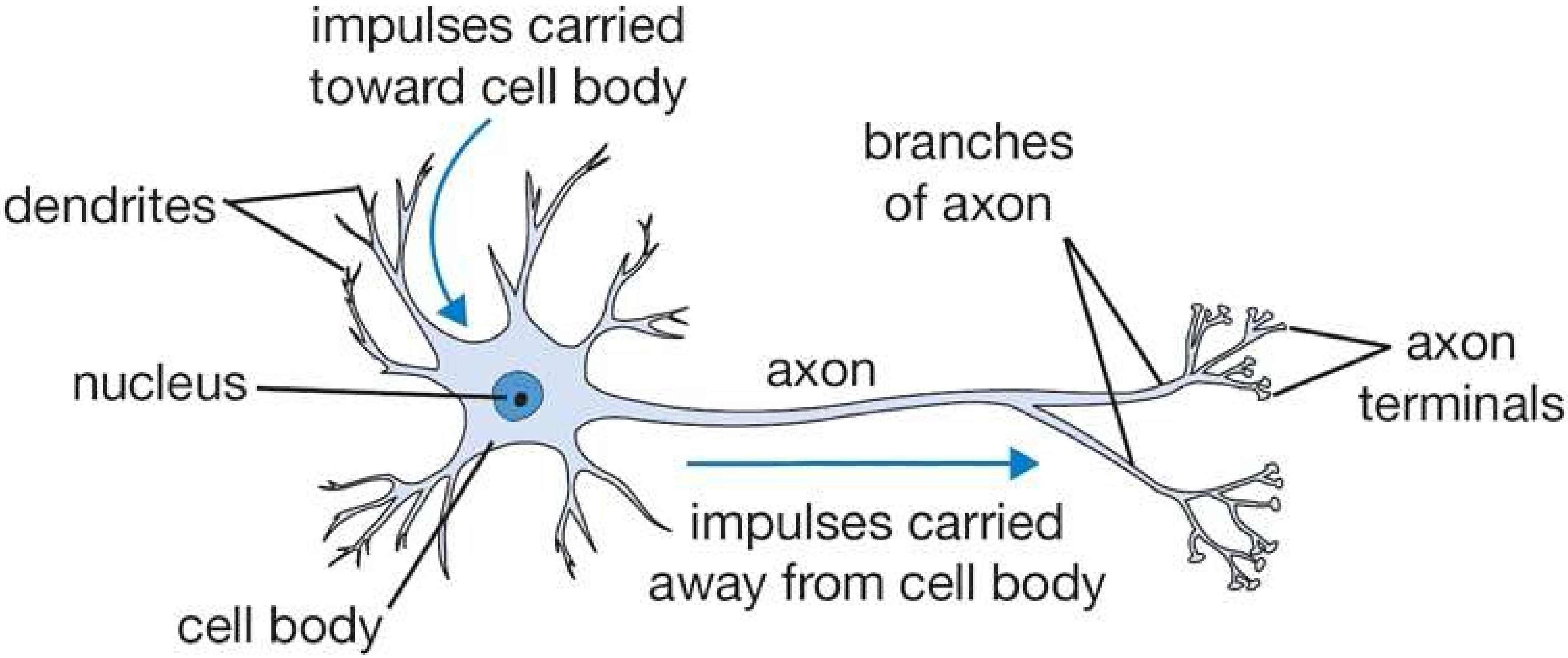
Agenda

- Biological and Artificial Neurons
- Neural Network
- Multi-Layer Perceptron (Fully-connected layers)
- Backpropagation

Biological and Artificial Neurons

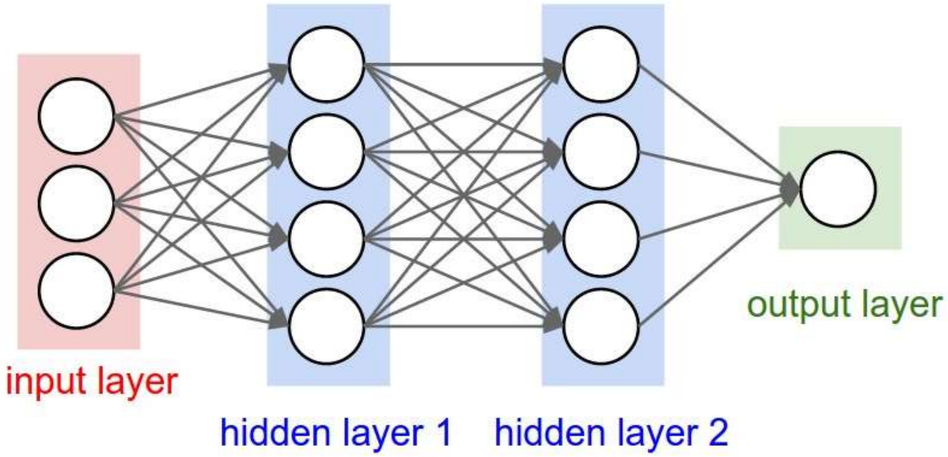
Neuron


impulses carried toward cell body
dendrites
branches of axon
nucleus
axon
axon terminals
impulses carried away from cell body
cell body

An Artificial Neural Network (Multi-Layer Perceptron)

