UniGe | MaLGa

[Deep] Neural Networks: an introduction

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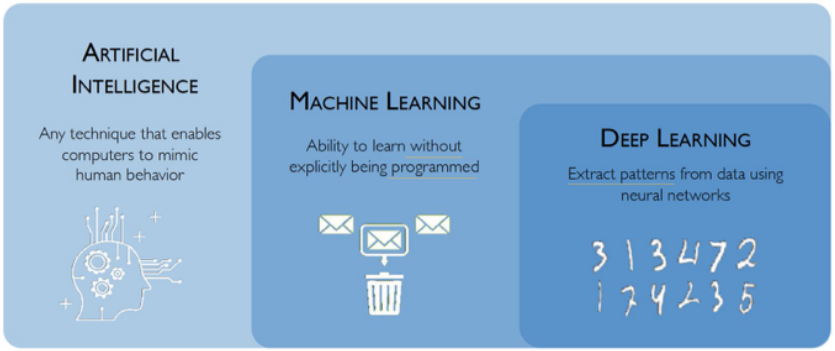
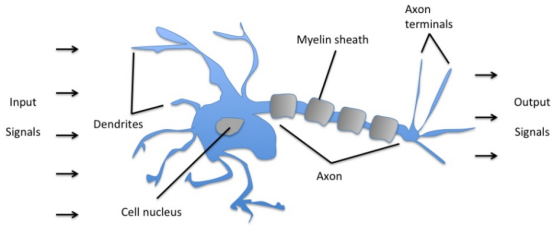
Some definitions

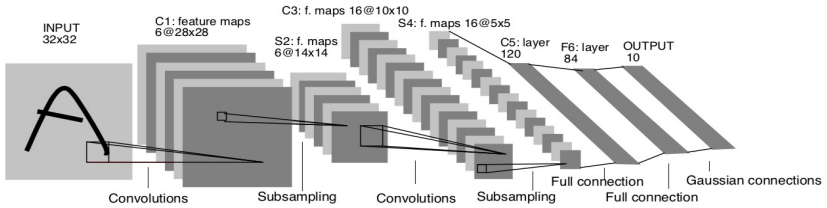


- Deep learning is a family of machine learning methods based on artificial neural networks (ANNs) that use multiple layers to progressively extract higher level features from raw input

