Neural Networks I

Machine Learning 1 — Lecture 7

2nd May 2023

Robert Peharz
Institute of Theoretical Computer Science
Graz University of Technology

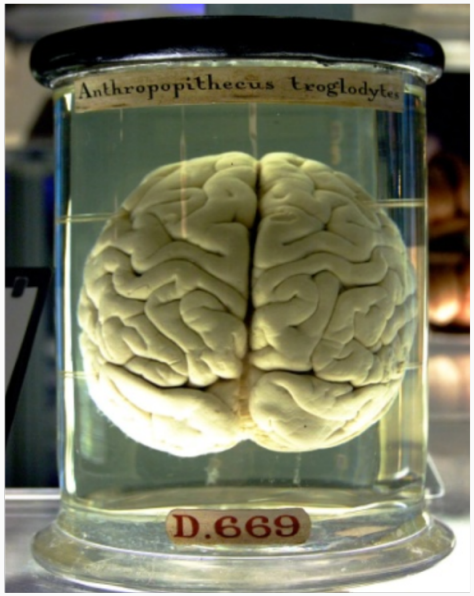
Brief Appetizer Video

https://www.youtube.com/watch?v=Suevq-kZdIw

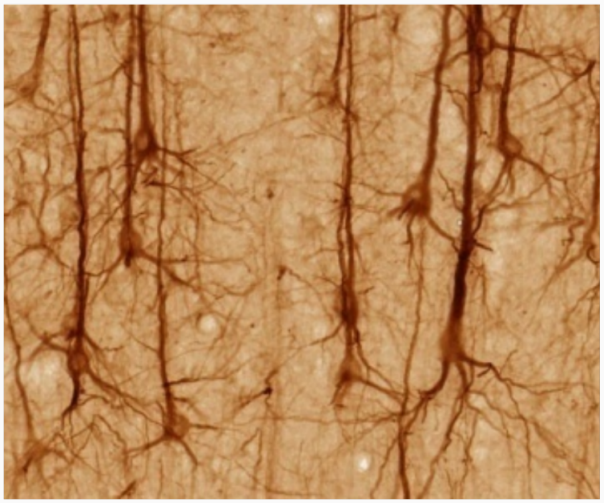
Excellent Tutorial by 3Blue1Brown [optional, recommended]

https://www.youtube.com/playlist?list=PLZHQObOWTQDNU6R1_67000Dx_ZCJB-3pi

Biological Neural Networks



- The brain: still the only "truly" intelligent device on earth
- A biological neural network of 100 billion **neurons**, connected via 100 trillions of **synapses**
- Extremely complex and parallel



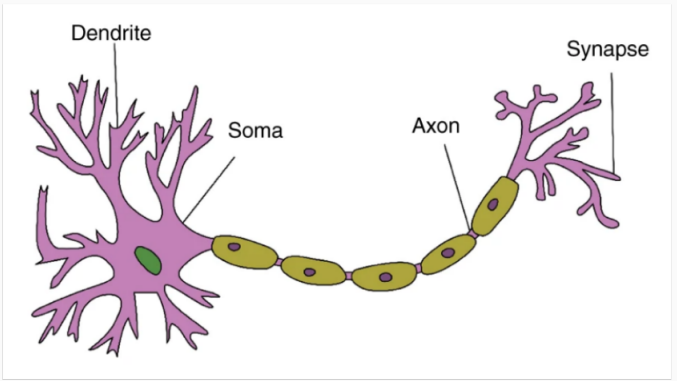


Image: Zhang et al., Artificial neural networks enabled by nanophotonics, 2019

Biological vs. Artificial Neuron

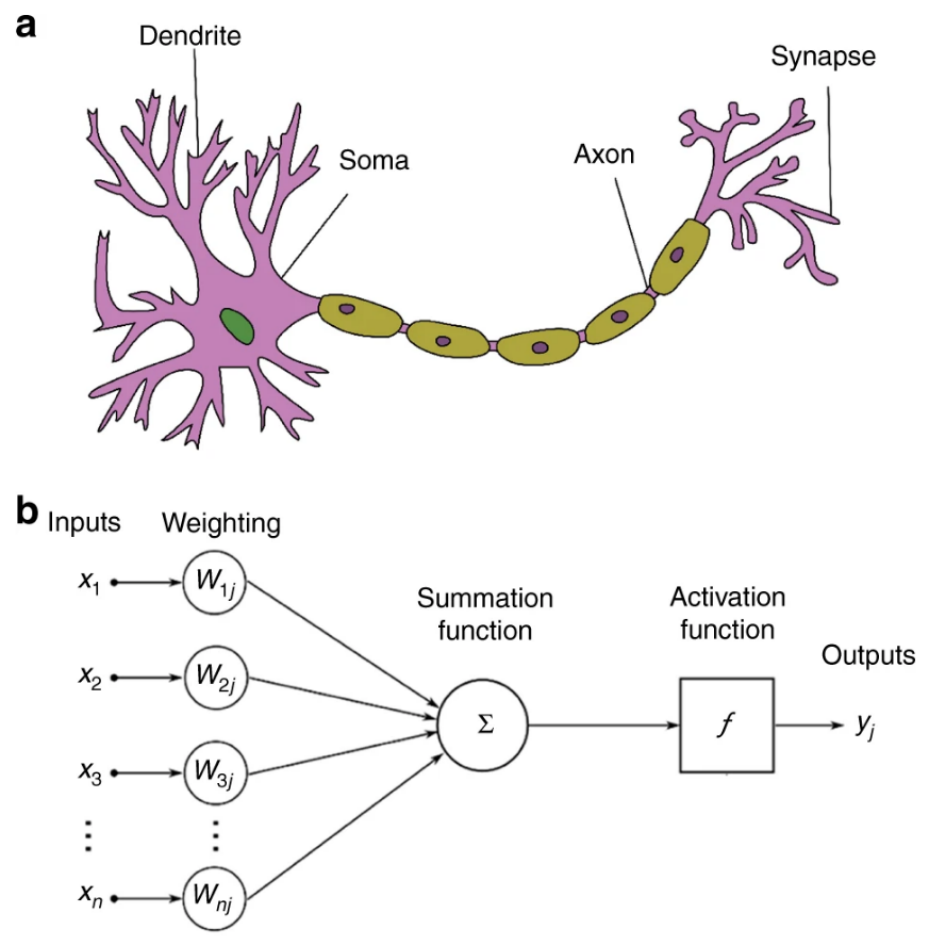
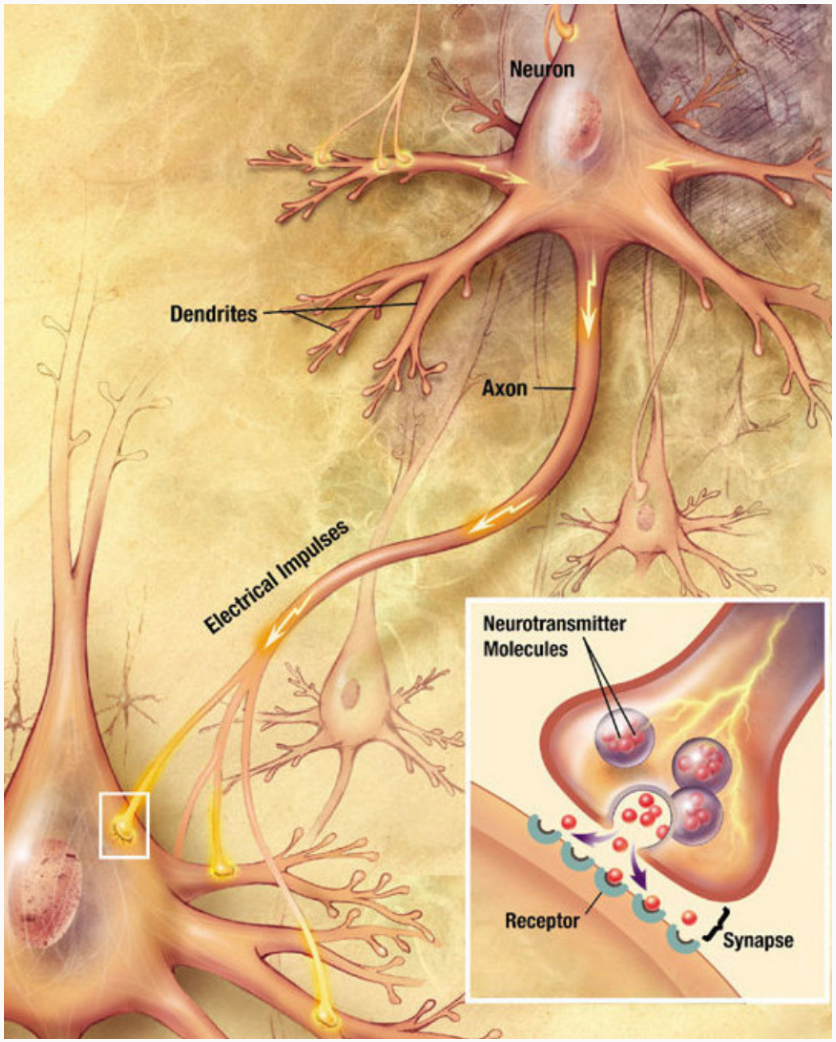


Image: Zhang et al., 2019

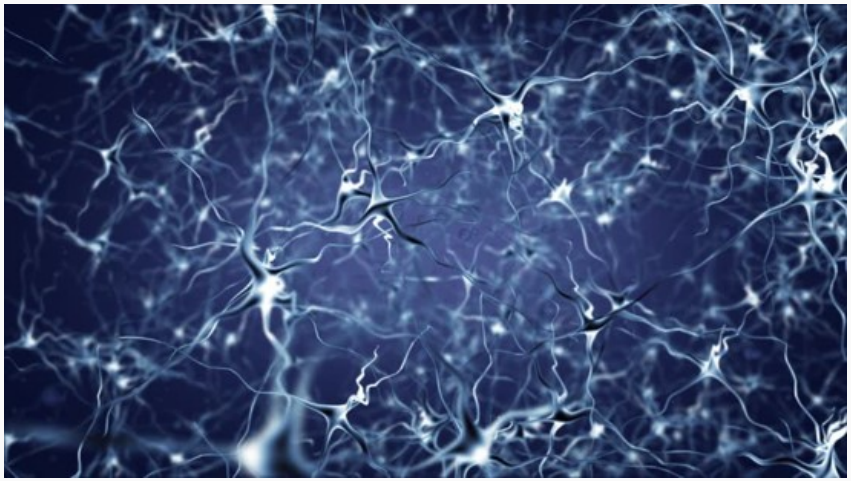
- **dendrite**: receive input spikes from previous neurons
- **soma**: accumulate input, fires/spikes if excited enough i)
- **axon**: long way transmission of spikes
- **synapses**: connection to next neurons (connection strength)
- **In ANNs:**
  - accumulation is $\approx \sum$
  - spiking is $\approx$ non-linear activation function
  - synapse strength is $\approx$ weights

Synapses

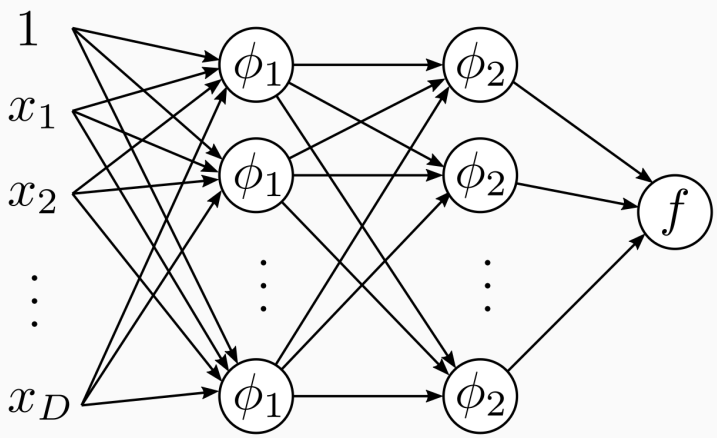


- Synapses are essential for the communication between neurons
- They are basically a link transmitting spikes from the pre-synaptic to the post-synaptic neuron
- **Synaptic strength** can be adapted; an essential mechanism for learning

Biological vs. Artificial Neural Networks



Biological neural network



Artificial neural network

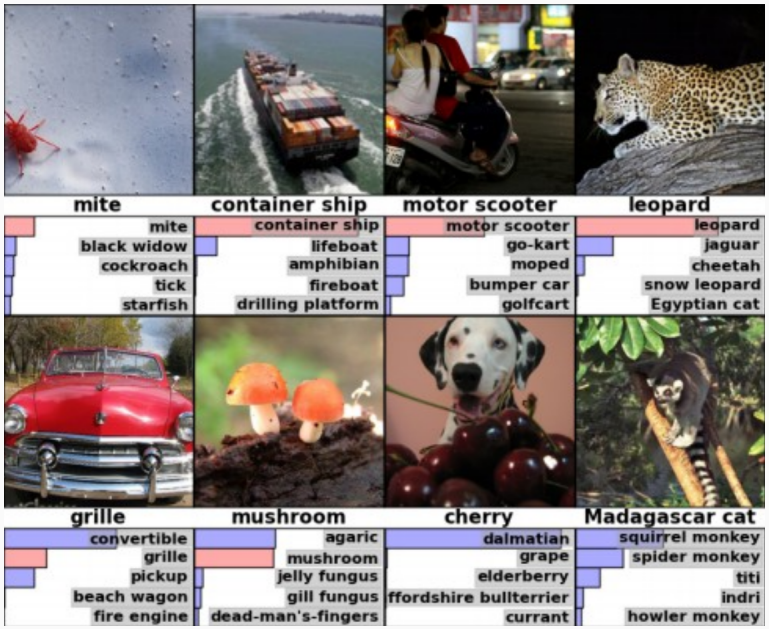
- Artificial neural networks (ANNs): learn from biology
- Two way street: Use ANNs to understand biological neural systems better
  - Develop biologically accurate neuron models
  - Simulations of biological neural networks
  - Spiking ANNs
- For ML purposes: **powerful function approximators**

Brief History

- 1943 – McCulloch and Pitts – *simple electrical circuit for connectionism*
- 1949 – Donald Hebb – *Hebbian learning*
- 1958 – Frank Rosenblatt – *Perceptron*
- $\approx$ 1970-1980 – "AI Winter"
- 1982 – Jon Hopfield – *Hopfield net*
- 1986 – Rumelhart, Hinton and Williams – *Backpropagation* (re-invented from 1960, actually autodiff/chain rule of calculus)
- 1989 – Yann LeCun – *Convolutional Neural Networks* (image models)
- 1997 – Sepp Hochreiter and Jürgen Schmidhuber – *Long Short Term Memory Networks*
- $\approx$ 1995–2006 – Neural networks were not popular (lighter models were preferred, e.g. support vector machines)
- 2006 – Hinton, Osindero, Teh – *Deep Learning, Deep Belief Networks*
- 2012 – Krizhevsky, Sutskever, Hinton: New state of the art on ImageNet
- After 2012 – extremely fast growth in popularity due to their success in real-world computer vision problems, natural language processing, etc.