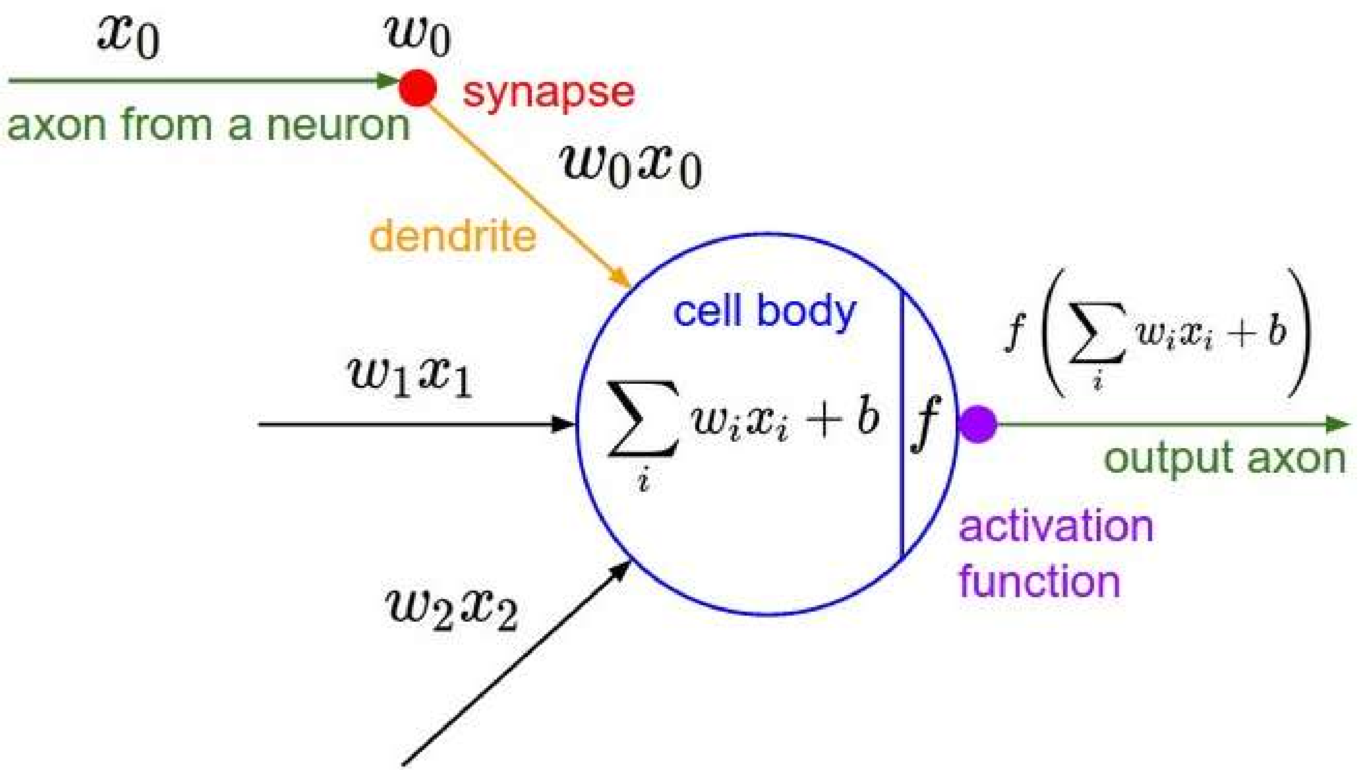
Idea:

- Use a simplified (mathematical) model of a neuron as building blocks
- Connect the neurons together in the following way:



- An **input layer**: feed in input features (e.g. like retinal cells in your eyes)
- A number of **hidden layers**: don't have specific meaning
- An **output layer**: interpret output like a "grandmother cell"

Modeling Individual Neurons



- $x_1, x_2, \ldots =$ inputs to the neuron
- $w_1, w_2, \ldots =$ the neuron's **weights**
- $b =$ the neuron's **bias**
- $f =$ an **activation function**
- $f(\sum_i x_i w_i + b) =$ the neuron's **activation** (output)

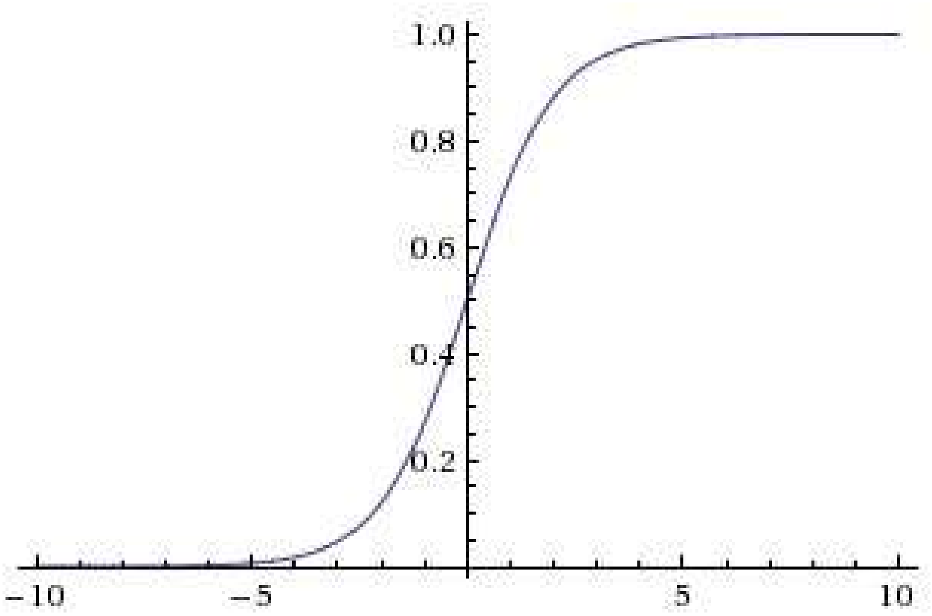
Activation Functions: common choices

Common Choices:

- Sigmoid activation
- Tanh activation
- ReLU activation

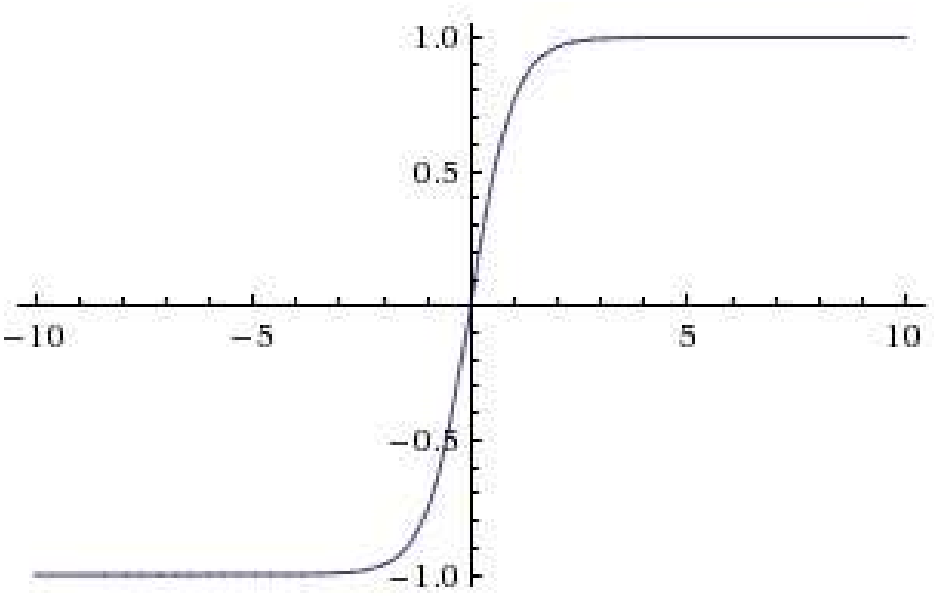
Rule of thumb: Start with ReLU activation. If necessary, try tanh.

