Deep Neural Networks - Lecture 3

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March 13, 2018

The perceptron

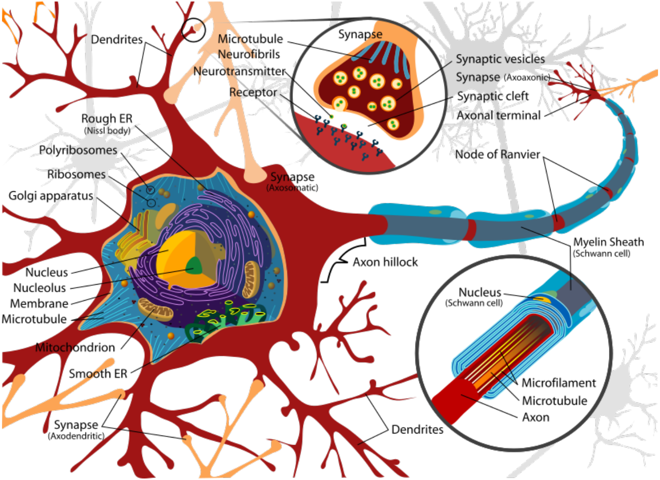
Neural Networks and Backpropagation

Trouble with neural networks

Where it all begins

- Many settings where humans outperform best algorithms.
- Idea: Emulate the human brain.
- 10^{11} neurons, 10^{14} connections in the brain. Trouble?
- Compare: a 10 TB drive can store 10^{14} bytes.

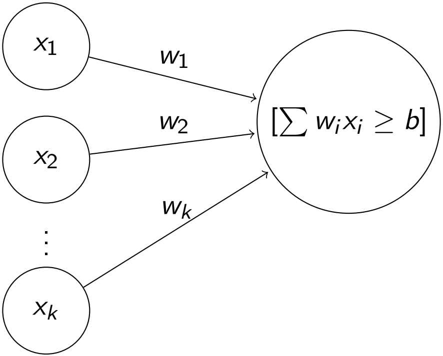
Where it all begins



The perceptron

The perceptron is a function that, given inputs $x_1, \ldots, x_k$ outputs $[\sum_i w_i x_i + b \geq 0]$ (or a specific GD-like algo for fitting these).

Think: x_i are factors contributing to a decision, they are weighted and the perceptron makes a decision automatically!



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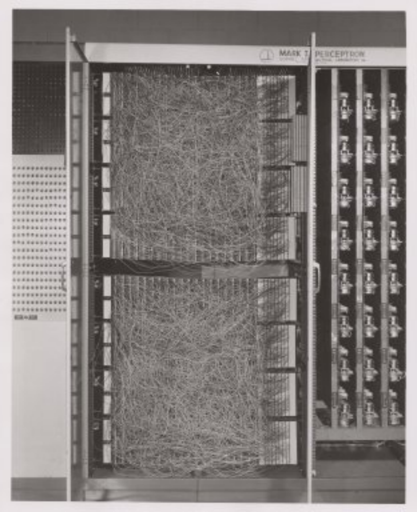

Mark I Perceptron (1957)

- Funded by US Navy.
- Photo recognition.
- 20x20 photo-cells.
- Weights in potentiometers.
- Trained with the perceptron algorithm - weights updated by electric motors.

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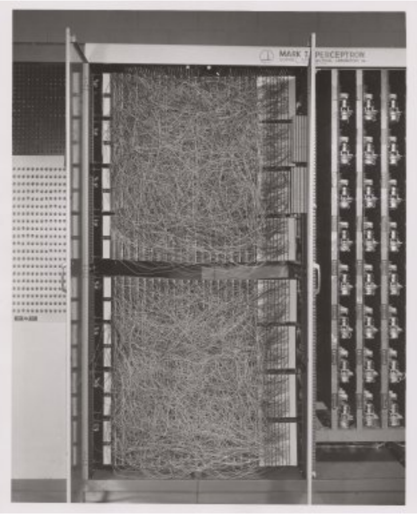

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...the embryo of an electronic computer that [the Navy] expects will be able to walk, talk, see, write, reproduce itself and be conscious of its existence...

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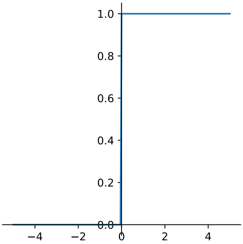

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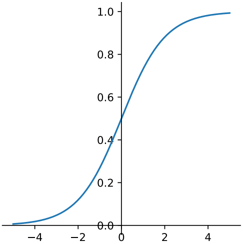

Train using a smooth approximation (not exactly what the perceptron algorithm was doing!).