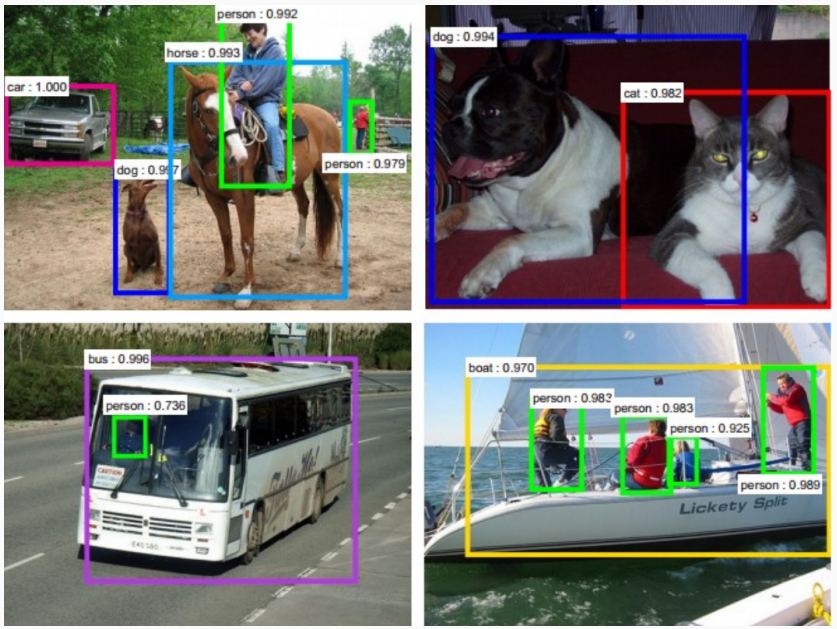
Deep Learning in Computer Vision

Image recognition



Krizhevsky et al., 2012

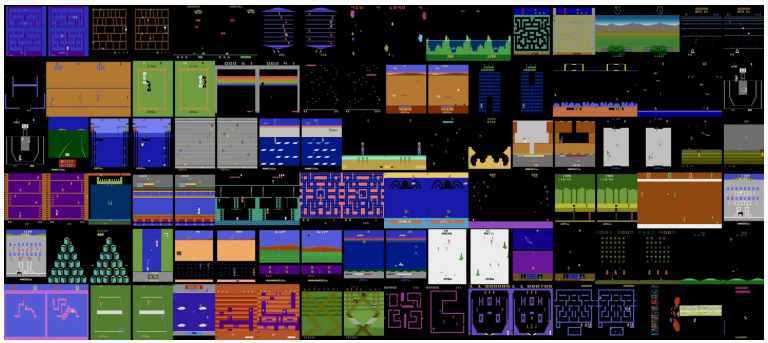
Object Detection



Ren et al., 2015

Deep Learning in Game Playing

Atari Games



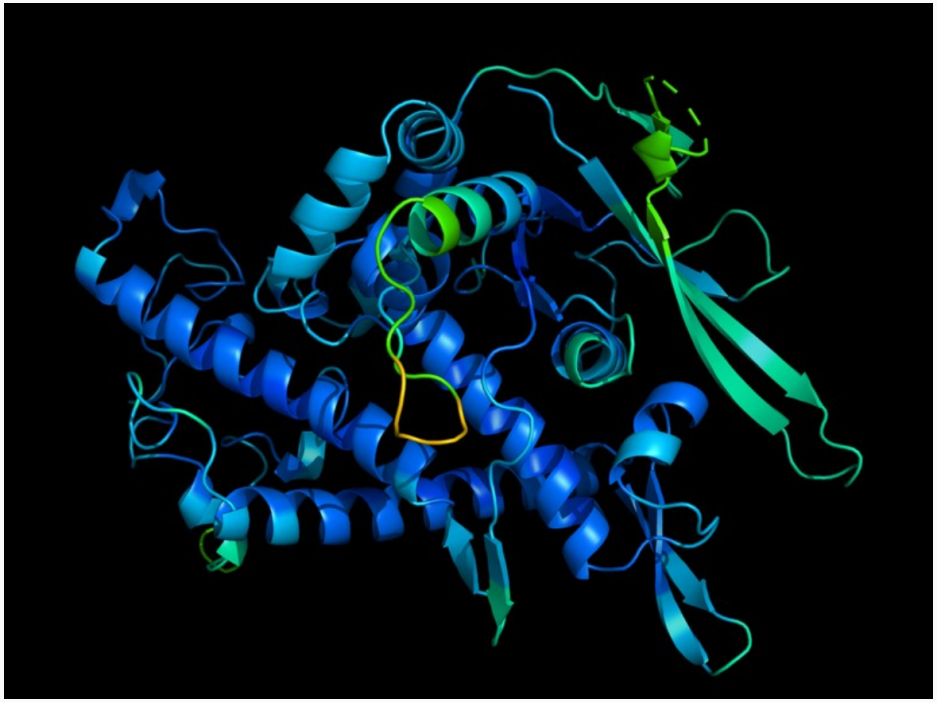
Mnih et al., 2015

Board Games

Silver et al., 2017

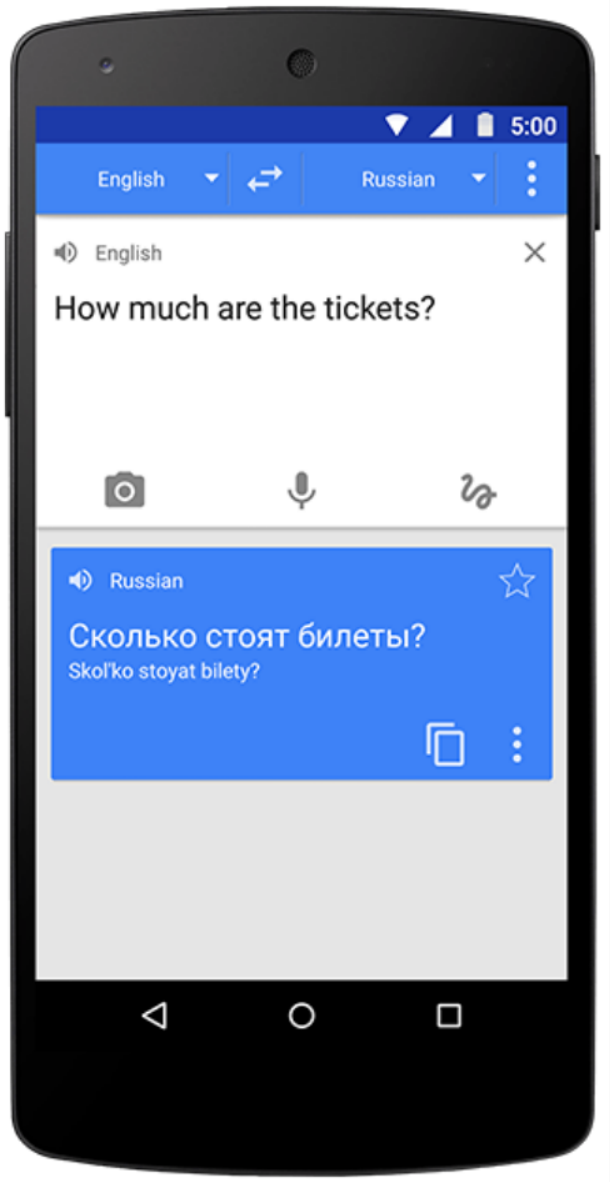
Deep Learning for Protein Folding

Alpha Fold



Senior et al., 2020

Deep Learning for Machine Translation



- **Long-short term memories**
  [Hochreiter and Schmidhuber, 1997]
- **Transformers** [Vaswani et al., 2017]

Neural Networks: Basics

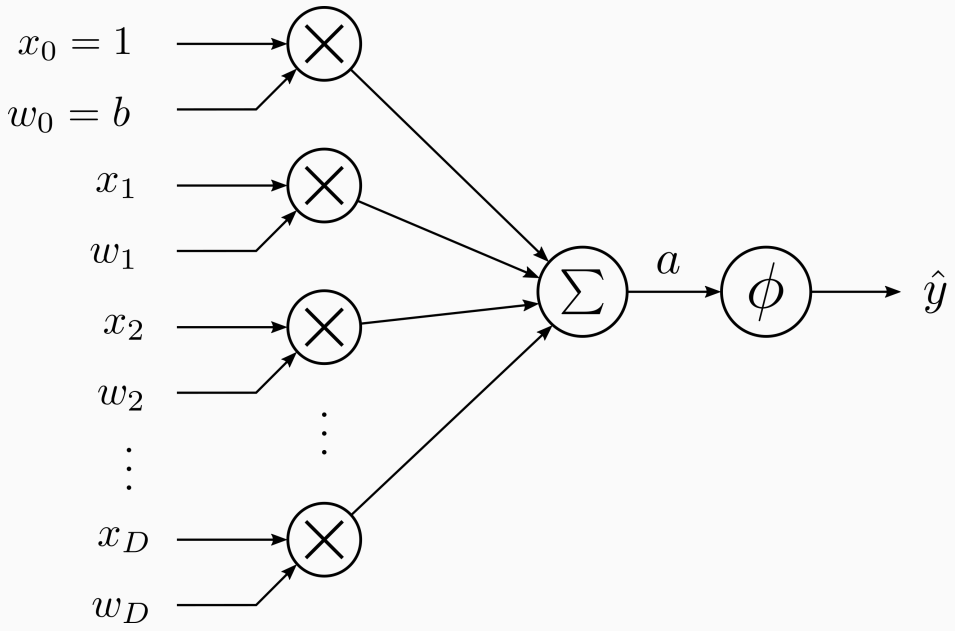
Neuron, Unit

The **neuron** (**unit**) is the basic building block of neural networks:

$$\hat{y} = \phi(a) = \phi\left(\sum_{i=0}^{D} w_i x_i\right)$$

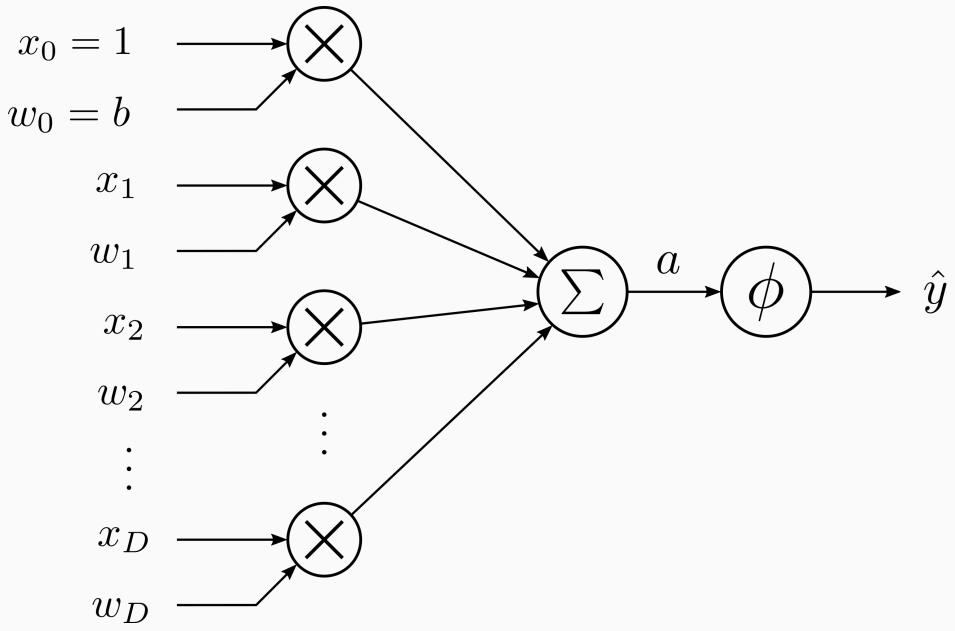
- D: number of inputs
- x_i: inputs (features, outputs from previous neurons)
- w_i: weights
- w_0: bias term ($x_0 \equiv 1$)
- ϕ: non-linear **activation function** (also called **non-linearity**)
- a: **activation** $\sum_{i=0}^{D} w_i x_i$
- $\hat{y}$: output $\phi(a)$
- **Affine function of x, followed by non-linearity ϕ**