Activation Function: Sigmoid



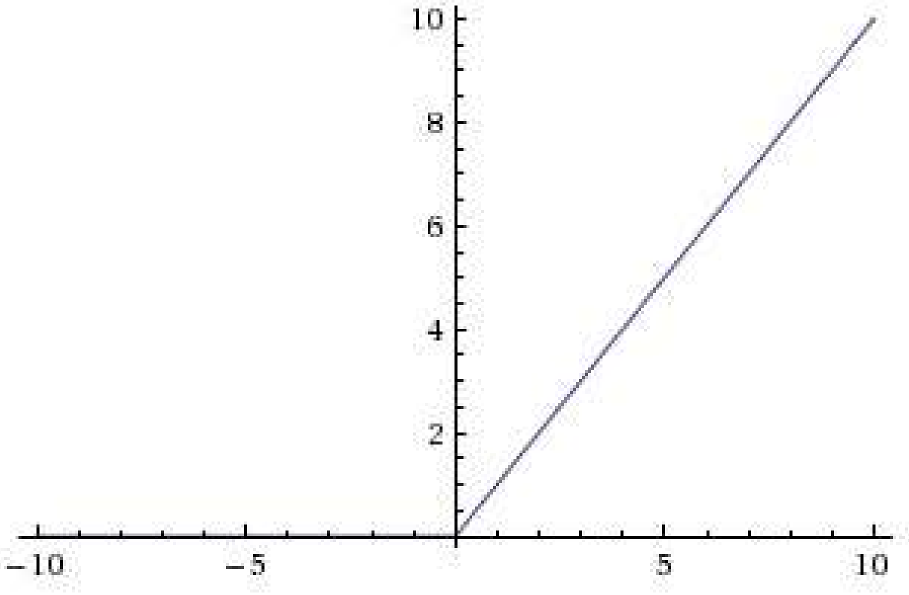
- somewhat problematic due to gradient signal
- all activations are positive

Activation Function: Tanh



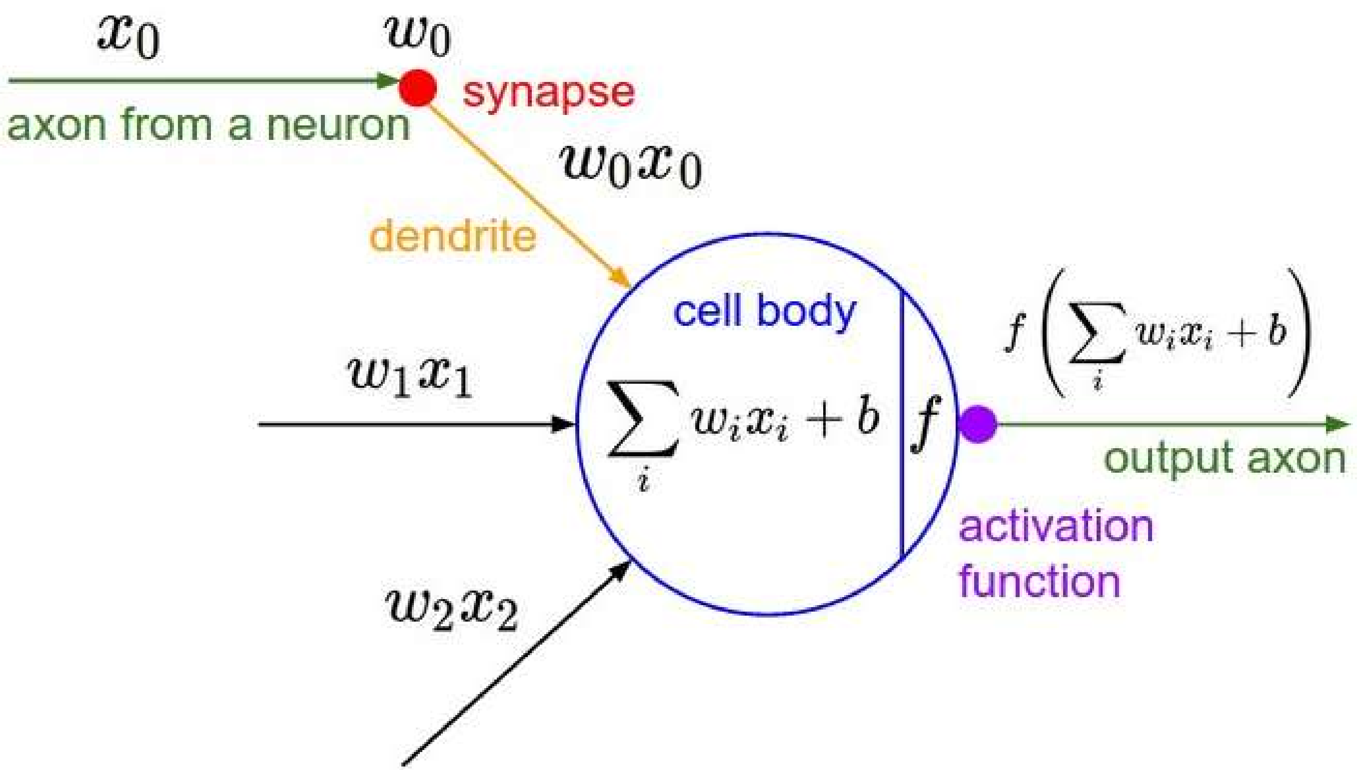
- scaled version of the sigmoid activation
- also somewhat problematic due to gradient signal
- activations can be positive or negative