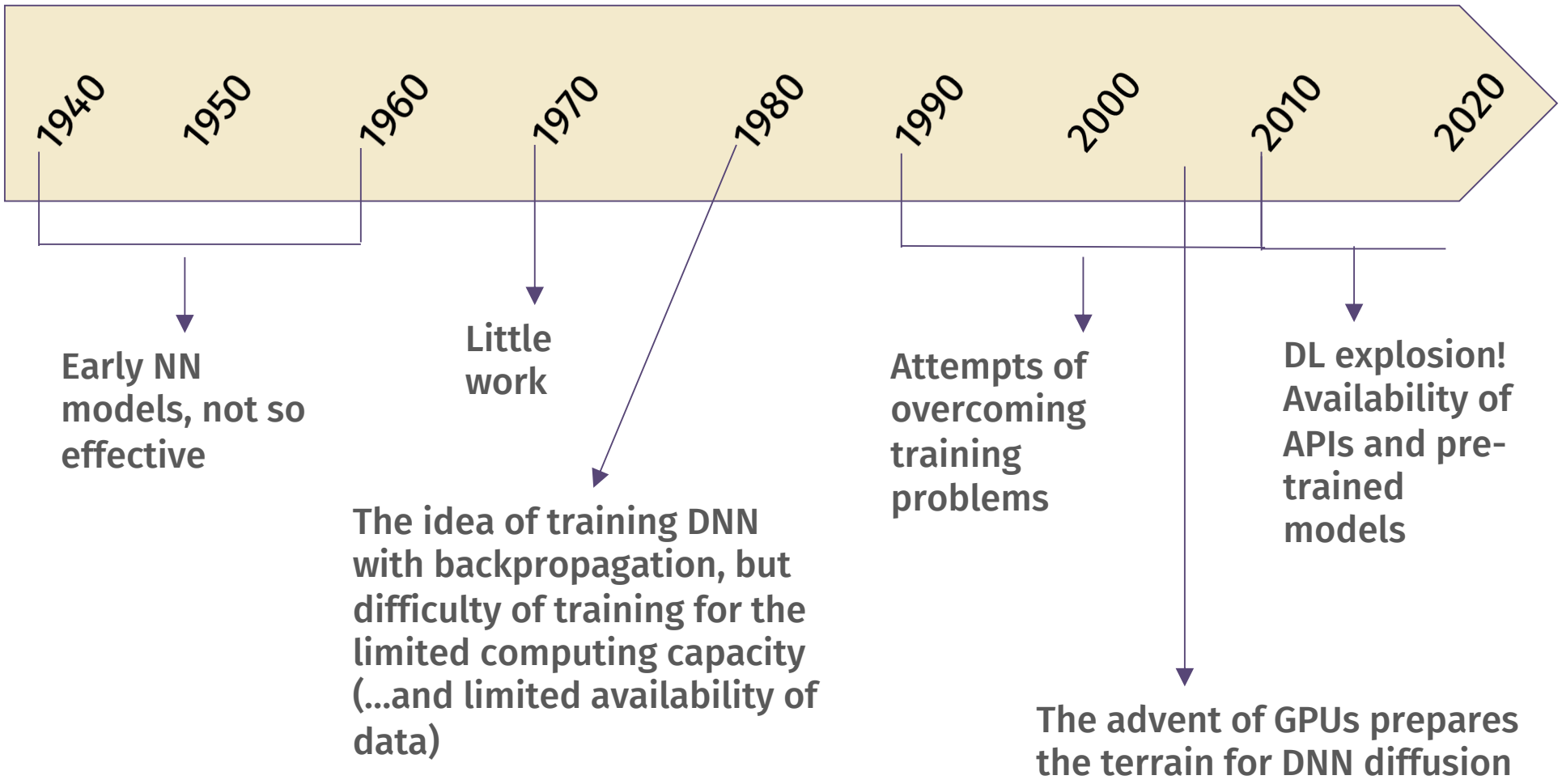
- ANNs are computing systems inspired by biological neural networks, based on a collection of units/nodes, artificial neurons, loosely modelling the neurons. biological brain



- But also: Deep learning methods are representation-learning methods with multiple levels of representation

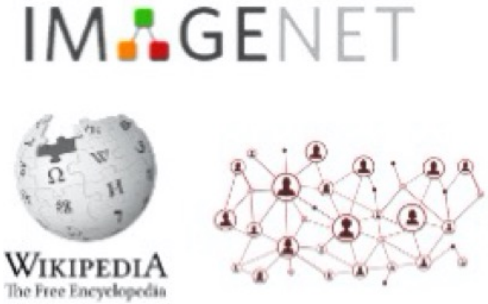


A bit of history



Why now?

Availability of data



Hardware

Software

What now?

Generative models

This person does not exist

Style transfer

Text-to-image

The street of a medieval fantasy town, ad dawn, dark, 4k, highly detailed

...have you ever heard about ChatGPT?

NI How should I introduce an introductory course on deep learning?

Introduction to Deep Learning: Unleashing the Power of Artificial Intelligence

Welcome to the world of deep learning! In this introductory course, we will embark on an exciting journey into the realm of artificial intelligence and explore the foundations of deep learning. Prepare to unlock the secrets behind one of the most transformative technologies of our time.

A change of paradigm

Feature engineering

$$\Phi(\Psi(x))$$

x

Data Representation (e.g. feature extraction)