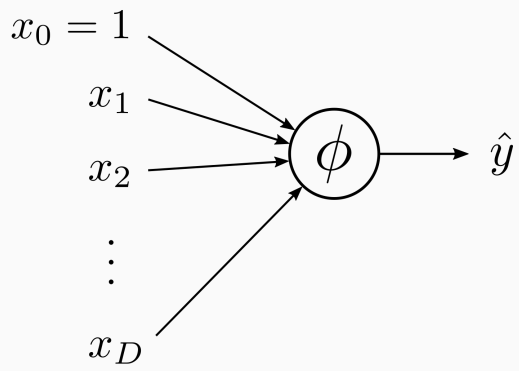
Neuron as Computational Graph



computational graph: directed acyclic graph whose leaves are inputs, roots are outputs, and internal nodes are computational operations; note that weights w_d can be seen as inputs as well

Neuron as Computational Graph



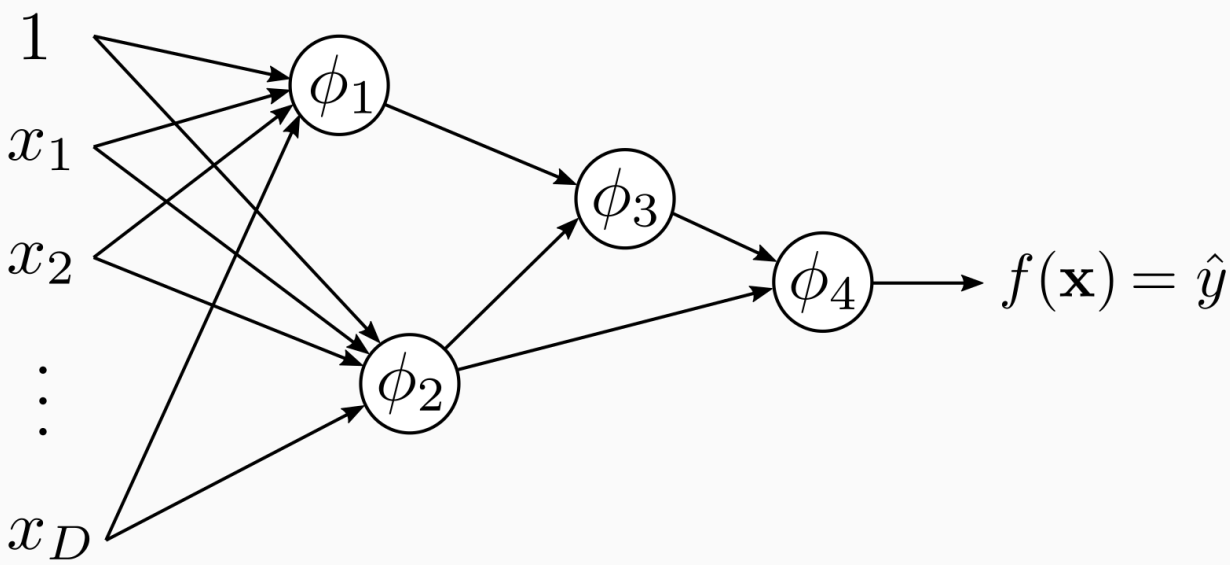


computational graph: directed acyclic graph whose leaves are inputs, roots are outputs, and internal nodes are computational operations; note that weights w_d can be seen as inputs as well

simplified graph: multiplication with weights w_d absorbed into edges, activation a absorbed into ϕ node

Neural Networks: Network of Neurons

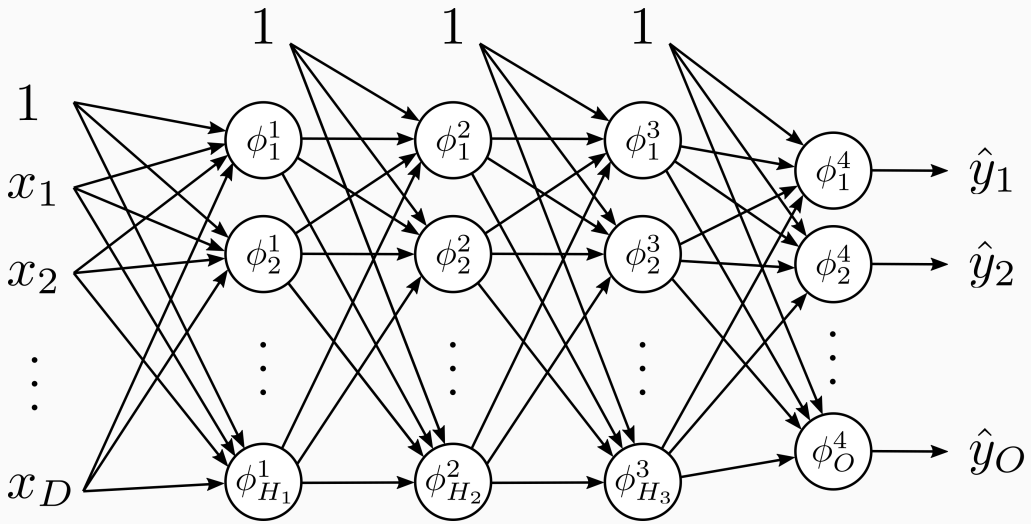
- Like in biological neural nets, ANNs are networks of neurons
- Each neuron is simple, but when combined, they can represent complicated functions $f(\boldsymbol{x})$, to be used for
  - Classification
  - Regression
  - Advanced applications
- Training by optimizing the weights (discussed later)



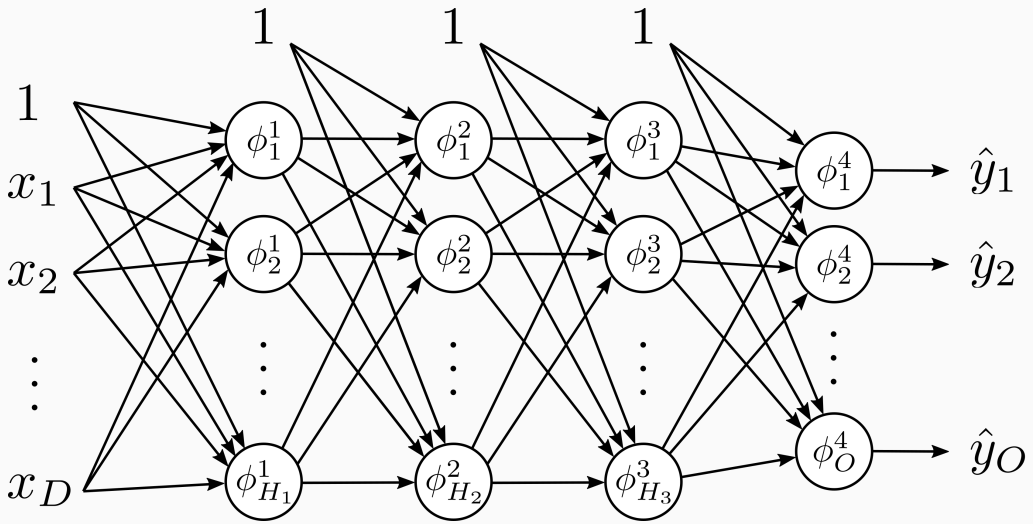
A regular architecture is the **multilayer perceptron (MLPs)**:

- consists of $L+1$ **layers** of neurons
- each neuron has all neurons of the previous layer as input
- $L+1^{\text{st}}$ layer is the **output layer** (**output neurons**)
- layers $1 \dots L$ are often called **hidden layers** (**hidden neurons**)
- inputs $\boldsymbol{x} = (1, x_1, \dots, x_D)^T$ interpreted as Layer 0 (**input layer**)

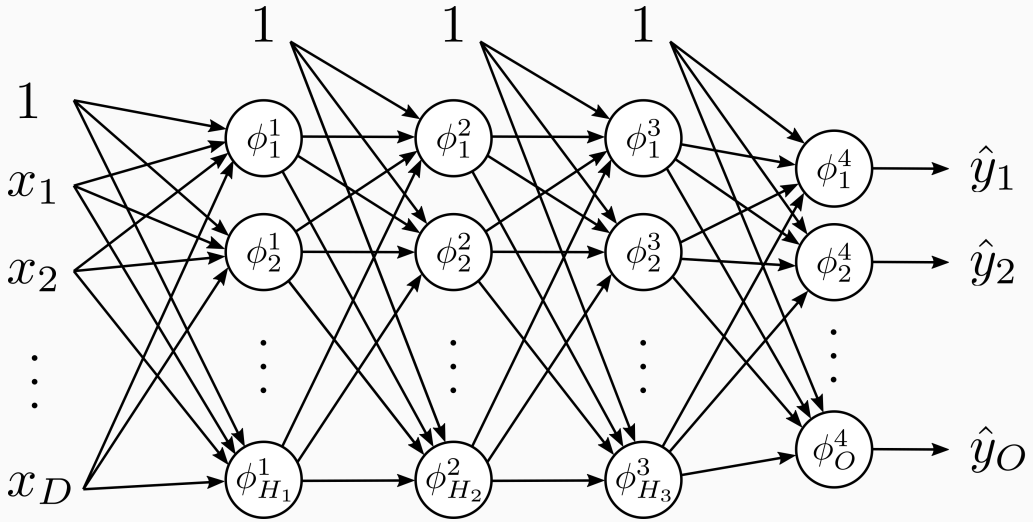
Example for $L = 3$



- D: number of inputs
- O: number of outputs
- H_l: number of neurons in l^{th} hidden layer
- ϕ_k^l: activation function of k^{th} neuron in l^{th} layer
- often the same activation function across each layer, i.e. $\phi_k^l = \phi^l$
- $L, H_1, \ldots, H_L$ are **hyper-parameters** of the architecture



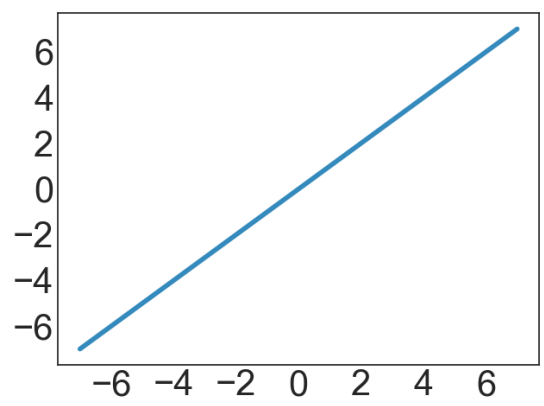
- $w^l_{i,j}$: weight for connection between i^{th} neuron in $l-1^{\text{st}}$ layer to j^{th} neuron in l^{th} layer
- let $H_0 := D$ and $h^0_i := x_i$
- let $h^l_0 \equiv 1$ (dummy features for biases)
- neuron activation $a^l_j = \sum_{i=0}^{H_{l-1}} w^l_{i,j}\, h^{l-1}_i$
- neuron output $\phi^l_j\left(a^l_j\right)$
- MLP output $\hat{y}_i := h^{L+1}_i$



Common Activation Functions ϕ

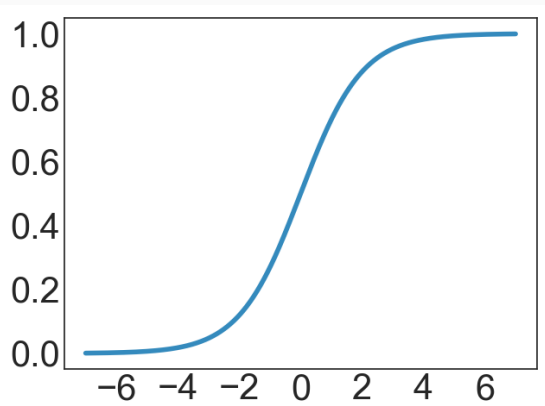
linear (identity function)

$\phi(x) = x$



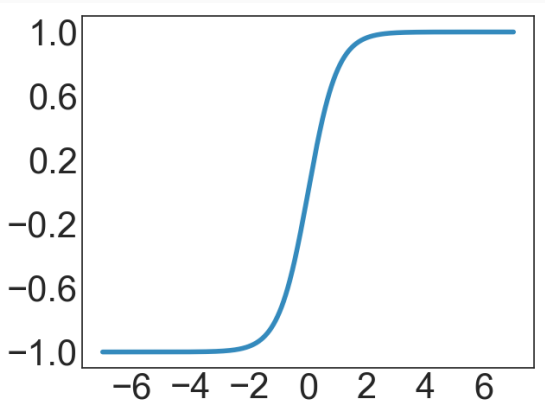
sigmoid (logistic function)

$\phi(x) = \frac{1}{1+e^{-x}}$



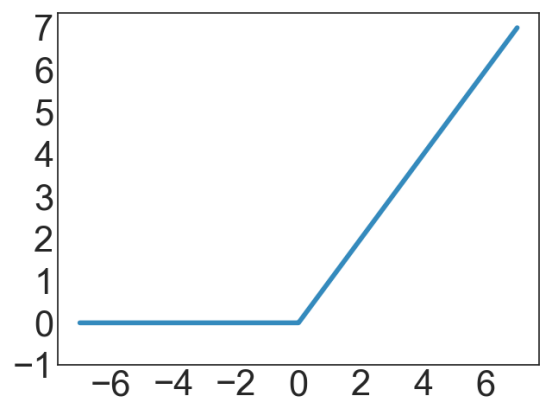
hyperbolic tangent

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



rectified linear unit (ReLU)

