CSC 411: Introduction to Machine Learning

CSC 411 Lecture 10: Neural Networks

Mengye Ren and Matthew MacKay

University of Toronto

Inspiration: The Brain

- Our brain has $\sim 10^{11}$ neurons, each of which communicates (is connected) to $\sim 10^4$ other neurons

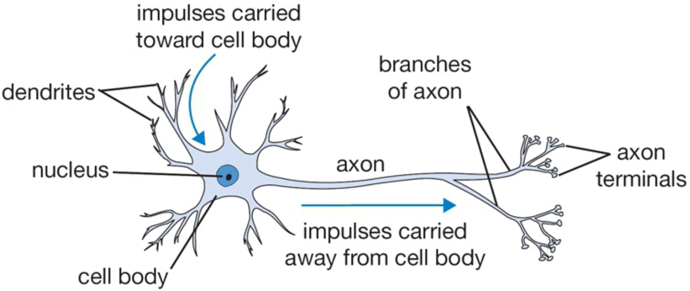
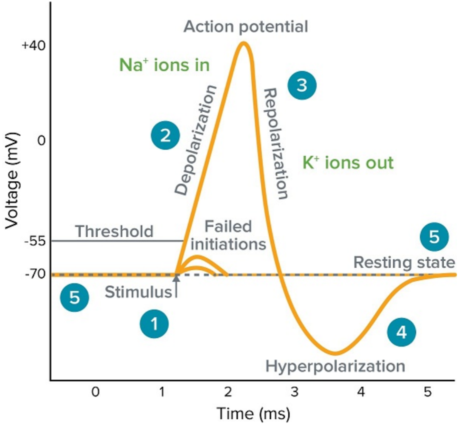


Figure: The basic computational unit of the brain: Neuron

[Pic credit: http://cs231n.github.io/neural-networks-1/]

Inspiration: The Brain

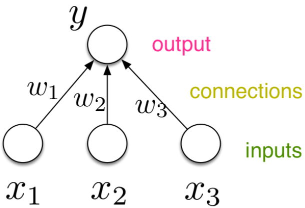
- Neurons receive input signals and accumulate voltage. After some threshold they will fire spiking responses.



[Pic credit: www.moleculardevices.com]

Inspiration: The Brain

- For neural nets, we use a much simpler model neuron, or **unit**:

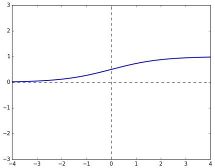


output weights bias

$$y = \phi\left(\mathbf{w}^\top \mathbf{x} + b\right)$$

activation function inputs

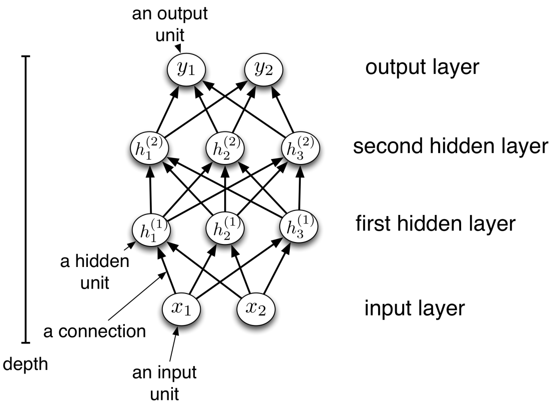
- Compare with logistic regression: $y = \sigma(\mathbf{w}^\top \mathbf{x} + b)$



- By throwing together lots of these incredibly simplistic neuron-like processing units, we can do some powerful computations!

Multilayer Perceptrons

- We can connect lots of units together into a **directed acyclic graph**.
- Typically, units are grouped together into **layers**.
- This gives a **feed-forward neural network**. That's in contrast to **recurrent neural networks**, which can have cycles.



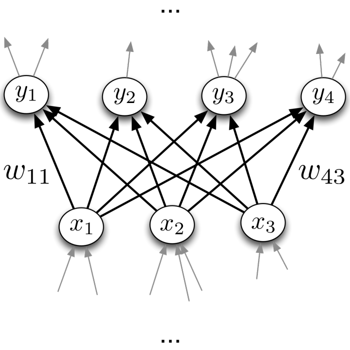
Multilayer Perceptrons

- Each layer connects N input units to M output units.
- In the simplest case, all input units are connected to all output units. We call this a **fully connected layer**. We'll consider other layer types later.
- Note: the inputs and outputs for a layer are distinct from the inputs and outputs to the network.