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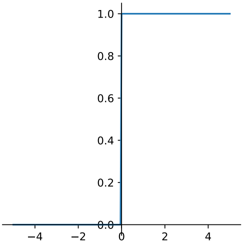

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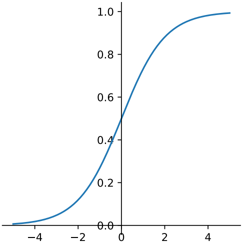

Train using a smooth approximation (not exactly what the perceptron algorithm was doing!).
Many smooth step functions possible, e.g. the sigmoid function $\sigma(x) = \frac{1}{1+e^{-x}}$. Rings a bell?

The power of perceptrons

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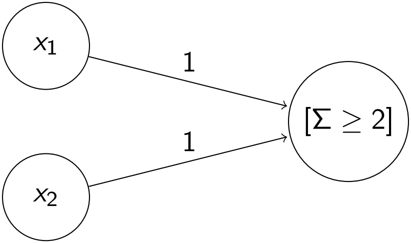

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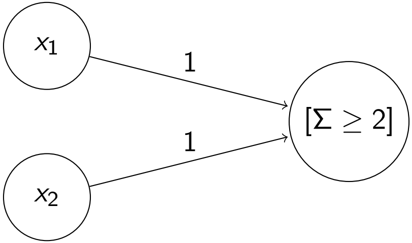

Exercise: Can a perceptron compute XOR?

Network of perceptrons

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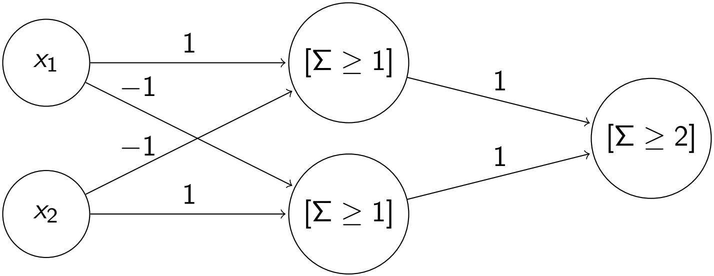

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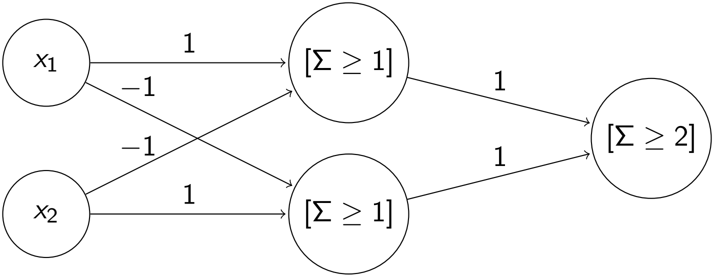

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Note that this DAG can be very large (think: SAT).

Training a DAG of perceptrons

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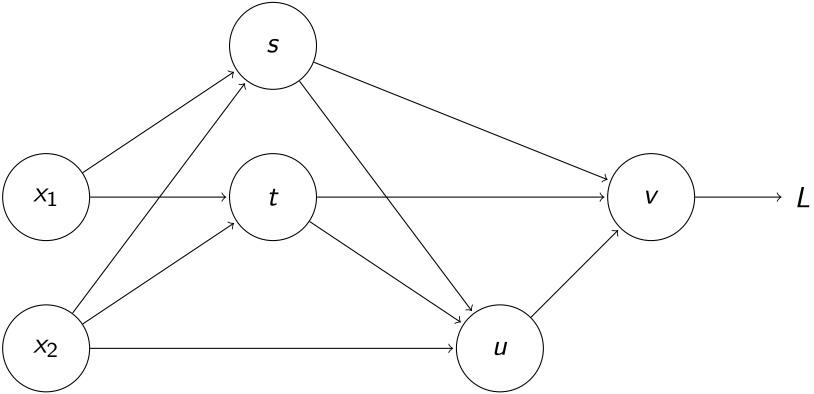
More specifically: Given a DAG of sigmoid approximations to the perceptron, can we compute gradients of the loss function?