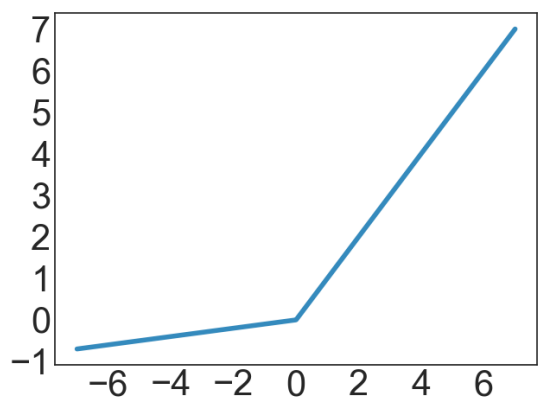
$\phi(x) = \max(x, 0)$



leaky ReLU

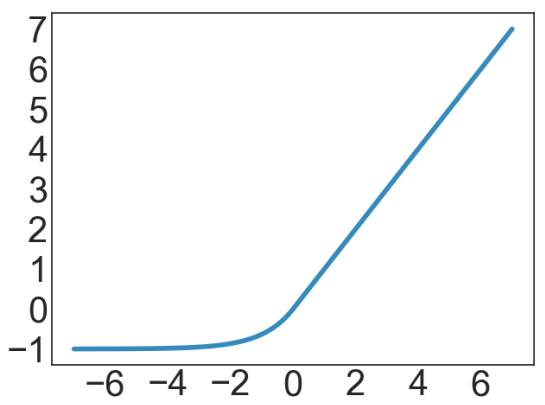
$\phi(x) = \max(x, ax)$

(e.g. $a = 0.1$)



exponential linear unit

$$\phi(x) = \begin{cases} x & x \geq 0 \\ a(e^x - 1) & x < 0 \end{cases}$$

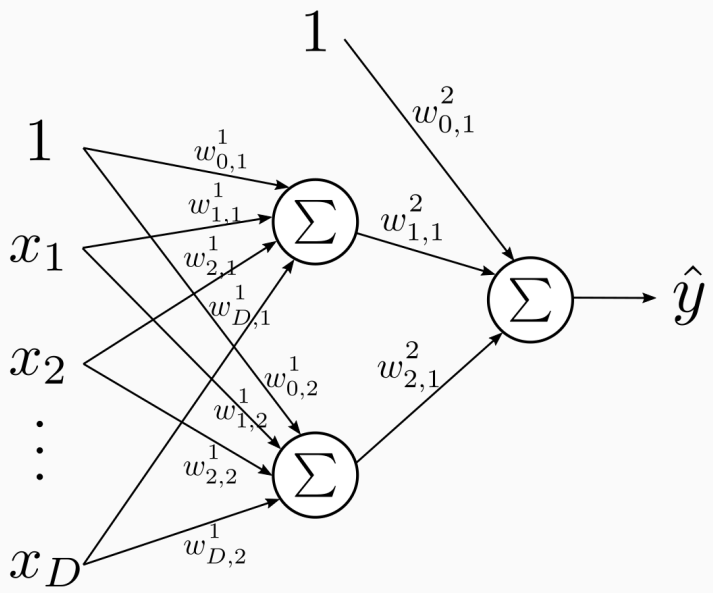


Why do we need non-linear activation functions ϕ?

Why do we need non-linear activation functions ϕ?

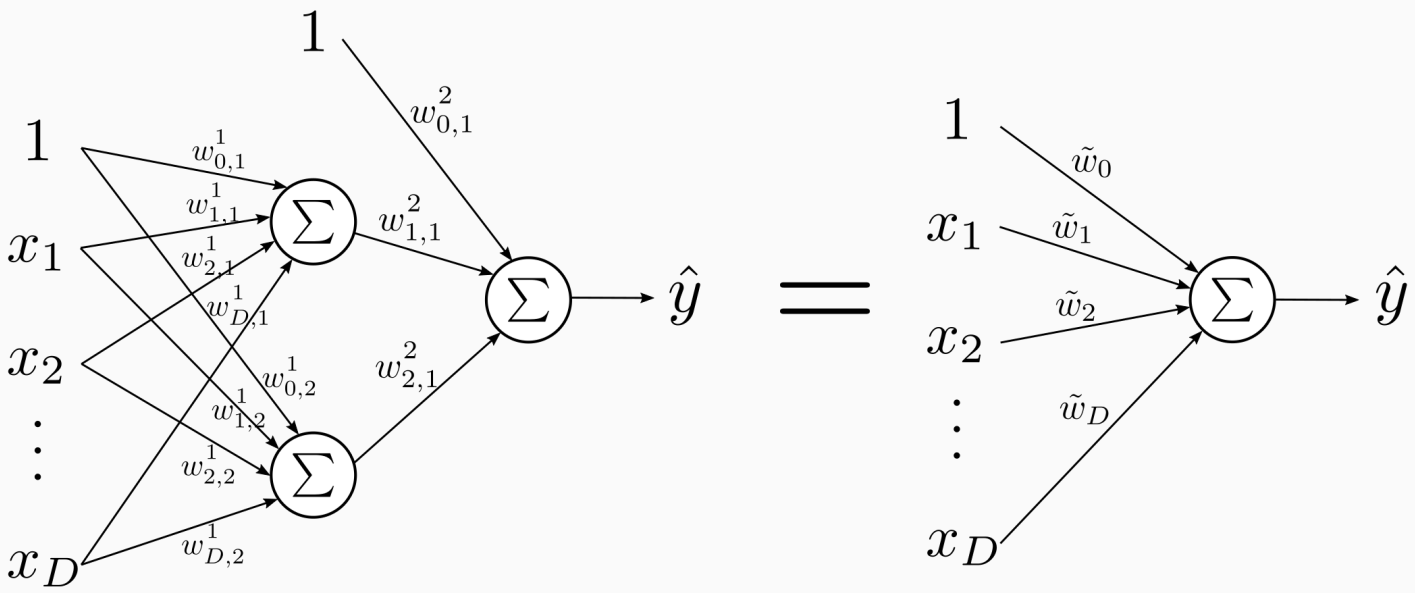
1. Linear functions often not adequate for real-world datasets.
2. Plug-and-play philosophy of ANNs: Construct complicated functions out of simple ones.
   This does not work with linear neurons!

Assume **linear units**, i.e. using $\phi(x) = x$:



$$\hat{y} = w^2_{0,1} + \sum_{i=1}^{2} w^2_{i,1} \left(\sum_{j=0}^{D} w^1_{j,i} x_j \right)$$

Assume **linear units**, i.e. using $\phi(x) = x$:



$$\hat{y} = w^2_{0,1} + \sum_{i=1}^{2} w^2_{i,1} \left(\sum_{j=0}^{D} w^1_{j,i} x_j \right) = \sum_{j=0}^{D} \tilde{w}_j x_j$$

$$\tilde{w}_0 = w^2_{0,1} + w^1_{0,1}\, w^2_{1,1} + w^1_{0,2}\, w^2_{2,1}$$
$$\tilde{w}_j = w^1_{j,1}\, w^2_{1,1} + w^1_{j,2}\, w^2_{2,1}$$

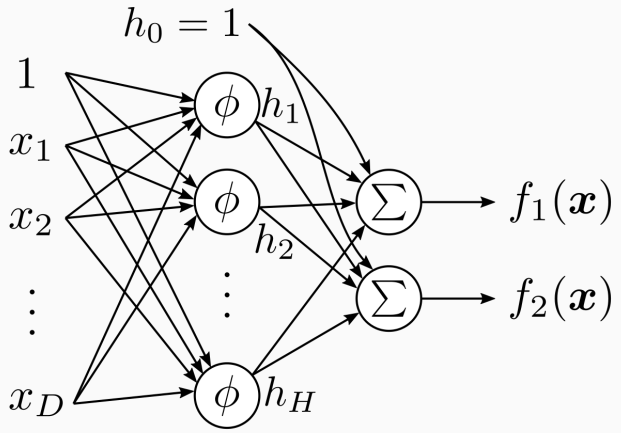
No matter how many linear units, or how they are connected:
Neural network of linear units = single linear unit!

No matter how many linear units, or how they are connected:
Neural network of linear units = single linear unit!

Does non-linearity save us?

Universal Approximation Theorem

Consider **single-layer neural nets**, i.e. MLPs with $L = 1$. Further assume that all hidden units have the same non-linearity ϕ and that all outputs are linear units.



Theorem **[Cybenko (1989), Pinkus (1999)]**

Any continuous function $f : \mathbb{R}^D \mapsto \mathbb{R}^O$ can be arbitrarily well approximated (on any compact set) by a single-layer neural network, for a wide range of non-linearities ϕ (specifically, ϕ just needs to be non-polynomial).

A **single-layer net** is already a **universal approximator**!

Why should we then even consider MLPs with more than one hidden layer?

Expressive Efficiency

- **Shallow networks** (1 hidden layer)
  - **universal approximators**
  - However, some function classes require **exponentially** many neurons, in the number of inputs
- **Deep networks** (many hidden layers)
  - can typically represent represent the same function classes with only **polynomial size**
  - This phenomenon is called **expressive efficiency** – Deep networks can represent non-linear function more efficiently than shallow ones
- Classical example: **parity function** – requires exponential size in shallow networks, but only polynomial size in deep networks

Expressive Efficiency – Intuition

- Non-linearities ϕ are "simple", like sigmoid, ReLU, etc.
- Real-world problems like "predict apple/pear from an image" are "highly non-linear"
- Cascading non-linear layers improves their flexibility to express non-linear functions
- Lower layers tend to extract low-level features, while higher levels tend to learn more abstract features

Deep Vs. Shallow Networks

- **Traditional downside** of deep networks: harder to train (to be discussed later)
- **"Neural network winter" ($\sim$1990-2005):** "Neural networks with more than two layers cannot reliably be trained."
- **Deep learning (2006–):** Tricks of the trade to train deep networks
- Neural networks can nowadays be scaled to hundreds or even thousands of layers

From Linear Models to Neural Networks

- In Lecture 4, we introduced **linear models**:

$$\hat{y} = \sum_{i=0}^{D} w_i x_i$$

- In Lecture 5, we generalized them by considering fixed **non-linear** features:

$$\hat{y} = \sum_{i=0}^{H} w_i \, \phi_i(\boldsymbol{x})$$

- Single-layer neural nets can be seen as linear models (output layer) with **learnable** non-linear features (hidden layer):

$$\hat{y} = \sum_{j=0}^{H} w^2_{j,1} \, \phi\Big(\sum_{i=0}^{D} w^1_{i,j} x_i \Big)$$

- **Deep neural networks: stacked feature extractors**

Automatic Differentiation

Neural networks are powerful function approximators, with hundreds to hundreds of billions of parameters.

How do we learn these parameters?

Neural networks are powerful function approximators, with hundreds to hundreds of billions of parameters.

How do we learn these parameters?

Gradient descent!

Training Setup

- We collect all network parameters in one vector $\boldsymbol{\theta}$
- Let $\hat{y} = f(\boldsymbol{x}, \boldsymbol{\theta})$ be the network's output for input $\boldsymbol{x}$ and parameters $\boldsymbol{\theta}$
- Training loss: $\mathcal{L}_{train}(\boldsymbol{\theta}) = \frac{1}{N} \sum_{i=1}^{N} \ell(y^{(i)}, f(\boldsymbol{x}^{(i)}, \boldsymbol{\theta}))$
- ℓ is some sample-wise loss, e.g. quadratic loss for regression, or cross-entropy for classification
- Minimize with gradient descent with $\nabla_{\boldsymbol{\theta}} \mathcal{L}_{train}$
- However, the structure of neural nets is complicated...
- How to compute the gradient? 

A Little Simplification

$$\mathcal{L}_{train}(\boldsymbol{\theta}) = \frac{1}{N}\sum_{i=1}^{N} \ell(y^{(i)}, f(\boldsymbol{x}^{(i)}, \boldsymbol{\theta}))$$

First simplification: gradient of sum is sum of gradients:

$$\nabla_{\boldsymbol{\theta}} \mathcal{L}_{train}(\boldsymbol{\theta}) = \nabla_{\boldsymbol{\theta}} \frac{1}{N}\sum_{i=1}^{N} \ell(y^{(i)}, f(\boldsymbol{x}^{(i)}, \boldsymbol{\theta})) = \frac{1}{N}\sum_{i=1}^{N} \nabla_{\boldsymbol{\theta}} \ell(y^{(i)}, f(\boldsymbol{x}^{(i)}, \boldsymbol{\theta}))$$

Thus, we just need to understand how to **compute the gradient for single sample $\boldsymbol{x}, y$**:

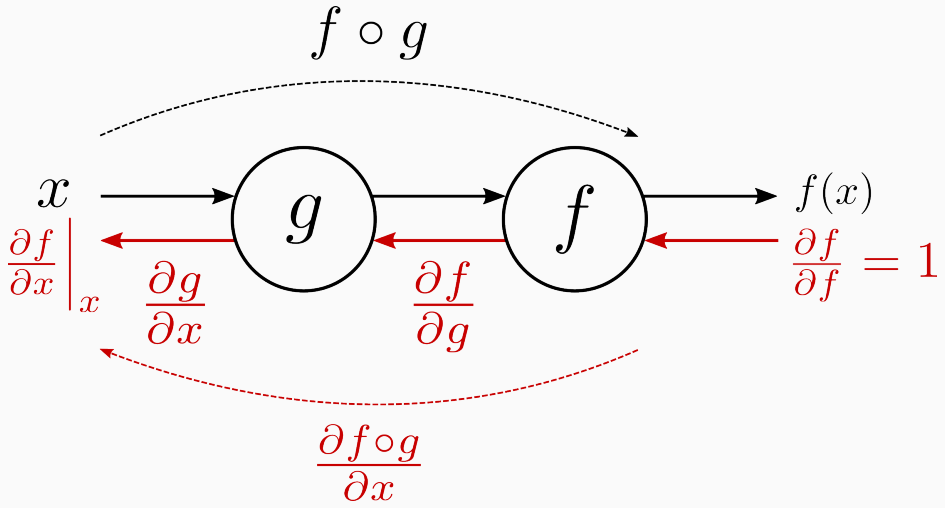
$$\nabla_{\boldsymbol{\theta}} \ell(y, f(\boldsymbol{x}, \boldsymbol{\theta}))$$