Activation Function: ReLU



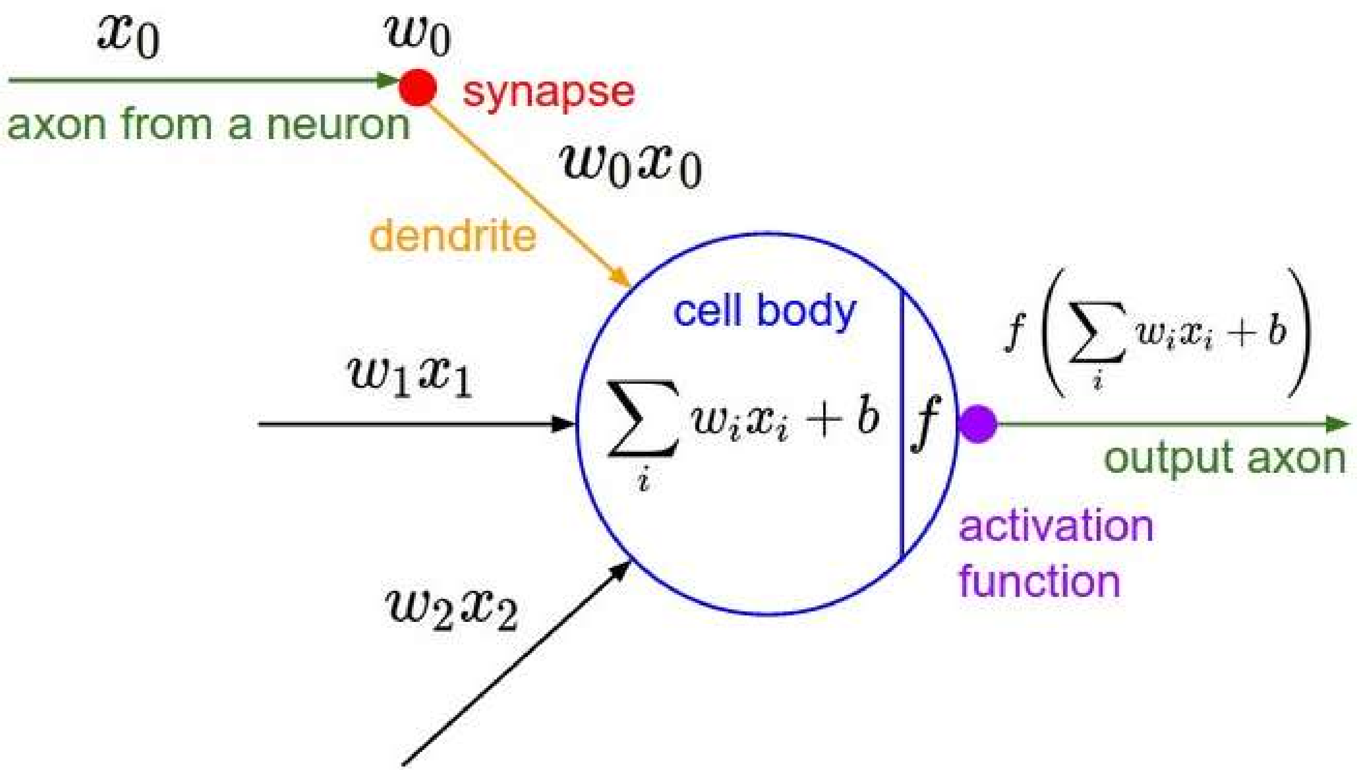
- most often used nowadays
- all activations are positive
- easy to compute gradients
- can be problematic if the bias is too large and negative, so the activations are always 0

Linear Regression as a Single Neuron



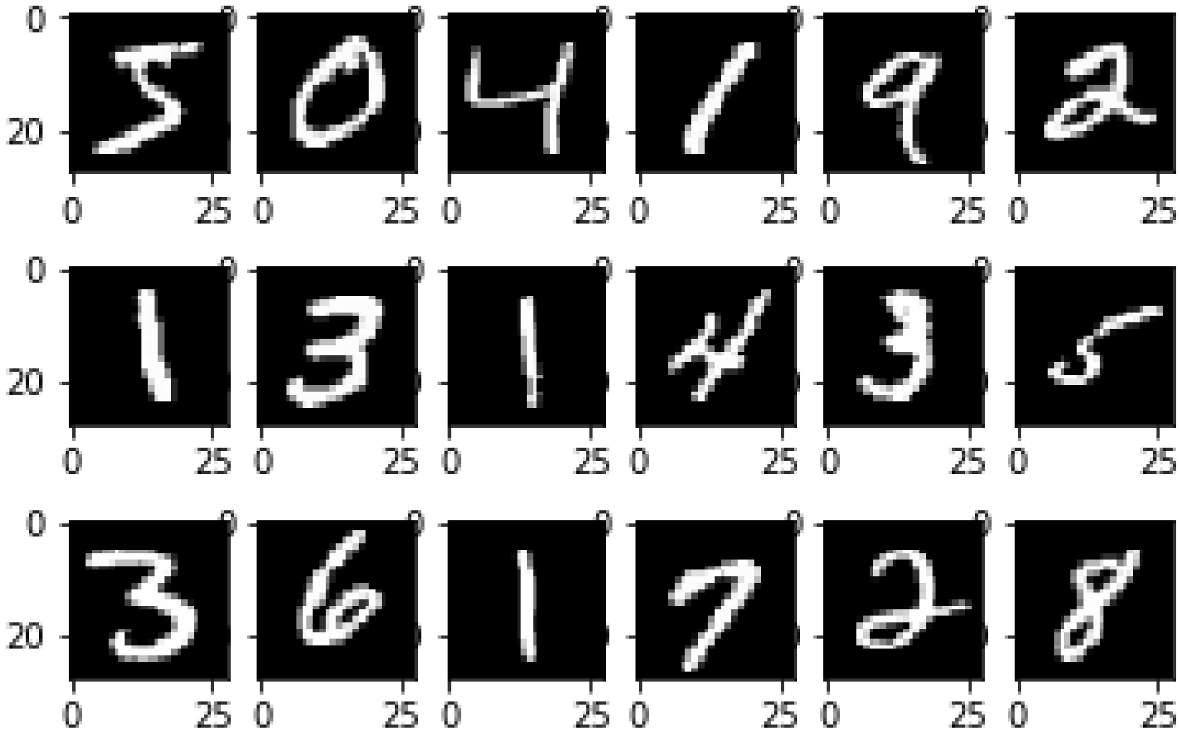
- $x_1, x_2, \ldots$: inputs
- $w_1, w_2, \ldots$: components of the **weight vector w**
- b : the **bias**
- f : identity function
- $y = \sum_i x_i w_i + b = \mathbf{w}^T \mathbf{x} + b$

Binary Classification (Logistic Regression) as a Single Neuron



- $x_1, x_2, \ldots$: inputs
- $w_1, w_2, \ldots$: components of the **weight vector w**
- b : the **bias**
- $f = \sigma$
- $y = \sigma(\sum_i x_i w_i + b) = \sigma(\mathbf{w}^T \mathbf{x} + b)$