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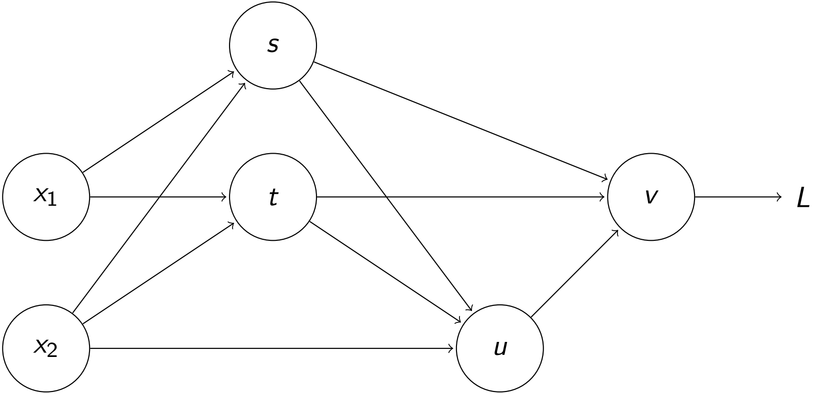

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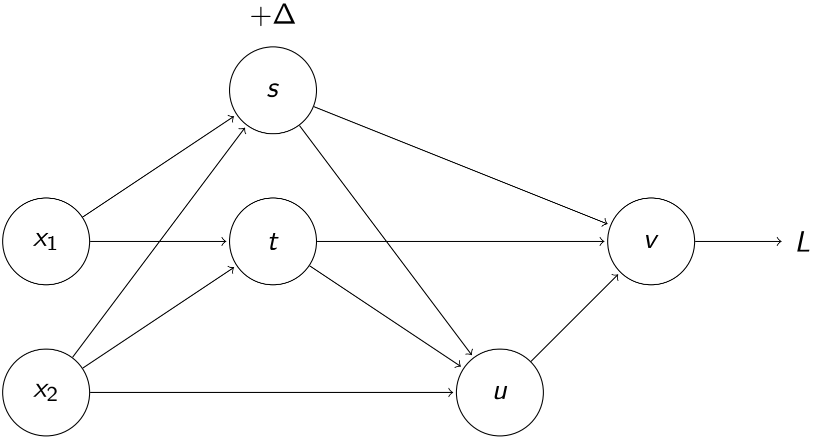

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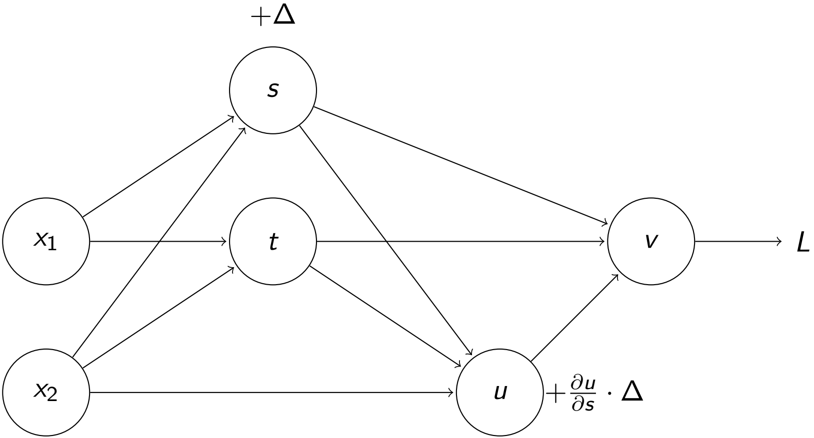

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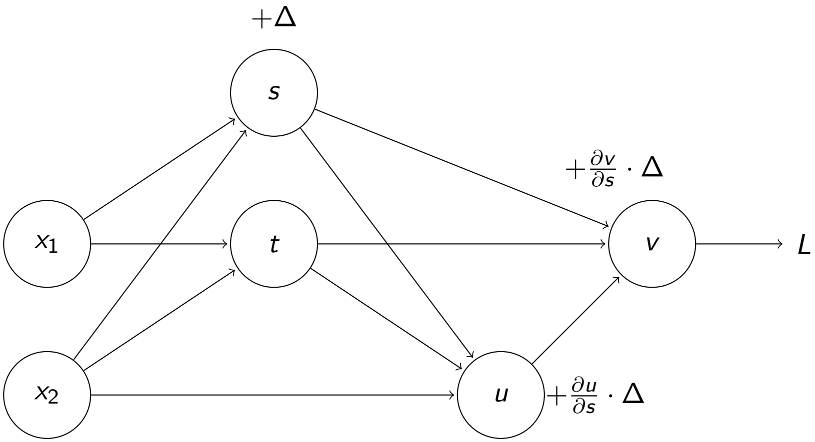