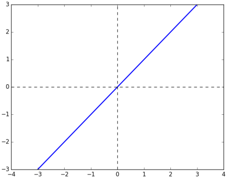
- We need to compute M outputs from N inputs. We can do so in parallel using matrix multiplication. This means we'll be using a $M \times N$ matrix
- The output units are a function of the input units:

$$\mathbf{y} = f(\mathbf{x}) = \phi(\mathbf{W}\mathbf{x} + \mathbf{b})$$

- A multilayer network consisting of fully connected layers is called a **multilayer perceptron**. Despite the name, it has nothing to do with perceptrons!

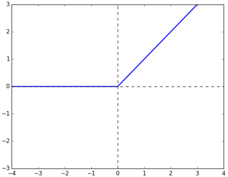


Some activation functions:



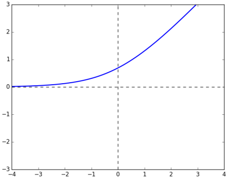
Identity

$$y = z$$



Rectified Linear Unit (ReLU)

$$y = \max(0, z)$$

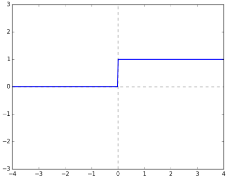


Soft ReLU

$$y = \log 1 + e^z$$

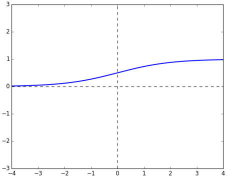
Multilayer Perceptrons

Some activation functions:



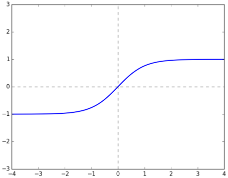
Hard Threshold

$$y = \begin{cases} 1 & \text{if } z > 0 \\ 0 & \text{if } z \leq 0 \end{cases}$$



Logistic

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



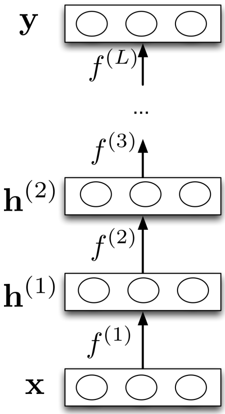
Hyperbolic Tangent (tanh)

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

Multilayer Perceptrons

- Each layer computes a function, so the network computes a composition of functions:

$$
\begin{aligned}
\mathbf{h}^{(1)} &= f^{(1)}(\mathbf{x}) = \phi(\mathbf{W}^{(1)}\mathbf{x} + \mathbf{b}^{(1)}) \\
\mathbf{h}^{(2)} &= f^{(2)}(\mathbf{h}^{(1)}) = \phi(\mathbf{W}^{(2)}\mathbf{h}^{(1)} + \mathbf{b}^{(2)}) \\
&\vdots \\
\mathbf{y} &= f^{(L)}(\mathbf{h}^{(L-1)})
\end{aligned}
$$



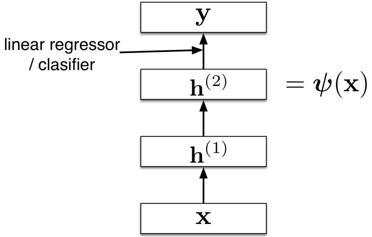
- Or more simply:

$$
\mathbf{y} = f^{(L)} \circ \cdots \circ f^{(1)}(\mathbf{x}).
$$

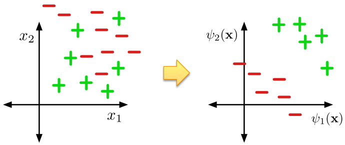
- Neural nets provide modularity: we can implement each layer's computations as a black box.