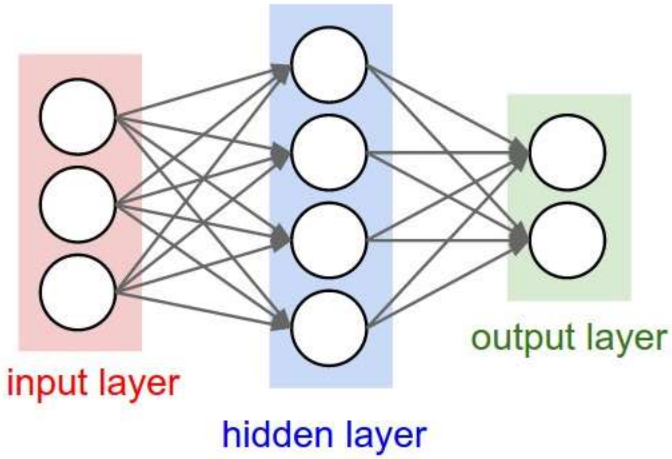
MNIST Digit Recognition



- Input: An 28x28 pixel image
    - $\mathbf{x}$ is a vector of length 784
- Target: The digit represented in the image
    - $\mathbf{t}$ is a one-hot vector of length 10
- Model (from tutorial 4)
    - $\mathbf{y} = \text{softmax}(W\mathbf{x} + \mathbf{b})$

Adding a Hidden Layer

Two layer neural network



- Input size: 784 (number of features)
- Hidden size: 50 (we choose this number)
- Output size: 10 (number of classes)

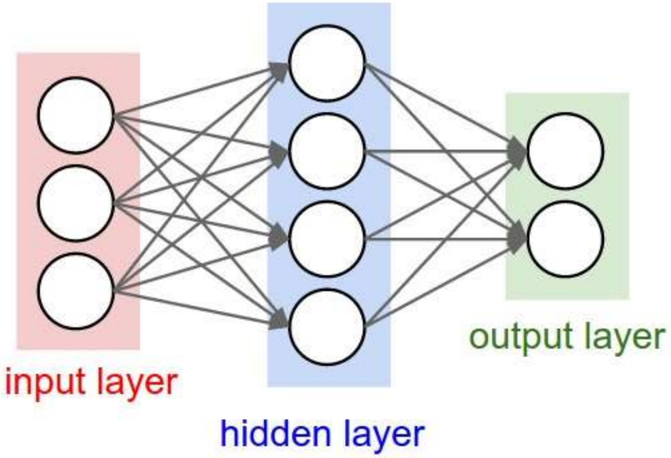
Side note about machine learning models

When discussing machine learning models, we usually

- first talk about **how to make predictions** assume the weights are trained
- *then* talk about how to traing the weights

Often the second step requires gradient descent or some other optimization method

Making Predictions: computing the hidden layer

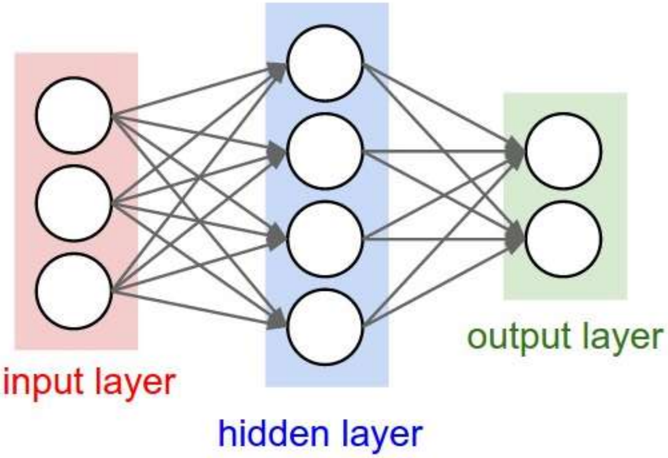


$$h_1 = f(\sum_{i=1}^{784} w_{1,i}^{(1)} x_i + b_1^{(1)})$$

$$h_2 = f(\sum_{i=1}^{784} w_{2,i}^{(1)} x_i + b_2^{(1)})$$

$\ldots$

Making Predictions: computing the output (pre-activation)

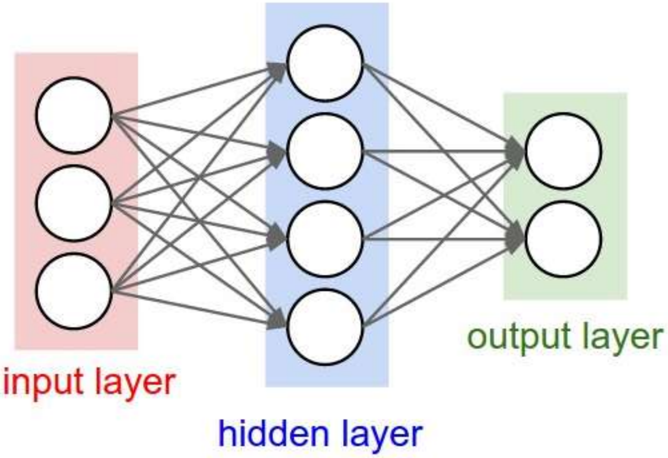


$$z_1 = \sum_{j=1}^{50} w_{1,j}^{(2)} h_j + b_1^{(2)}$$

$$z_2 = \sum_{j=1}^{50} w_{2,j}^{(2)} h_j + b_2^{(2)}$$

$$\dots$$

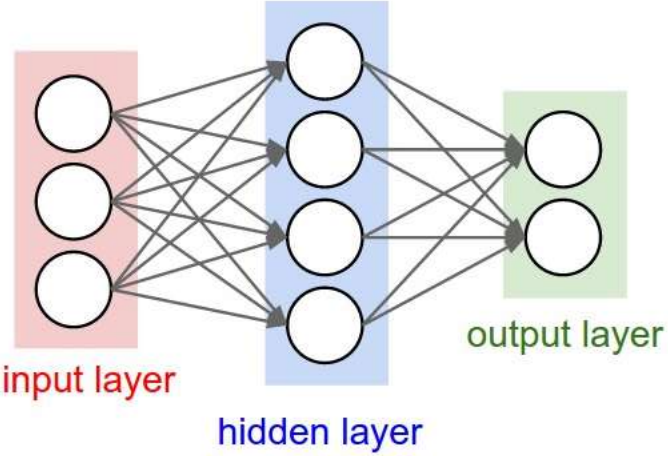
Making Predictions: applying the output activation



$$\mathbf{z} = \begin{bmatrix} z_1 \\ z_2 \\ \dots \\ z_{10} \end{bmatrix}$$

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

Making Predictions: Vectorized



$$\mathbf{h} = f(W^{(1)}\mathbf{x} + \mathbf{b}^{(1)})$$

$$\mathbf{z} = f(W^{(2)}\mathbf{h} + \mathbf{b}^{(2)})$$

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

Expressive Power: Linear Layers (No Activation Function)

- We've seen that there are some functions that linear classifiers can't represent. Are deep networks any better?
- Any sequence of *linear* layers (with no activation function) can be equivalently represented with a single linear layer.

$$\begin{aligned} \mathbf{y} &= \underbrace{W^{(3)} W^{(2)} W^{(1)}} \mathbf{x} \\ &= W' \mathbf{x} \end{aligned}$$

Deep linear networks are no more expressive than linear regression!