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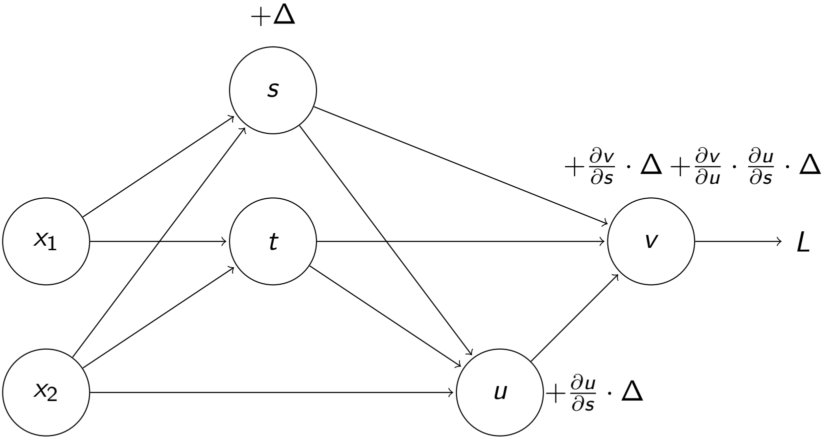

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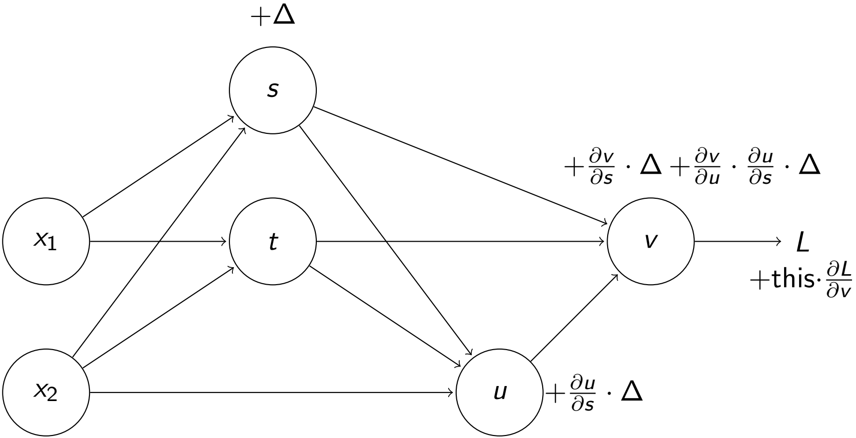

Backpropagation

It seems that for a node z, we have

$$\frac{\partial L}{\partial z} = \sum_{z=z_0 \to \ldots \to z_l = L} \prod_{i=1}^{l-1} \frac{\partial z_{i+1}}{\partial z_i}.$$

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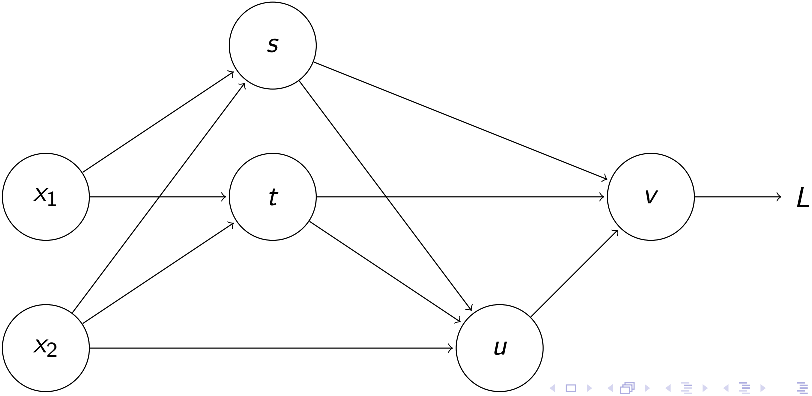

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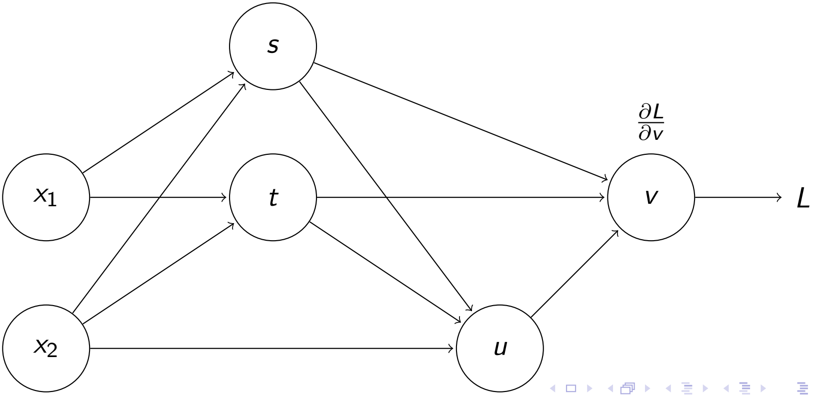