Automatic Differentiation in Computational Graphs

- A neural network $f(\boldsymbol{x}, \boldsymbol{\theta})$ is really just a special case of a **computational graph** with $\boldsymbol{x}$ and $\boldsymbol{\theta}$ as input
- **Automatic Differentiation (AD)** is a family of techniques to compute the partial derivatives (gradient) in computations graphs—thus, AD is immediately applicable to neural nets
- In neural networks a special case of AD, namely **reverse mode AD** is usually called **backpropagation of error (backprop)**
- Backprop is often attributed to Rumelhart, Hinton and Williams (1986), but actually also they just rediscovered the method for neural nets

Automatic Differentiation = Chain Rule of Calculus

- Recall that the chain rule says: $\frac{\partial f \circ g}{\partial x} = \frac{\partial f}{\partial g}\frac{\partial g}{\partial x}$
- This can be interpreted as **message passing** on a (chain-shaped) **computational graph**:

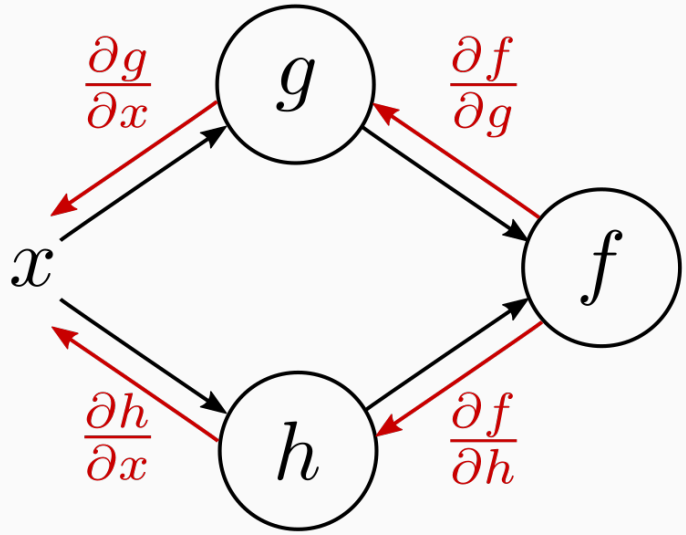


- Backwards pass starts with the trivial derivative $\frac{\partial f}{\partial f} = 1$
- Recursion: if derivatives of a node's output is known, the derivative of the node itself is just a multiplicative update with a **local derivative** (known and easy)

Automatic Differentiation = Chain Rule of Calculus

- More generally, we need a chain rule in multiple dimensions
- Consider a function of the form $f(x) = f(g(x), h(x))$ which is a composition of a $\mathbb{R} \mapsto \mathbb{R}^2$ (g, h) and a $\mathbb{R}^2 \mapsto \mathbb{R}$ (f) function
- Derivatives of several output branches simply add up:

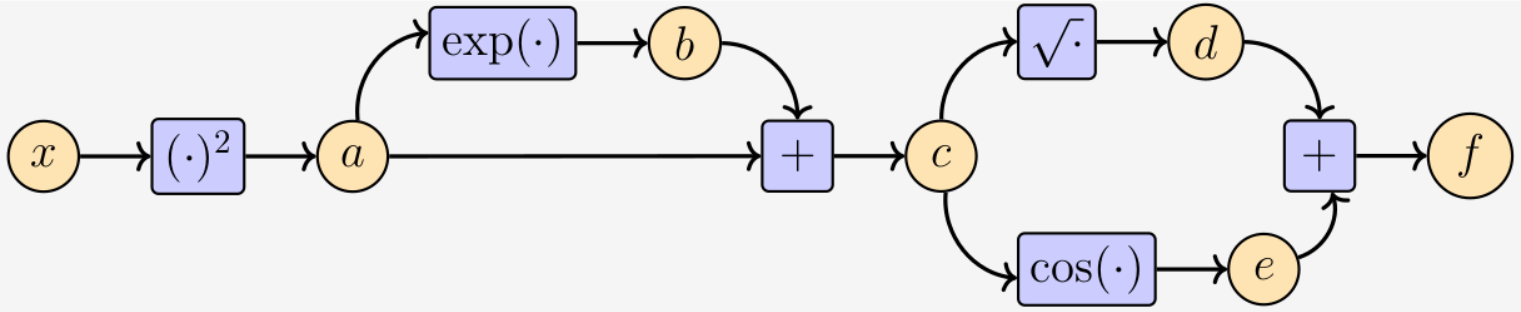
$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial g}\frac{\partial g}{\partial x} + \frac{\partial f}{\partial h}\frac{\partial h}{\partial x}$$



- In general, if $f(x) = f(g_1(x), g_2(x), \ldots, g_K(x))$ then

$$\frac{\partial f}{\partial x} = \sum_{k=1}^{K} \frac{\partial f}{\partial g_k}\frac{\partial g_k}{\partial x}$$

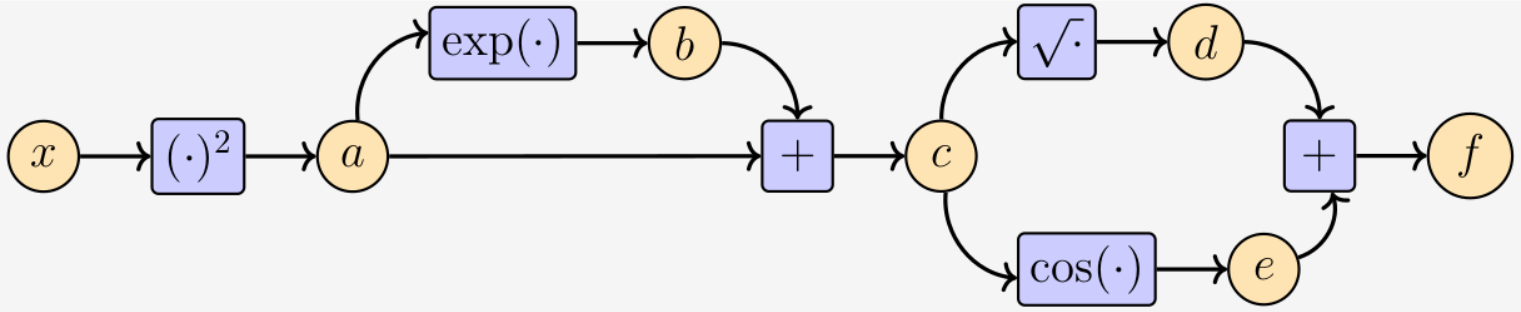
- Consider following computational graph (Deisenroth et al.):



- Here, the blue nodes are operations, while the orange nodes are intermediate results
- The computational graph implements the function

$$f(x) = \sqrt{x^2 + \exp(x^2)} + \cos(x^2 + \exp(x^2))$$

- Note that there might be many graphs implementing the same function (graph is not unique for given f)

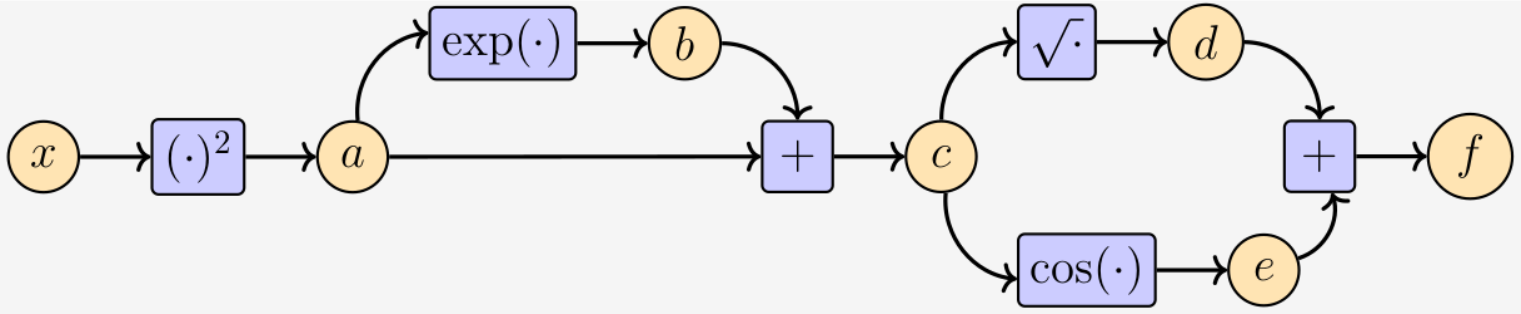


What is $f(x)$ for $x = 2$?

- $a = x^2 = 4$
- $b = \exp(a) = 54.598$
- $c = a + b = 58.598$
- $d = \sqrt{c} = 7.6549$
- $e = \cos(c) = -0.46$
- $f = d + e = 7.194$

Let's store forward messages a, b, c, d, e, f in the orange nodes

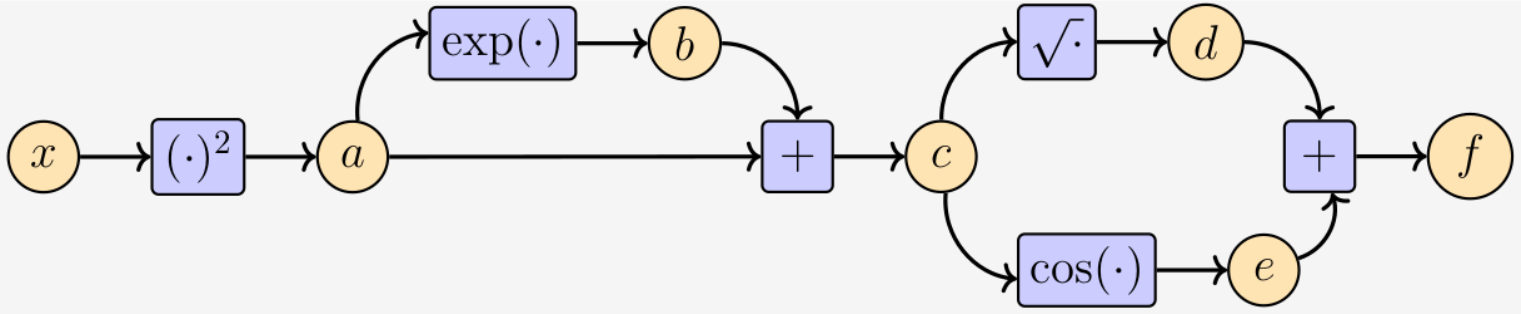
Backwards Pass (Autodiff, Backprop) Example



What is $\frac{\partial f}{\partial x}$? (more precisely, $\frac{\partial f}{\partial x}\big|_{x=2}$)

- $\frac{\partial f}{\partial f} =$
- $\frac{\partial f}{\partial e} =$
- $\frac{\partial f}{\partial d} =$
- $\frac{\partial f}{\partial c} =$
- $\frac{\partial f}{\partial b} =$
- $\frac{\partial f}{\partial a} =$
- $\frac{\partial f}{\partial x} =$

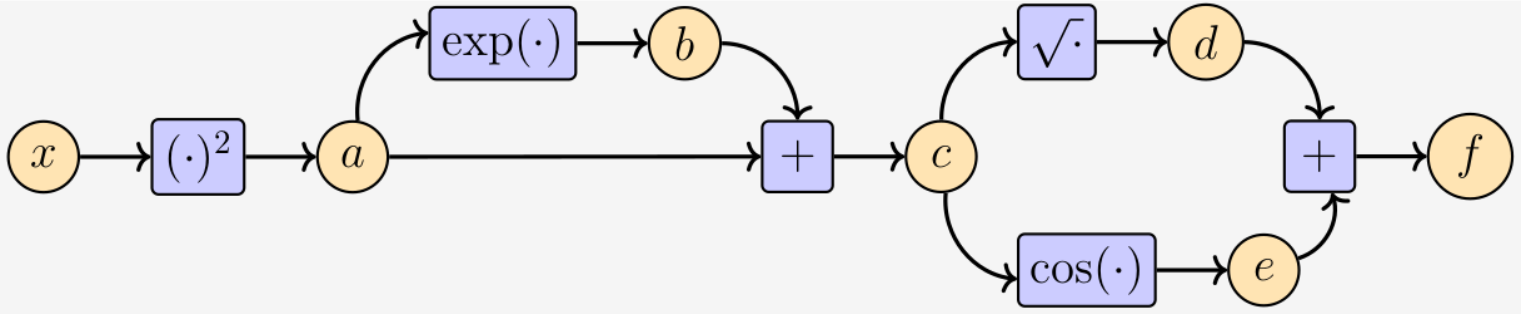
Backwards Pass (Autodiff, Backprop) Example



What is $\frac{\partial f}{\partial x}$? (more precisely, $\frac{\partial f}{\partial x}\big|_{x=2}$)

- $\frac{\partial f}{\partial f} = 1$
- $\frac{\partial f}{\partial e} =$
- $\frac{\partial f}{\partial d} =$
- $\frac{\partial f}{\partial c} =$
- $\frac{\partial f}{\partial b} =$
- $\frac{\partial f}{\partial a} =$
- $\frac{\partial f}{\partial x} =$