Expressive Power: MLP (nonlinear activation)

- Multilayer feed-forward neural nets with *nonlinear* activation functions are **universal approximators**: they can approximate any function arbitrarily well.
- This has been shown for various activation functions (thresholds, logistic, ReLU, etc.)
  - Even though ReLU is "almost" linear, it's nonlinear enough!

Universality for binary inputs and targets

- Hard threshold hidden units, linear output
- Strategy: 2^D hidden units, each of which responds to one particular input configuration
    - Only requires one hidden layer, though it needs to be extremely wide!

Limits of universality

- You may need to represent an exponentially large network.
- If you can learn any function, you'll just overfit.
- Really, we desire a *compact* representation!

Backpropagation

Training Neural Networks

- How do we find good weights for the neural network?
- We can continue to use the loss functions:
  - cross-entropy loss for classification
  - square loss for regression
- The neural network operations we used (weights, etc) are continuous

We can use gradient descent!

Gradient Descent Recap

- Start with a set of parameters (initialize to some value)
- Compute the gradient $\frac{\partial \mathcal{E}}{\partial w}$ for each parameter (also $\frac{\partial \mathcal{E}}{\partial b}$)
    - This computation can often vectorized
- Update the parameters towards the negative direction of the gradient

Gradient Descent for Neural Networks

- Conceptually, the exact same idea!
- However, we have more parameters than before
  - Higher dimensional
  - Harder to visualize
  - More “steps”

Since $\frac{\partial \mathcal{E}}{\partial w}$, is the average of $\frac{\partial \mathcal{L}}{\partial w}$ across training examples, we’ll focus on computing $\frac{\partial \mathcal{L}}{\partial w}$

Univariate Chain Rule

Recall: if $f(x)$ and $x(t)$ are univariate functions, then

$$\frac{d}{dt}f(x(t)) = \frac{df}{dx}\frac{dx}{dt}$$

Univariate Chain Rule for Logistic Least Square

Recall: Univariate logistic least squares model

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

Let's compute the loss derivative

Univariate Chain Rule Computation (1)

How you would have done it in calculus class

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

Univariate Chain Rule Computation (2)

Similarly for $\frac{\partial \mathcal{L}}{\partial b}$

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

Univariate Chain Rule Computation (2)

Similarly for $\frac{\partial \mathcal{L}}{\partial b}$

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

Q: What are the disadvantages of this approach?

A More Structured Way to Compute the Derivatives

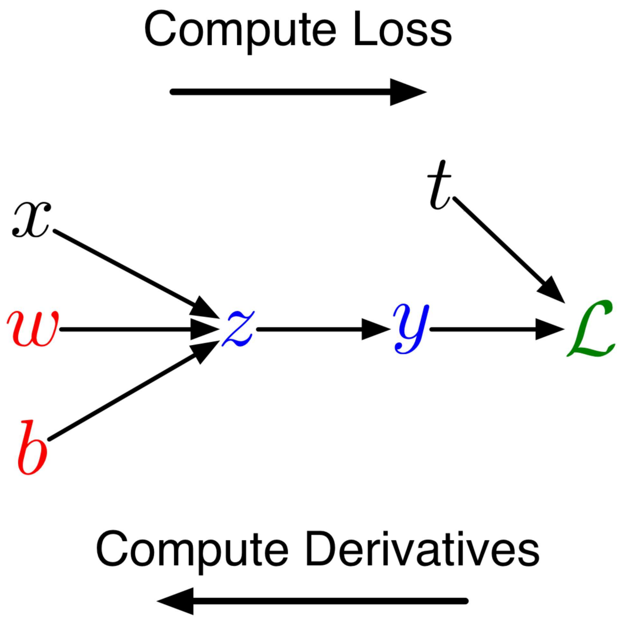
$$
\begin{aligned}
z &= wx + b \\
y &= \sigma(z) \\
\mathcal{L} &= \frac{1}{2}(y - t)^2
\end{aligned}
$$

$$
\begin{aligned}
\frac{d\mathcal{L}}{dy} &= y - t \\
\frac{d\mathcal{L}}{dz} &= \frac{d\mathcal{L}}{dy}\sigma'(z) \\
\frac{\partial\mathcal{L}}{\partial w} &= \frac{d\mathcal{L}}{dz}\, x \\
\frac{\partial\mathcal{L}}{\partial b} &= \frac{d\mathcal{L}}{dz}
\end{aligned}
$$

Less repeated work; easier to write a program to efficiently compute derivatives

Computation Graph

We can diagram out the computations using a *computation graph*.



The *nodes* represent all the inputs and computed quantities

The *edges* represent which nodes are computed directly as a function of which other nodes.

Chain Rule (Error Signal) Notation

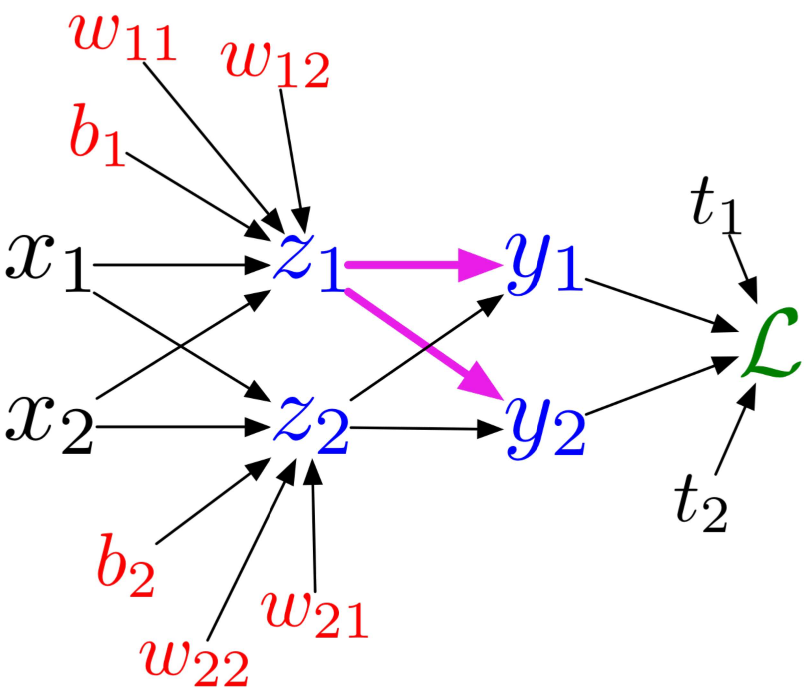
- Use $\overline{y}$ to denote the derivative $\frac{d\mathcal{L}}{dy}$
  - sometimes called the **error signal**
- This notation emphasizes that the error signals are just values our program is computing (rather than a mathematical operation).