Feature Learning

- If task is regression: choose $\mathbf{y} = f^{(L)}(\mathbf{h}^{(L-1)}) = (\mathbf{w}^{(L)})^T \mathbf{h}^{(L-1)} + b^{(L)}$
- If task is binary classification: choose $\mathbf{y} = f^{(L)}(\mathbf{h}^{(L-1)}) = \sigma((\mathbf{w}^{(L)})^T \mathbf{h}^{(L-1)} + b^{(L)})$
- Neural nets can be viewed as a way of learning features:

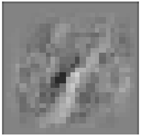


- The goal:



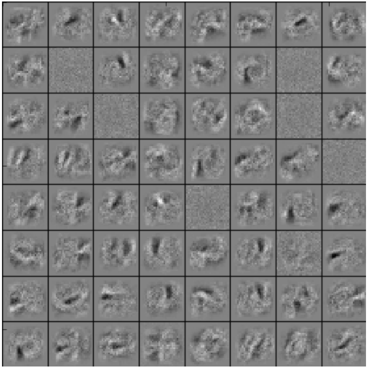
Feature Learning

- Suppose we're trying to classify images of handwritten digits. Each image is represented as a vector of $28 \times 28 = 784$ pixel values.
- Each first-layer hidden unit computes $\phi(\mathbf{w}_i^T \mathbf{x})$. It acts as a **feature detector**.
- We can visualize $\mathbf{w}$ by reshaping it into an image. Here's an example that responds to a diagonal stroke.



Feature Learning

Here are some of the features learned by the first hidden layer of a handwritten digit classifier:



Expressive Power

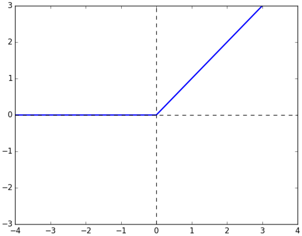
- We've seen that there are some functions that linear classifiers can't represent. Are deep networks any better?
- Suppose a layer's activation function was the identity, so the layer just computes a affine transformation of the input
  - We call this a linear layer
- Any sequence of *linear* layers can be equivalently represented with a single linear layer.

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

  - Deep linear networks are no more expressive than linear regression.
  - Linear layers do have their uses

Expressive Power

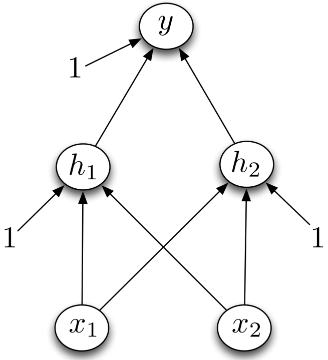
- Multilayer feed-forward neural nets with *nonlinear* activation functions are **universal function approximators**: they can approximate any function arbitrarily well.
- This has been shown for various activation functions (thresholds, logistic, ReLU, etc.)
    - Even though ReLU is "almost" linear,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



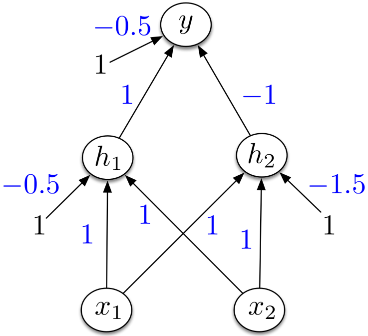
Multilayer Perceptrons

Designing a network to classify XOR:

Assume hard threshold activation function



Multilayer Perceptrons



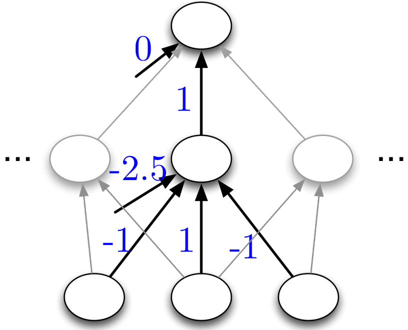
- h_1 computes $\mathbb{I}[x_1 + x_2 - 0.5 > 0]$
  - i.e. x_1 OR x_2
- h_2 computes $\mathbb{I}[x_1 + x_2 - 1.5 > 0]$
  - i.e. x_1 AND x_2
- y computes $\mathbb{I}[h_1 - h_2 - 0.5 > 0] \equiv \mathbb{I}[h_1 + (1 - h_2) - 1.5 > 0]$
  - i.e. h_1 AND (NOT h_2)

Expressive Power

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

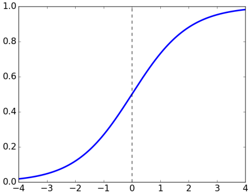
x_1	x_2	x_3	t
	$\vdots$		$\vdots$
-1	-1	1	-1
-1	1	-1	1
-1	1	1	1
	$\vdots$		$\vdots$



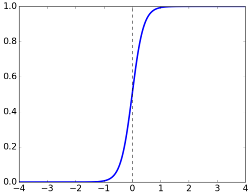
- Only requires one hidden layer, though it needs to be extremely wide.