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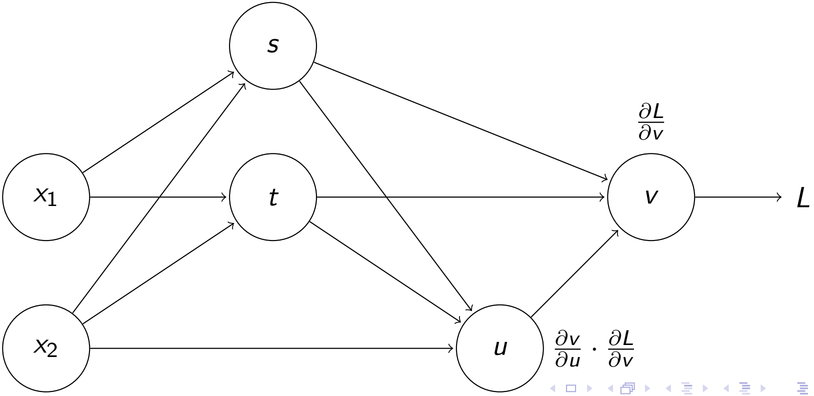

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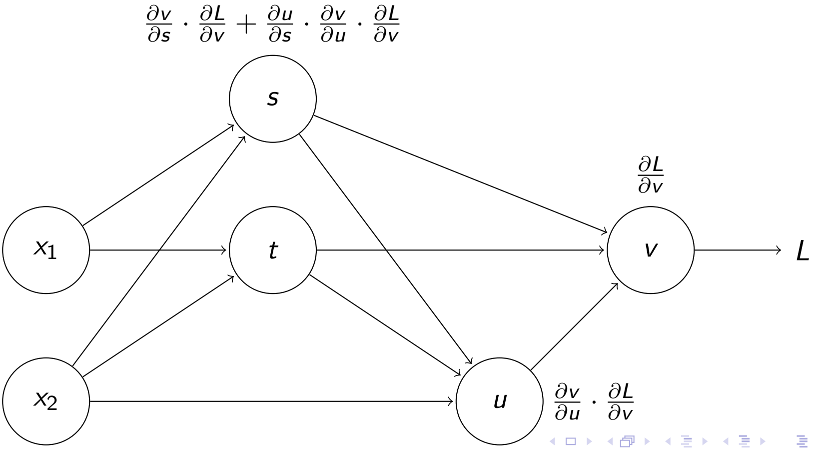

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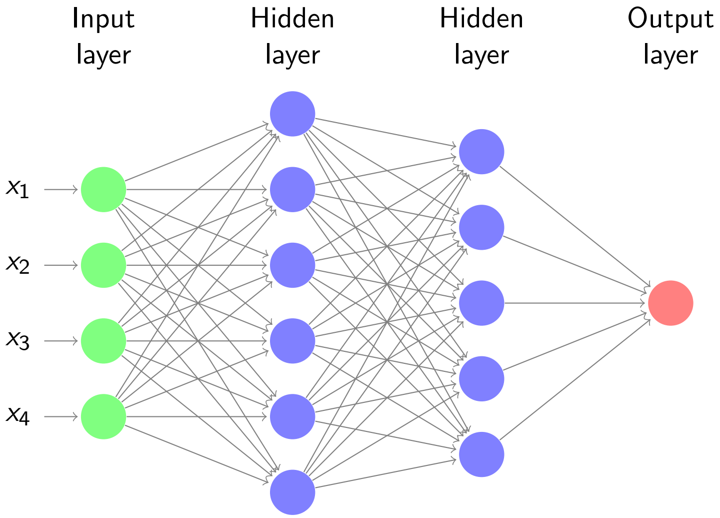
Computing the derivatives of nodes over their parameters is trivial.

Multilayer Perceptron (MLP)

- *Multilayer Perceptron (MLP)*, or a *Feedforward Neural Network* consists of several layers of units (sigmoid or other), each connected with previous and next.
- Number of layers (excluding inputs) is called the *depth*.
- The inner layers are called *hidden*.