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

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

Multiclass Logistic Regression Computation Graph

In general, the computation graph *fans out*:



$$z_l = \sum_j w_{lj} x_j + b_l$$

$$y_k = \frac{e^{z_k}}{\sum_l e^{z_l}}$$

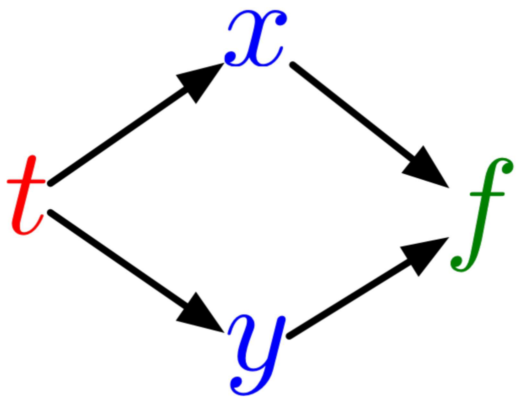
$$\mathcal{L} = -\sum_k t_k \log y_k$$

There are multiple paths for which a weight like w_{11} affects the loss L.

Multivariate Chain Rule

Suppose we have a function $f(x, y)$ and functions $x(t)$ and $y(t)$. (All the variables here are scalar-valued.) Then

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



Multivariate Chain Rule Example

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

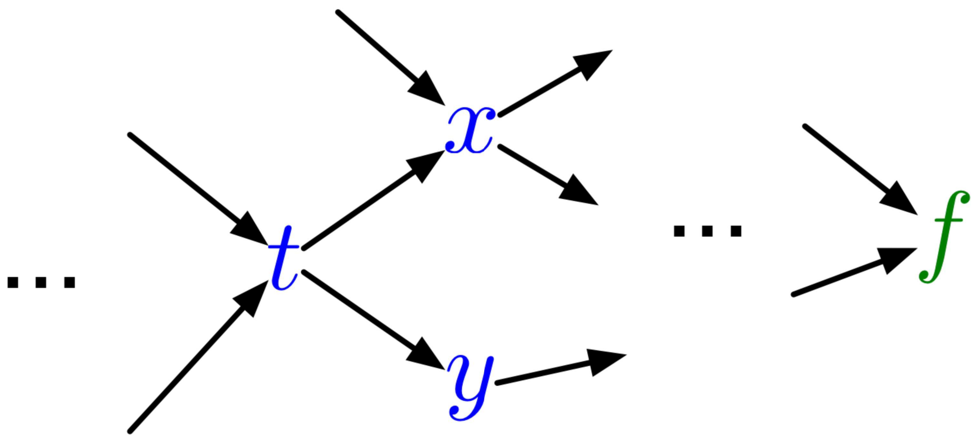
$$\begin{aligned}\frac{d}{dt} f(x(t), y(t)) &= \frac{\partial f}{\partial x}\frac{dx}{dt} + \frac{\partial f}{\partial y}\frac{dy}{dt} \\ &= (ye^{xy}) \cdot (-\sin t) + (1 + xe^{xy}) \cdot 2t\end{aligned}$$