Expressive Power

- What about the logistic activation function?
- You can approximate a hard threshold by scaling up the weights and biases:



$$y = \sigma(x)$$



$$y = \sigma(5x)$$

- This is good: logistic units are differentiable, so we can train them with gradient descent.

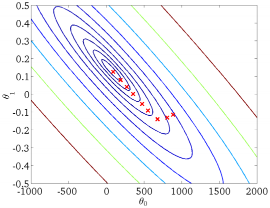
Expressive Power

- Limits of universality
  - You may need to represent an exponentially large network.
  - How can you find the appropriate weights to represent a given function?
  - If you can learn any function, you'll just overfit.
  - Really, we desire a *compact* representation.

Training neural networks with backpropagation

Recap: Gradient Descent

- **Recall:** gradient descent moves opposite the gradient (the direction of steepest descent)



- Weight space for a multilayer neural net: one coordinate for each weight or bias of the network, in *all* the layers
- Conceptually, not any different from what we've seen so far — just higher dimensional and harder to visualize!
- We want to compute the cost gradient $\mathrm{d}\mathcal{J}/\mathrm{d}\mathbf{w}$, which is the vector of partial derivatives.
  - This is the average of $\mathrm{d}\mathcal{L}/\mathrm{d}\mathbf{w}$ over all the training examples, so in this lecture we focus on computing $\mathrm{d}\mathcal{L}/\mathrm{d}\mathbf{w}$.

Univariate Chain Rule

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

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

Univariate Chain Rule

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 derivatives $\frac{\partial \mathcal{L}}{\partial w}, \frac{\partial \mathcal{L}}{\partial b}$

Univariate Chain Rule

How you would have done it in calculus class

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

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

What are the disadvantages of this approach?

Univariate Chain Rule

A more structured way to do it

Computing the loss:

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

Computing the derivatives:

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

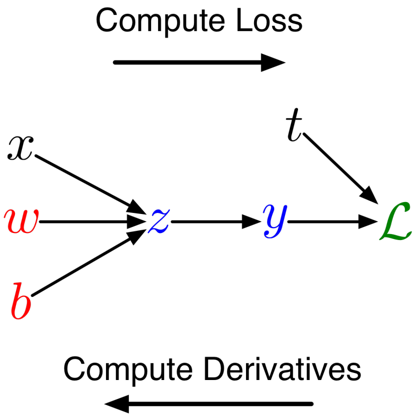
Remember, the goal isn't to obtain closed-form solutions, but to be able to write a program that efficiently computes the derivatives.

Univariate Chain Rule

- We can diagram out the computations using a **computation graph**.
- The nodes represent all the inputs and computed quantities, and the edges represent which nodes are computed directly as a function of which other nodes.

Computing the loss:

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



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**.
- This emphasizes that the error signals are just values our program is computing (rather than a mathematical operation).

Computing the loss:

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

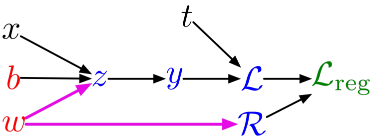
Computing the derivatives:

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

Multivariate Chain Rule

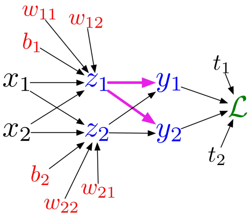
Problem: what if the computation graph has **fan-out** > 1?
This requires the **multivariate Chain Rule**!