$\Psi(x)$

Classifier

y

Feature learning

This part learns the representation

This part trains the classifier

x

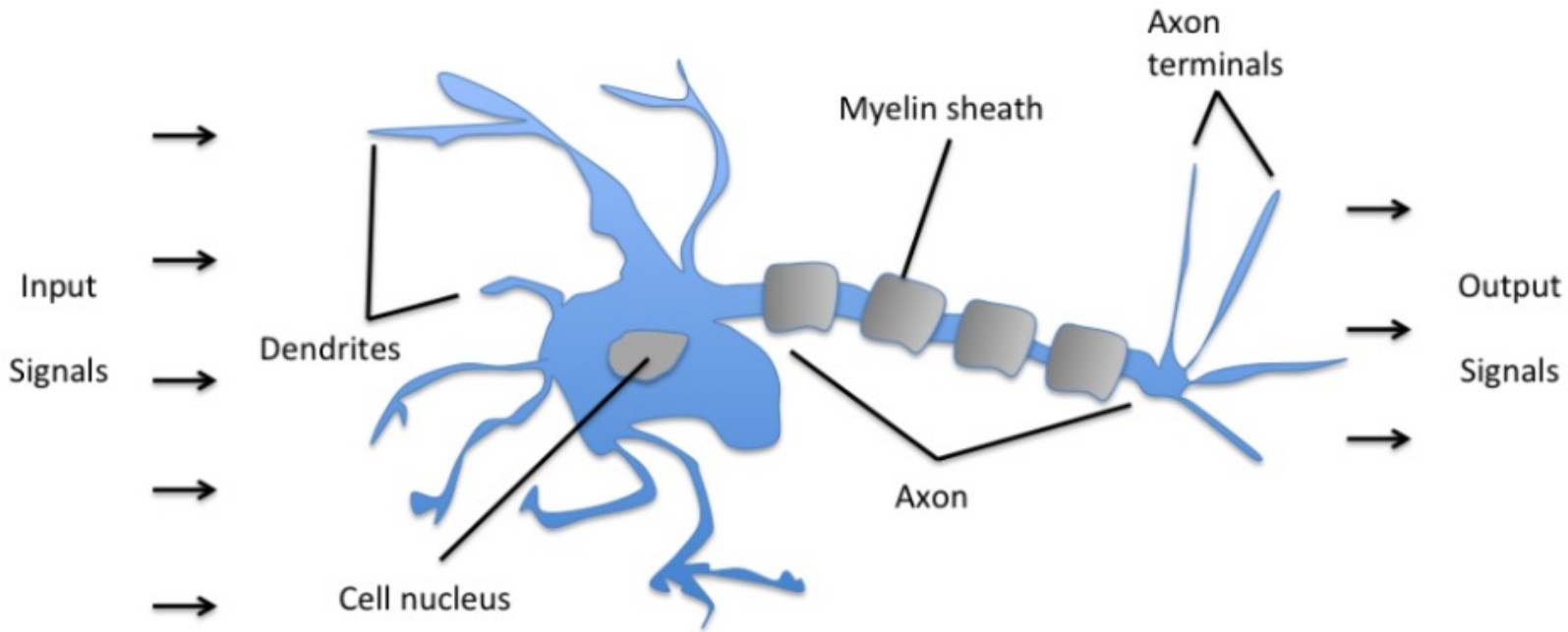
(Deep) NN

y

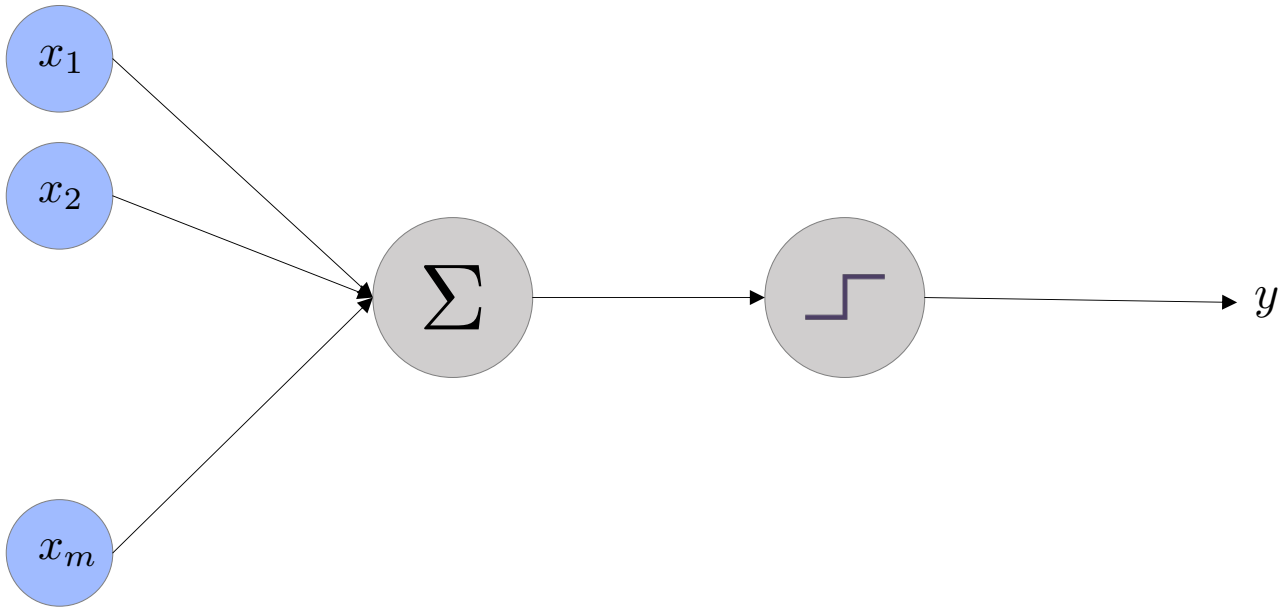
$f(x)$

Single Layer Perceptron

Biological neuron