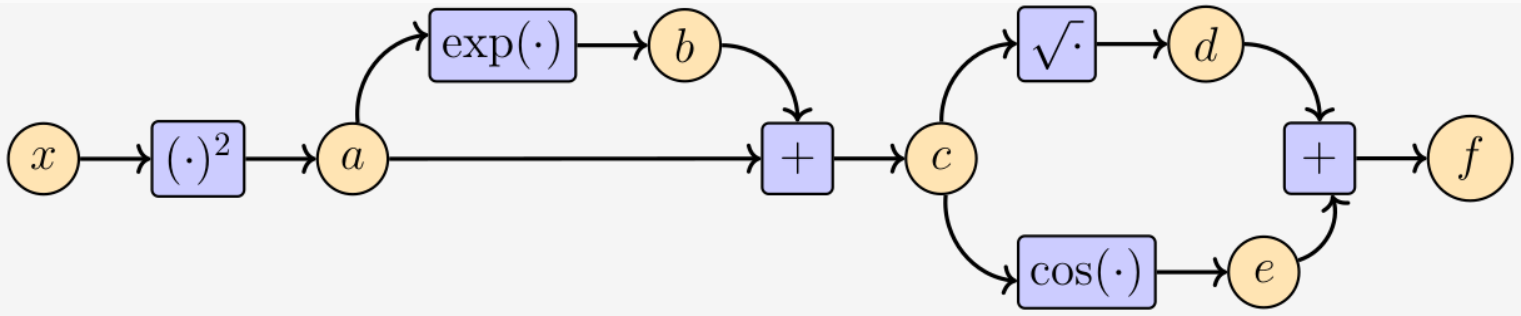
Backwards Pass (Autodiff, Backprop) Example



What is $\frac{\partial f}{\partial x}$? (more precisely, $\frac{\partial f}{\partial x}\big|_{x=2}$)

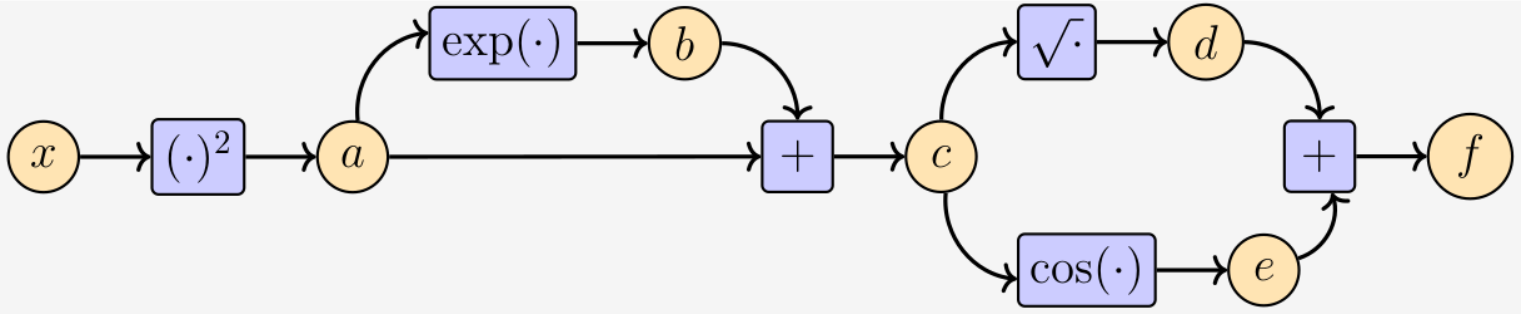
- $\frac{\partial f}{\partial f} = 1$
- $\frac{\partial f}{\partial e} = \frac{\partial f}{\partial f}\frac{\partial f}{\partial e} = 1 \times 1 = 1$
- $\frac{\partial f}{\partial d} =$
- $\frac{\partial f}{\partial c} =$
- $\frac{\partial f}{\partial b} =$
- $\frac{\partial f}{\partial a} =$
- $\frac{\partial f}{\partial x} =$

Backwards Pass (Autodiff, Backprop) Example



What is $\frac{\partial f}{\partial x}$? (more precisely, $\frac{\partial f}{\partial x}\big|_{x=2}$)

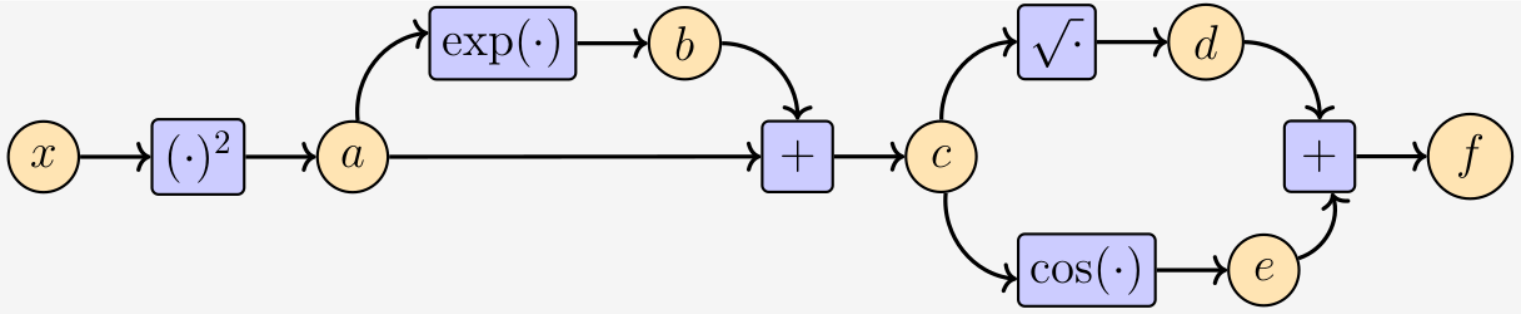
- $\frac{\partial f}{\partial f} = 1$
- $\frac{\partial f}{\partial e} = \frac{\partial f}{\partial f}\frac{\partial f}{\partial e} = 1 \times 1 = 1$
- $\frac{\partial f}{\partial d} = \frac{\partial f}{\partial f}\frac{\partial f}{\partial d} = 1 \times 1 = 1$
- $\frac{\partial f}{\partial c} =$
- $\frac{\partial f}{\partial b} =$
- $\frac{\partial f}{\partial a} =$
- $\frac{\partial f}{\partial x} =$



What is $\frac{\partial f}{\partial x}$? (more precisely, $\frac{\partial f}{\partial x}\big|_{x=2}$)

- $\frac{\partial f}{\partial f} = 1$
- $\frac{\partial f}{\partial e} = \frac{\partial f}{\partial f}\frac{\partial f}{\partial e} = 1 \times 1 = 1$
- $\frac{\partial f}{\partial d} = \frac{\partial f}{\partial f}\frac{\partial f}{\partial d} = 1 \times 1 = 1$
- $\frac{\partial f}{\partial c} = \frac{\partial f}{\partial e}\frac{\partial e}{\partial c} + \frac{\partial f}{\partial d}\frac{\partial d}{\partial c} = 1 \times -\sin(c) + 1 \times \frac{1}{2}c^{-\frac{1}{2}} = -0.822$
- $\frac{\partial f}{\partial b} =$
- $\frac{\partial f}{\partial a} =$
- $\frac{\partial f}{\partial x} =$

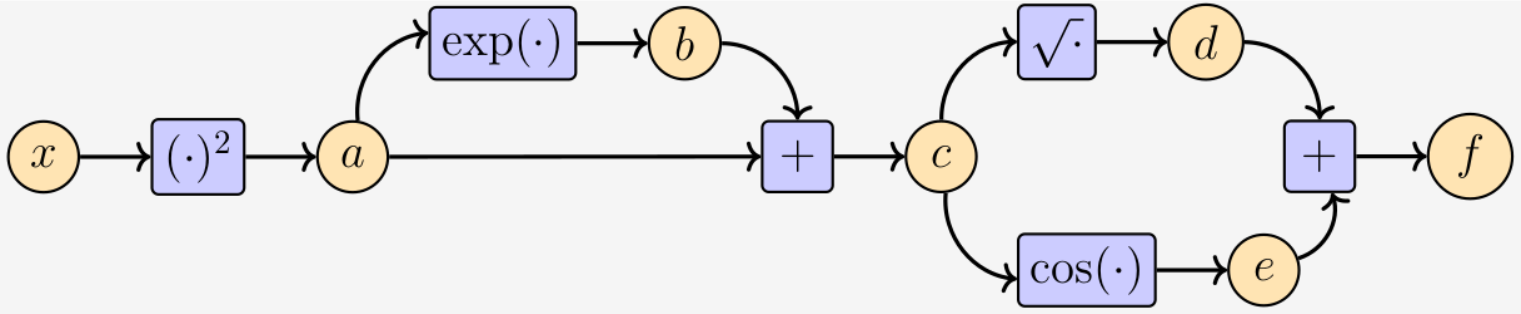
Backwards Pass (Autodiff, Backprop) Example



What is $\frac{\partial f}{\partial x}$? (more precisely, $\frac{\partial f}{\partial x}\big|_{x=2}$)

- $\frac{\partial f}{\partial f} = 1$
- $\frac{\partial f}{\partial e} = \frac{\partial f}{\partial f}\frac{\partial f}{\partial e} = 1 \times 1 = 1$
- $\frac{\partial f}{\partial d} = \frac{\partial f}{\partial f}\frac{\partial f}{\partial d} = 1 \times 1 = 1$
- $\frac{\partial f}{\partial c} = \frac{\partial f}{\partial e}\frac{\partial e}{\partial c} + \frac{\partial f}{\partial d}\frac{\partial d}{\partial c} = 1 \times -\sin(c) + 1 \times \frac{1}{2}c^{-\frac{1}{2}} = -0.822$
- $\frac{\partial f}{\partial b} = \frac{\partial f}{\partial c}\frac{\partial c}{\partial b} = -0.822 \times 1 = -0.822$
- $\frac{\partial f}{\partial a} =$
- $\frac{\partial f}{\partial x} =$

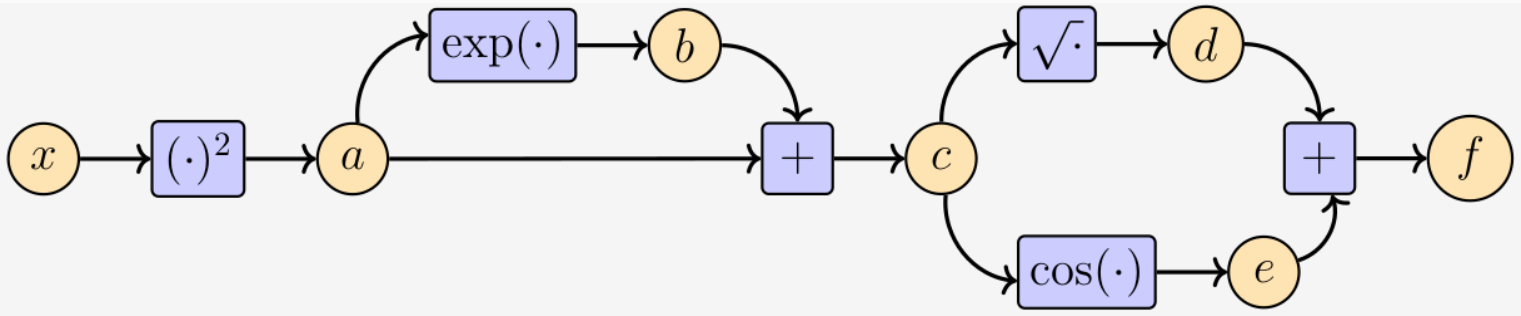
Backwards Pass (Autodiff, Backprop) Example



What is $\frac{\partial f}{\partial x}$? (more precisely, $\frac{\partial f}{\partial x}\big|_{x=2}$)

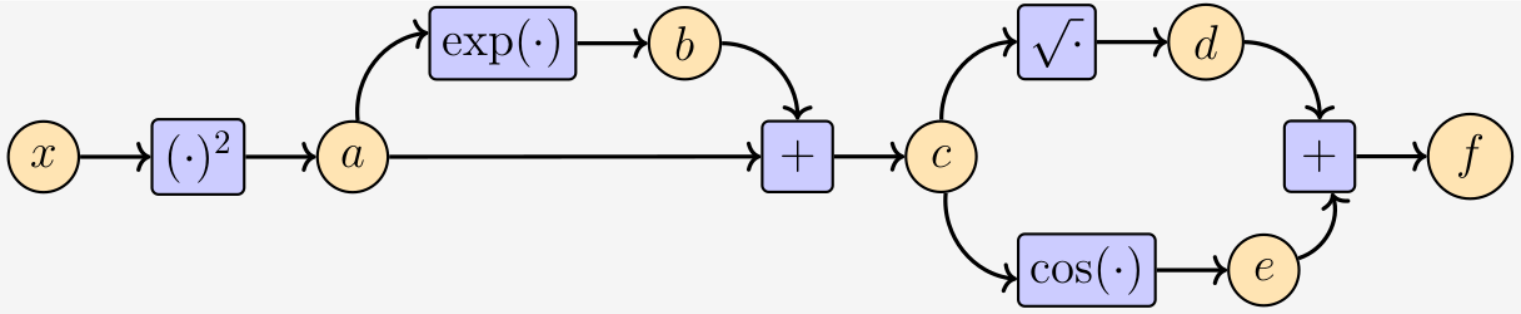
- $\frac{\partial f}{\partial f} = 1$
- $\frac{\partial f}{\partial e} = \frac{\partial f}{\partial f}\frac{\partial f}{\partial e} = 1 \times 1 = 1$
- $\frac{\partial f}{\partial d} = \frac{\partial f}{\partial f}\frac{\partial f}{\partial d} = 1 \times 1 = 1$
- $\frac{\partial f}{\partial c} = \frac{\partial f}{\partial e}\frac{\partial e}{\partial c} + \frac{\partial f}{\partial d}\frac{\partial d}{\partial c} = 1 \times -\sin(c) + 1 \times \frac{1}{2}c^{-\frac{1}{2}} = -0.822$
- $\frac{\partial f}{\partial b} = \frac{\partial f}{\partial c}\frac{\partial c}{\partial b} = -0.822 \times 1 = -0.822$
- $\frac{\partial f}{\partial a} = \frac{\partial f}{\partial c}\frac{\partial c}{\partial a} + \frac{\partial f}{\partial b}\frac{\partial b}{\partial a} = -0.822 \times 1 + -0.822 \times \exp(a) = -45.717$
- $\frac{\partial f}{\partial x} =$