L_2-Regularized regression



$$z = wx + b$$
$$y = \sigma(z)$$
$$\mathcal{L} = \frac{1}{2}(y - t)^2$$
$$\mathcal{R} = \frac{1}{2}w^2$$
$$\mathcal{L}_{\text{reg}} = \mathcal{L} + \lambda\mathcal{R}$$

Softmax regression

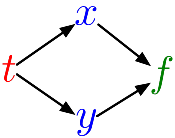


$$z_\ell = \sum_j w_{\ell j} x_j + b_\ell$$
$$y_k = \frac{e^{z_k}}{\sum_\ell e^{z_\ell}}$$
$$\mathcal{L} = -\sum_k t_k \log y_k$$

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

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



- Example:

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

- Plug in to Chain Rule:

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

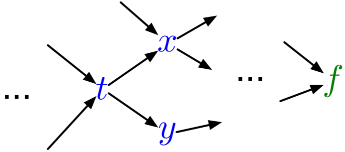
Multivariable Chain Rule

- In the context of backpropagation:

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



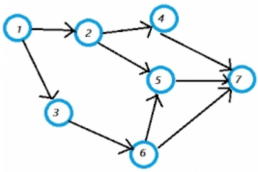
- In our notation:

$$\overline{t} = \overline{x}\,\frac{\mathrm{d}x}{\mathrm{d}t} + \overline{y}\,\frac{\mathrm{d}y}{\mathrm{d}t}$$

Backpropagation

Full backpropagation algorithm:

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

For $i = 1, \ldots, N$

Compute v_i as a function of $\mathrm{Pa}(v_i)$

backward pass

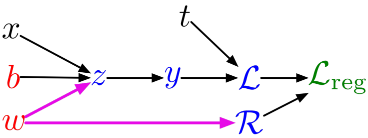
$\overline{v_N} = 1$

For $i = N-1, \ldots, 1$

$\overline{v_i} = \sum_{j \in \mathrm{Ch}(v_i)} \overline{v_j} \frac{\partial v_j}{\partial v_i}$

Backpropagation

Example: univariate logistic least squares regression



Forward pass:

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

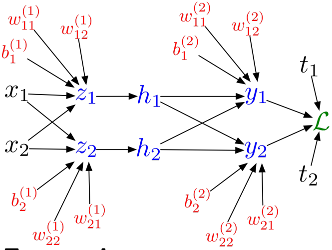
Backward pass:

$$
\begin{aligned}
\overline{\mathcal{L}_{\mathrm{reg}}} &= 1 \\
\overline{\mathcal{R}} &= \overline{\mathcal{L}_{\mathrm{reg}}} \frac{\mathrm{d}\mathcal{L}_{\mathrm{reg}}}{\mathrm{d}\mathcal{R}} \\
&= \overline{\mathcal{L}_{\mathrm{reg}}}\, \lambda \\
\overline{\mathcal{L}} &= \overline{\mathcal{L}_{\mathrm{reg}}} \frac{\mathrm{d}\mathcal{L}_{\mathrm{reg}}}{\mathrm{d}\mathcal{L}} \\
&= \overline{\mathcal{L}_{\mathrm{reg}}} \\
\overline{y} &= \overline{\mathcal{L}} \frac{\mathrm{d}\mathcal{L}}{\mathrm{d}y} \\
&= \overline{\mathcal{L}}\,(y - t)
\end{aligned}
$$

$$
\begin{aligned}
\overline{z} &= \overline{y} \frac{\mathrm{d}y}{\mathrm{d}z} \\
&= \overline{y}\, \sigma'(z) \\
\overline{w} &= \overline{z} \frac{\partial z}{\partial w} + \overline{\mathcal{R}} \frac{\mathrm{d}\mathcal{R}}{\mathrm{d}w} \\
&= \overline{z}\, x + \overline{\mathcal{R}}\, w \\
\overline{b} &= \overline{z} \frac{\partial z}{\partial b} \\
&= \overline{z}
\end{aligned}
$$

Backpropagation

Multilayer Perceptron (multiple outputs):



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:

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

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

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

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

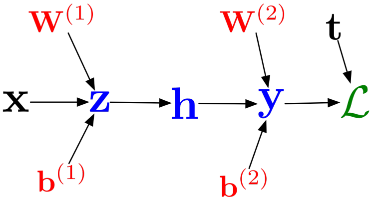
$$\overline{h_i} = \sum_k \overline{y_k} w_{ki}^{(2)}$$

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

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

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

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:

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

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

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

- Rule of thumb: 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.
  - Forward & backward weights are tied in backprop.
  - Backprop requires synchronous update (1 forward followed by 1 backward).
  - All the biologically plausible alternatives we know about learn much more slowly (on computers).