Multilayer Perceptron (MLP)

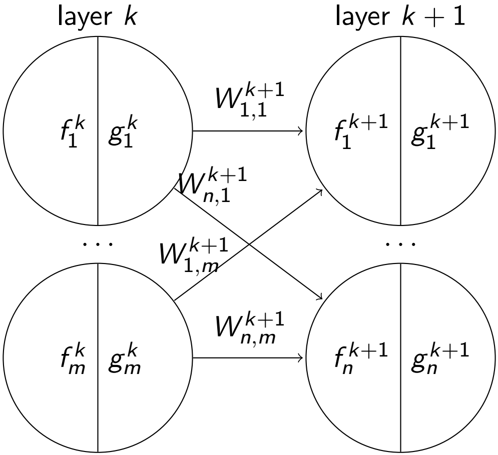


Universal approximation for MLP

Theorem (Universal approximation theorem for MLP)

Any continuous function on $[0, 1]^n$ can be approximated arbitrarily well by an MLP with a single hidden layer.

Matrix algebra - notation



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$$f^k = W^k g^{k-1}.$$

Here f^k and g^{k-1} could be vectors if single datapoint, or matrices.

$$\frac{\partial L}{\partial g^{k-1}} = W^T \frac{\partial L}{\partial f^k}.$$

Again, $\frac{\partial L}{\partial g^{k-1}}$ and $\frac{\partial L}{\partial f^k}$ can be vectors or matrices.

Matrix algebra

Exercise: Relate $\frac{\partial L}{\partial f^k}$ and $\frac{\partial L}{\partial g^k}$, if $g^k = \sigma(f^k)$ (coordinate-wise).

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Solution:

$$\frac{\partial L}{\partial f^k} = \frac{\partial L}{\partial g^k} \circ g^k \circ \left(1 - g^k\right).$$

$A \circ B$ is the Hadamard (element-wise) product.

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Solution:

$$\frac{\partial L}{\partial W^k} = \frac{\partial L}{\partial f^k} \left(g^{k-1}\right)^T .$$

Note that for batches summing up happens automagically!

The art of neural networks

In the non-modern setting, setting the parameters of neural networks was more art than science:

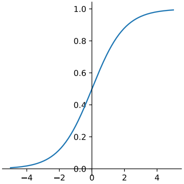
- Choosing the architecture.
- Choosing the units.
- Controlling the learning rate.
- Initializing the weights.
- And other (regularization, mini-batch size, etc.)

These issues were addressed by recent developments.

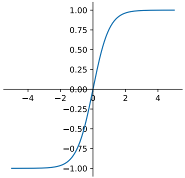
Architecture

- *If your deep neural net is not overfitting you should be using a bigger one!* – G. Hinton
- Bigger network is more expressive.
- Bigger networks take longer to train.
- Deeper networks are much harder to train.
- Modern variants of SGD are much better at training deep nets. And we have stronger hardware. And better ideas (e.g. ResNet)

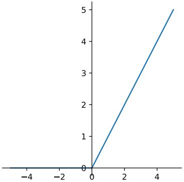
Units



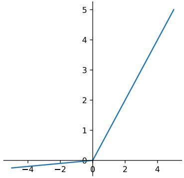
sigmoid: $\sigma(x) = \frac{1}{1+e^{-x}}$



tanh: $\tanh(x) = \frac{e^{x}+e^{-x}}{e^{x}+e^{-x}}$



ReLU: $\text{ReLU}(x) = \max(0, x)$



leaky ReLU: $\text{LReLU}(x) = \max(ax, x)$

Learning rate

- If the learning rate is too small, convergence is very slow.
- Learning rate that is too high results in oscillations.
- Some modern variants of SGD can automatically adapt.

Initialization

- Very small initial weights slow down learning initially, or even completely vanish.
- Very large initial weights can lead to oscillations and random-like behaviour or even blow-up with no regularization.
- Heuristics, e.g. Glorot initialization: draw a weight from normal distribution with variance $\frac{2}{n_{in}+n_{out}}$.
- Modern techniques like batch normalization make initialization less of an issue.

Recap

- Perceptron and its biological and computational motivation.
- Multilayer perceptron and how to compute its gradients fast.
- Tricky decisions when tuning MLPs.

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- Multilayer perceptron and how to compute its gradients fast.
- Tricky decisions when tuning MLPs.

But do not worry:

- Sometimes MLPs work well even without excessive tuning.
- Next lecture, we will make things much more stable.