Backwards Pass (Autodiff, Backprop) Example



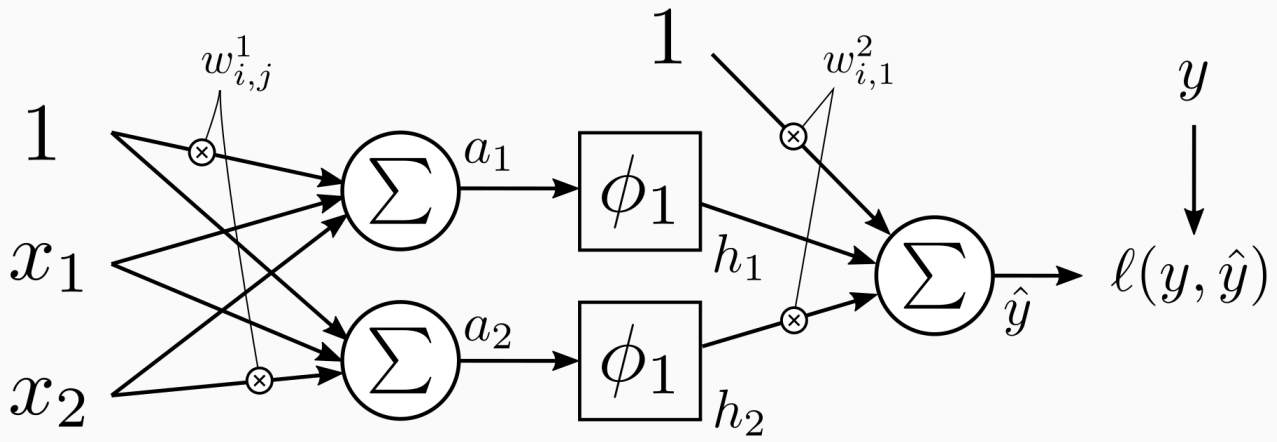
What is $\frac{\partial f}{\partial x}$? (more precisely, $\frac{\partial f}{\partial x}\big|_{x=2}$)

- $\frac{\partial f}{\partial f} = 1$
- $\frac{\partial f}{\partial e} = \frac{\partial f}{\partial f}\frac{\partial f}{\partial e} = 1 \times 1 = 1$
- $\frac{\partial f}{\partial d} = \frac{\partial f}{\partial f}\frac{\partial f}{\partial d} = 1 \times 1 = 1$
- $\frac{\partial f}{\partial c} = \frac{\partial f}{\partial e}\frac{\partial e}{\partial c} + \frac{\partial f}{\partial d}\frac{\partial d}{\partial c} = 1 \times -\sin(c) + 1 \times \frac{1}{2}c^{-\frac{1}{2}} = -0.822$
- $\frac{\partial f}{\partial b} = \frac{\partial f}{\partial c}\frac{\partial c}{\partial b} = -0.822 \times 1 = -0.822$
- $\frac{\partial f}{\partial a} = \frac{\partial f}{\partial c}\frac{\partial c}{\partial a} + \frac{\partial f}{\partial b}\frac{\partial b}{\partial a} = -0.822 \times 1 + -0.822 \times \exp(a) = -45.717$
- $\frac{\partial f}{\partial x} = \frac{\partial f}{\partial a}\frac{\partial a}{\partial x} = -45.717 \times 2x = -182.87$

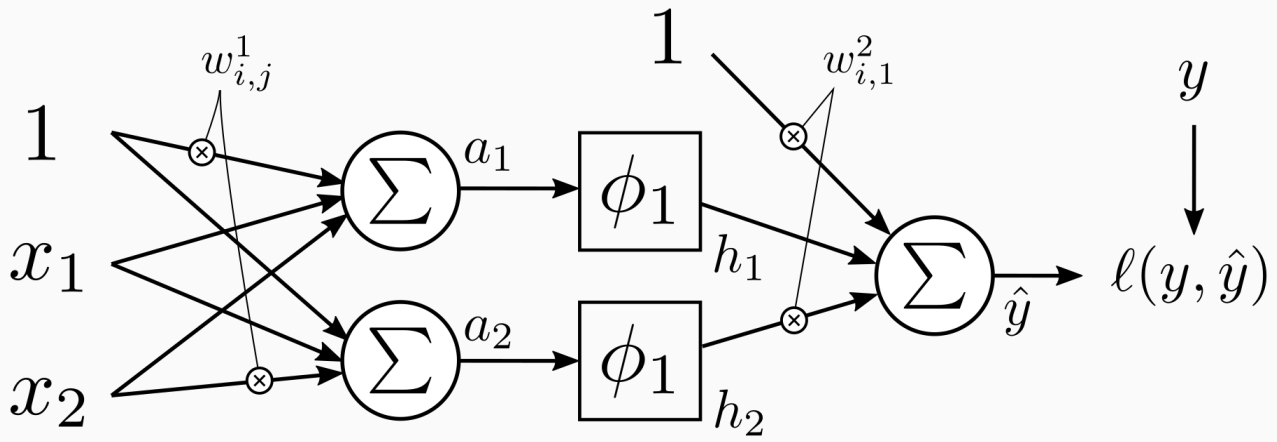


What is $\frac{\partial f}{\partial x}$? (more precisely, $\frac{\partial f}{\partial x}\big|_{x=2}$)

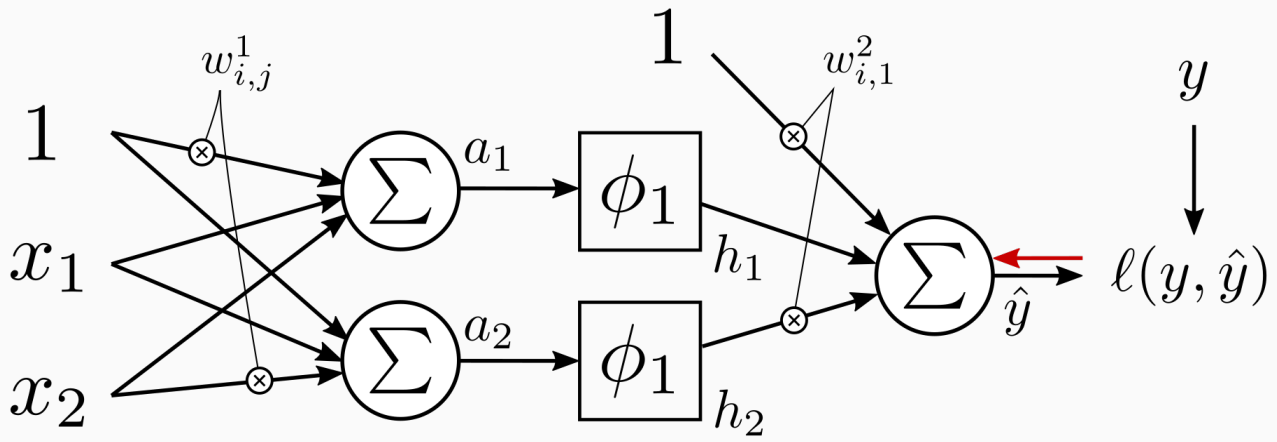
- $\frac{\partial f}{\partial f} = 1$
- $\frac{\partial f}{\partial e} = \frac{\partial f}{\partial f}\frac{\partial f}{\partial e} = 1 \times 1 = 1$
- $\frac{\partial f}{\partial d} = \frac{\partial f}{\partial f}\frac{\partial f}{\partial d} = 1 \times 1 = 1$
- $\frac{\partial f}{\partial c} = \frac{\partial f}{\partial e}\frac{\partial e}{\partial c} + \frac{\partial f}{\partial d}\frac{\partial d}{\partial c} = 1 \times -\sin(c) + 1 \times \frac{1}{2}c^{-\frac{1}{2}} = -0.822$
- $\frac{\partial f}{\partial b} = \frac{\partial f}{\partial c}\frac{\partial c}{\partial b} = -0.822 \times 1 = -0.822$
- $\frac{\partial f}{\partial a} = \frac{\partial f}{\partial c}\frac{\partial c}{\partial a} + \frac{\partial f}{\partial b}\frac{\partial b}{\partial a} = -0.822 \times 1 + -0.822 \times \exp(a) = -45.717$
- $\frac{\partial f}{\partial x} = \frac{\partial f}{\partial a}\frac{\partial a}{\partial x} = -45.717 \times 2x = -182.87$
- Note we get derivatives for **all nodes**, not only x!



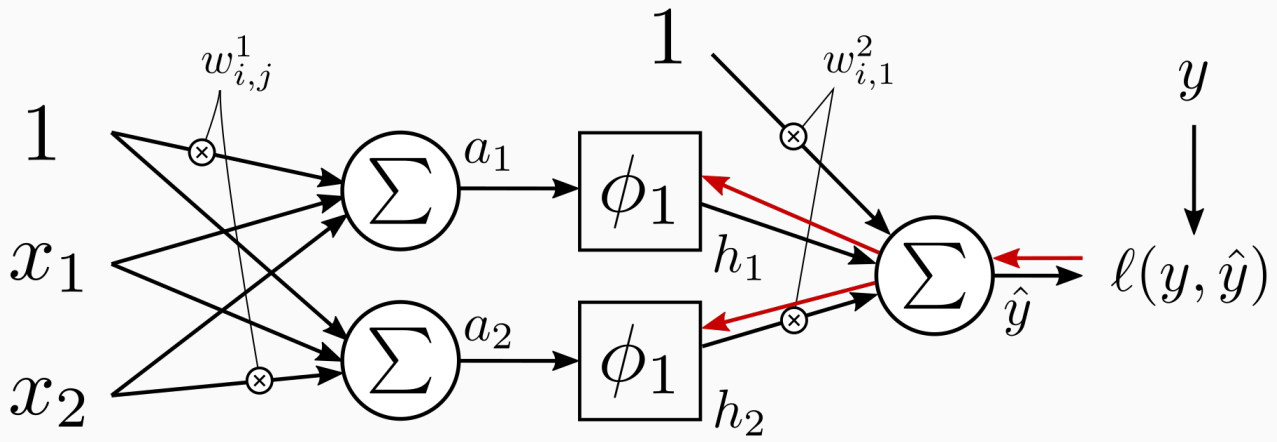
- Neural nets are simply computational graphs
- Inputs to the graph:
  - features $x_1, x_2, \ldots, x_D$
  - weights $w^l_{i,j}$
  - targets y
- The loss ℓ is also a node in the graph!



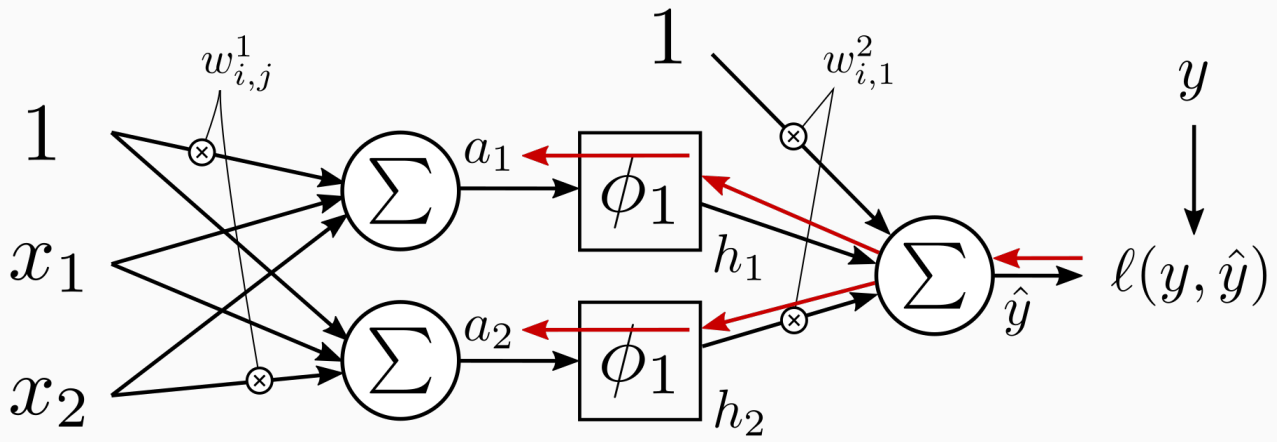
- $\frac{\partial \ell}{\partial \ell} = 1$



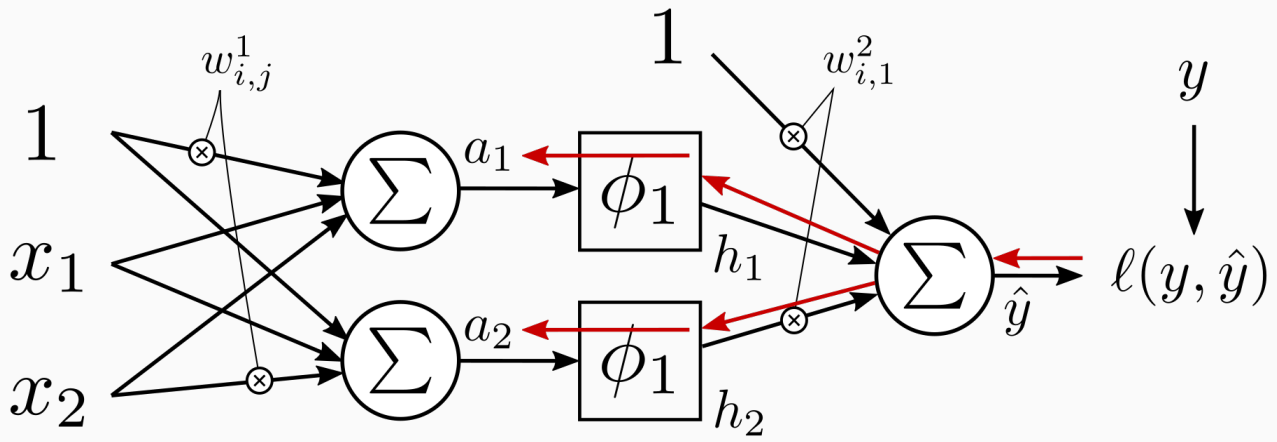
- $\frac{\partial \ell}{\partial \ell} = 1$
- $\frac{\partial \ell}{\partial \hat{y}} = \frac{\partial \ell}{\partial \ell} \frac{\partial \ell}{\partial \hat{y}} =: B_1$ (closed form for most losses)