Multivariate Chain Rule Notation

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



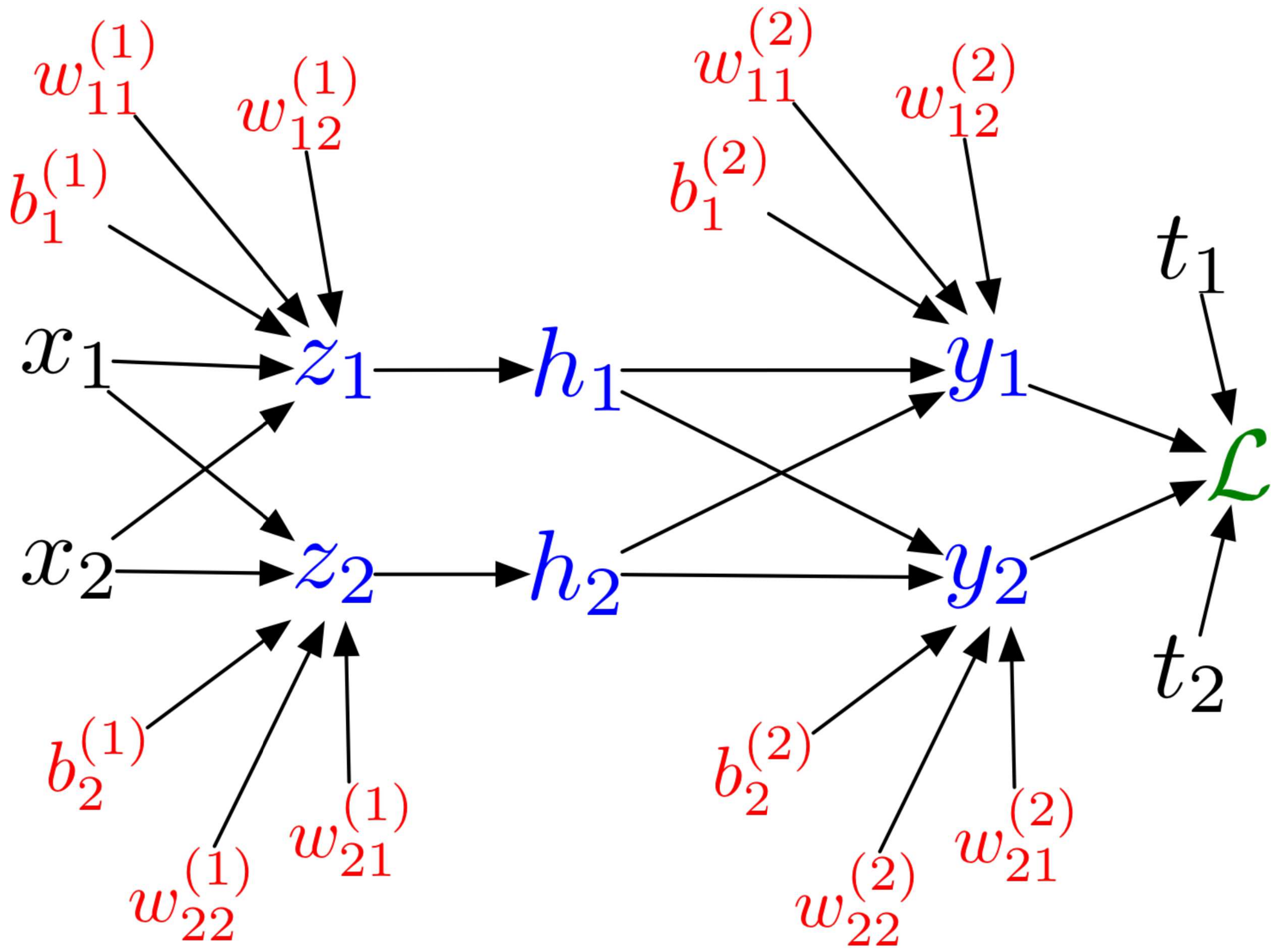
In our notation

$$\bar{t} = \bar{x}\frac{dx}{dt} + \bar{y}\frac{dy}{dt}$$

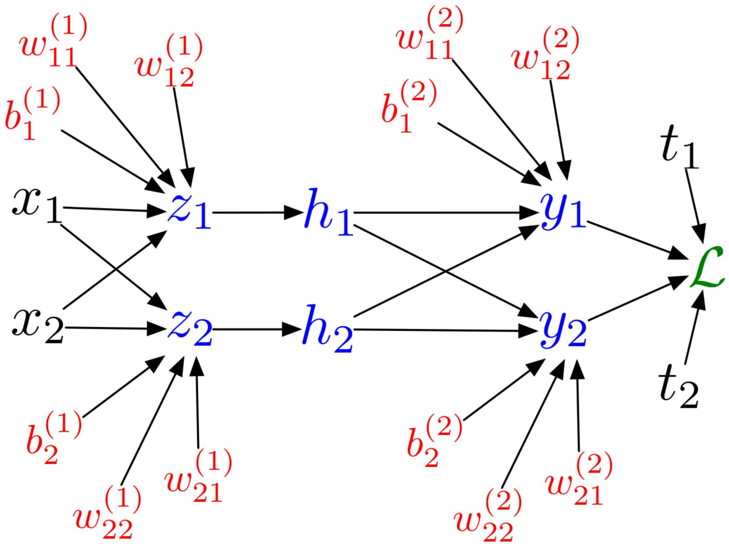
The Backpropagation Algorithm

- Backpropagation is an *algorithm* to compute gradients efficiency
  - Forward Pass: Compute predictions (and save intermediate values)
  - Backwards Pass: Compute gradients
- The idea behind backpropagation is very similar to *dynamic programming*
  - Use chain rule, and be careful about the order in which we compute the derivatives

Backpropagation Example



Backpropagation for a MLP



Forward pass:

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

$$h_i = \sigma(z_i)$$

$$y_k = \sum_i w_{ki}^{(2)} h_i + b_k^{(2)}$$

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

Backward pass:

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

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

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

$$\overline{b_k^{(2)}} = \overline{y_k}$$

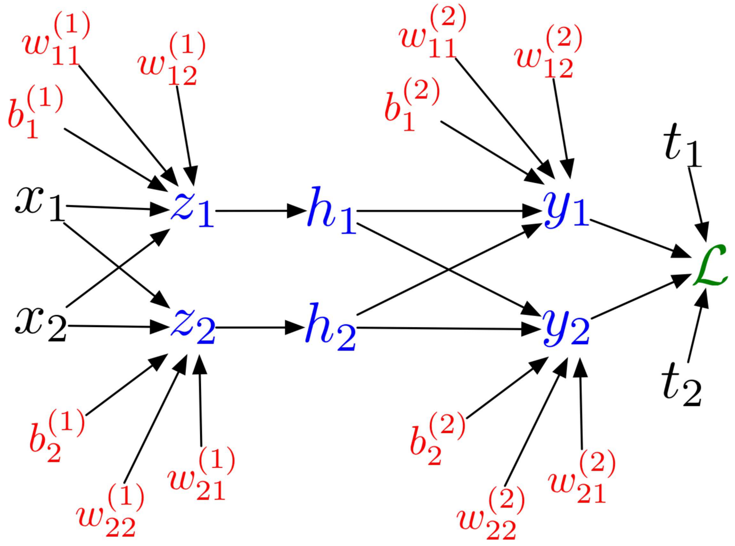
$$\overline{h_i} = \sum_k \overline{y_k} w_{ki}^{(2)}$$

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

$$\overline{w_{ij}^{(1)}} = \overline{z_i} x_j$$

$$\overline{b_i^{(1)}} = \overline{z_i}$$

Backpropagation for a MLP (Vectorized)



Forward pass:

$$\mathbf{z} = W^{(1)}\mathbf{x} + \mathbf{b}^{(1)}$$

$$\mathbf{h} = \sigma(\mathbf{z})$$

$$\mathbf{y} = W^{(2)}\mathbf{h} + \mathbf{b}^{(2)}$$

$$\mathcal{L} = \frac{1}{2}||\mathbf{y} - \mathbf{t}||^2$$

Backward pass:

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

$$\overline{\mathbf{y}} = \overline{\mathcal{L}}(\mathbf{y} - \mathbf{t})$$

$$\overline{W^{(2)}} = \overline{\mathbf{y}}\mathbf{h}^T$$

$$\overline{\mathbf{b}^{(2)}} = \overline{\mathbf{y}}$$

$$\overline{\mathbf{h}} = W^{(2)}{}^T\overline{y}$$

$$\overline{\mathbf{z}} = \overline{\mathbf{h}} \circ \sigma'(\mathbf{z})$$

$$\overline{W^{(1)}} = \overline{\mathbf{z}}\mathbf{x}^T$$

$$\overline{\mathbf{b}^{(1)}} = \overline{\mathbf{z}}$$