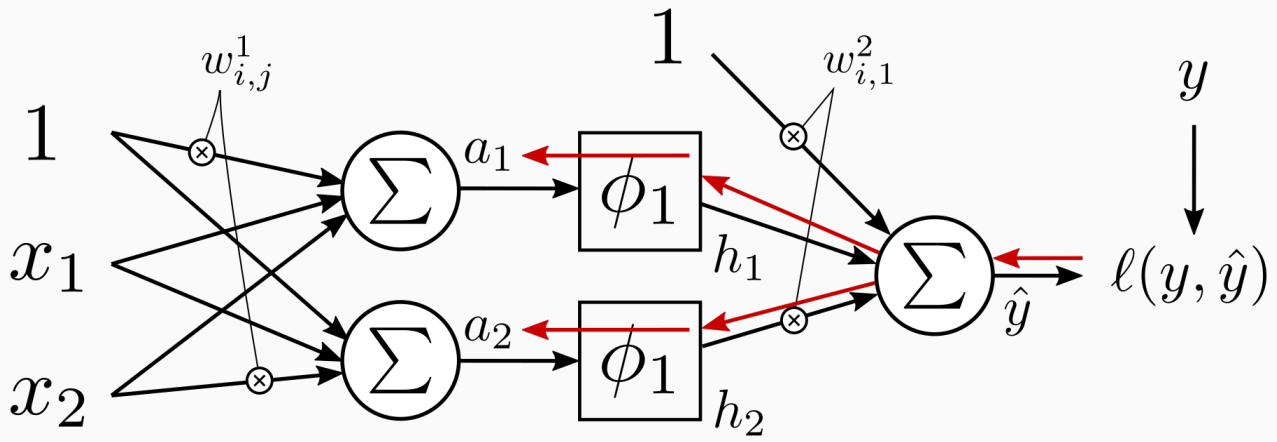
- $\frac{\partial \ell}{\partial \ell} = 1$
- $\frac{\partial \ell}{\partial \hat{y}} = \frac{\partial \ell}{\partial \ell} \frac{\partial \ell}{\partial \hat{y}} =: B_1$ (closed form for most losses)
- $\frac{\partial \ell}{\partial h_i} = \frac{\partial \ell}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial h_i} = B_1 w^2_{i,1} =: B_{2,i}$ $(\hat{y} = \sum_{i=0}^{2} w^2_{i,1} h_i)$



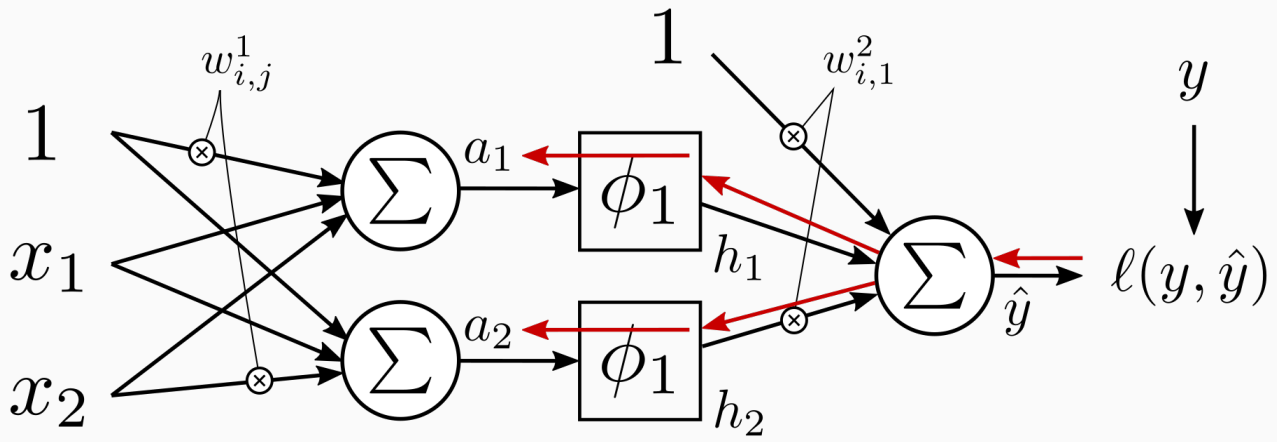
- $\frac{\partial \ell}{\partial \ell} = 1$
- $\frac{\partial \ell}{\partial \hat{y}} = \frac{\partial \ell}{\partial \ell}\frac{\partial \ell}{\partial \hat{y}} =: B_1$ (closed form for most losses)
- $\frac{\partial \ell}{\partial h_i} = \frac{\partial \ell}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial h_i} = B_1 w^2_{i,1} =: B_{2,i}$ $(\hat{y} = \sum_{i=0}^{2} w^2_{i,1} h_i)$
- $\frac{\partial \ell}{\partial a_i} = \frac{\partial \ell}{\partial h_i}\frac{\partial h_i}{\partial a_i} = B_{2,i}\, \phi_1'(a_i) =: B_{3,i}$ (known, closed form ϕ_1')



- $\frac{\partial \ell}{\partial \ell} = 1$
- $\frac{\partial \ell}{\partial \hat{y}} = \frac{\partial \ell}{\partial \ell}\frac{\partial \ell}{\partial \hat{y}} =: B_1$ (closed form for most losses)
- $\frac{\partial \ell}{\partial h_i} = \frac{\partial \ell}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial h_i} = B_1 w^2_{i,1} =: B_{2,i}$ $(\hat{y} = \sum_{i=0}^{2} w^2_{i,1} h_i)$
- $\frac{\partial \ell}{\partial a_i} = \frac{\partial \ell}{\partial h_i}\frac{\partial h_i}{\partial a_i} = B_{2,i}\,\phi_1'(a_i) =: B_{3,i}$ (known, closed form ϕ_1')
- $\frac{\partial \ell}{\partial w^2_{i,1}} = \frac{\partial \ell}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial w^2_{i,1}} = B_1 h_i$ $(\hat{y} = \sum_{i=0}^{2} w^2_{i,1} h_i)$



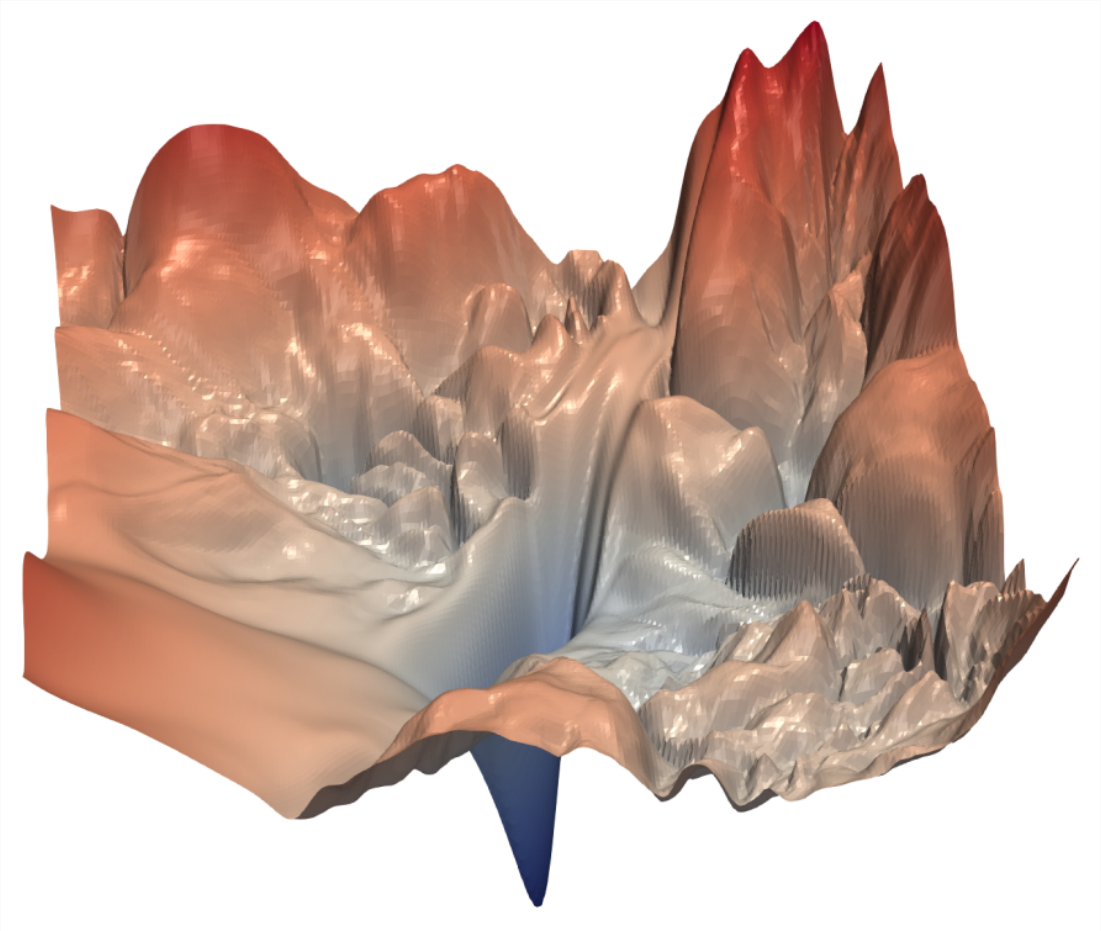
- $\frac{\partial \ell}{\partial \ell} = 1$
- $\frac{\partial \ell}{\partial \hat{y}} = \frac{\partial \ell}{\partial \ell}\frac{\partial \ell}{\partial \hat{y}} =: B_1$ (closed form for most losses)
- $\frac{\partial \ell}{\partial h_i} = \frac{\partial \ell}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial h_i} = B_1 w^2_{i,1} =: B_{2,i}$ $(\hat{y} = \sum_{i=0}^{2} w^2_{i,1} h_i)$
- $\frac{\partial \ell}{\partial a_i} = \frac{\partial \ell}{\partial h_i}\frac{\partial h_i}{\partial a_i} = B_{2,i}\,\phi_1'(a_i) =: B_{3,i}$ (known, closed form ϕ_1')
- $\frac{\partial \ell}{\partial w^2_{i,1}} = \frac{\partial \ell}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial w^2_{i,1}} = B_1 h_i$ $(\hat{y} = \sum_{i=0}^{2} w^2_{i,1} h_i)$
- $\frac{\partial \ell}{\partial w^1_{i,j}} = \frac{\partial \ell}{\partial a_j}\frac{\partial a_j}{\partial w^1_{i,j}} = B_{3,j} x_i$ $(a_j = \sum_{i=0}^{2} w^1_{i,j} x_i)$



- $\frac{\partial \ell}{\partial \ell} = 1$
- $\frac{\partial \ell}{\partial \hat{y}} = \frac{\partial \ell}{\partial \ell}\frac{\partial \ell}{\partial \hat{y}} =: B_1$ (closed form for most losses)
- $\frac{\partial \ell}{\partial h_i} = \frac{\partial \ell}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial h_i} = B_1 w^2_{i,1} =: B_{2,i}$ $(\hat{y} = \sum_{i=0}^{2} w^2_{i,1} h_i)$
- $\frac{\partial \ell}{\partial a_i} = \frac{\partial \ell}{\partial h_i}\frac{\partial h_i}{\partial a_i} = B_{2,i}\,\phi_1'(a_i) =: B_{3,i}$ (known, closed form ϕ_1')
- $\frac{\partial \ell}{\partial w^2_{i,1}} = \frac{\partial \ell}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial w^2_{i,1}} = B_1 h_i$ $(\hat{y} = \sum_{i=0}^{2} w^2_{i,1} h_i)$
- $\frac{\partial \ell}{\partial w^1_{i,j}} = \frac{\partial \ell}{\partial a_j}\frac{\partial a_j}{\partial w^1_{i,j}} = B_{3,j} x_i$ $(a_j = \sum_{i=0}^{2} w^1_{i,j} x_i)$
- $\frac{\partial \ell}{\partial x_i} = \sum_j \frac{\partial \ell}{\partial a_j}\frac{\partial a_j}{\partial x_i} = \sum_j B_{3,j} w^1_{i,j}$ (if needed)

Loss Landscape of Neural Networks (Non-Convex)

Training loss in neural networks is highly non-convex, and we can find only local minima. However, in practice they work very well.



Source: Li et al., *Visualizing the Loss Landscape of Neural Nets*, NeurIPS 2018.

Summary

- ANN: network of artificial neurons
- Non-linearity is key, otherwise ANNs "collapse" to a linear function
- Universal function approximators, even for one hidden layer
- Deep networks are more expressive efficient
- Learning via gradient descent
- Gradients computed via **automatic differentiation** (**backpropagation**, **chain rule**)