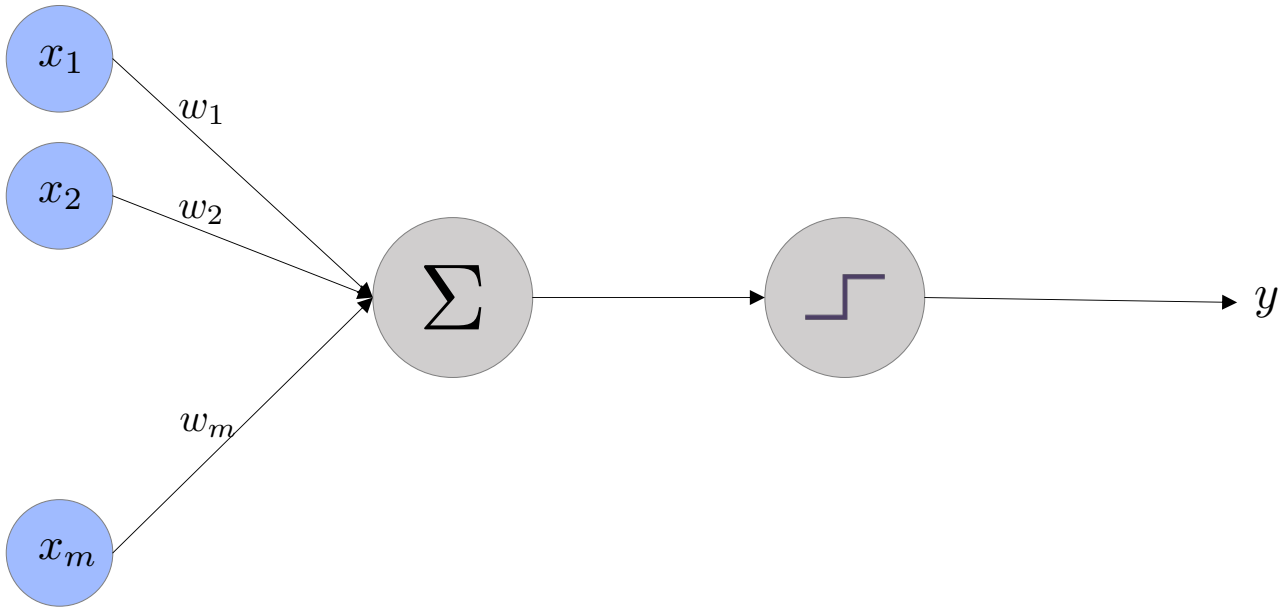
McCulloch & Pitts Neuron Model (1943)



$$f_\theta : \mathbb{R}^m \rightarrow \mathbb{R}$$

$$y = f_\theta(\mathbf{x}) = \begin{cases} 1 & \text{if } \sum_{i=1}^{m} x_i > \theta \\ 0 & \text{otherwise} \end{cases}$$

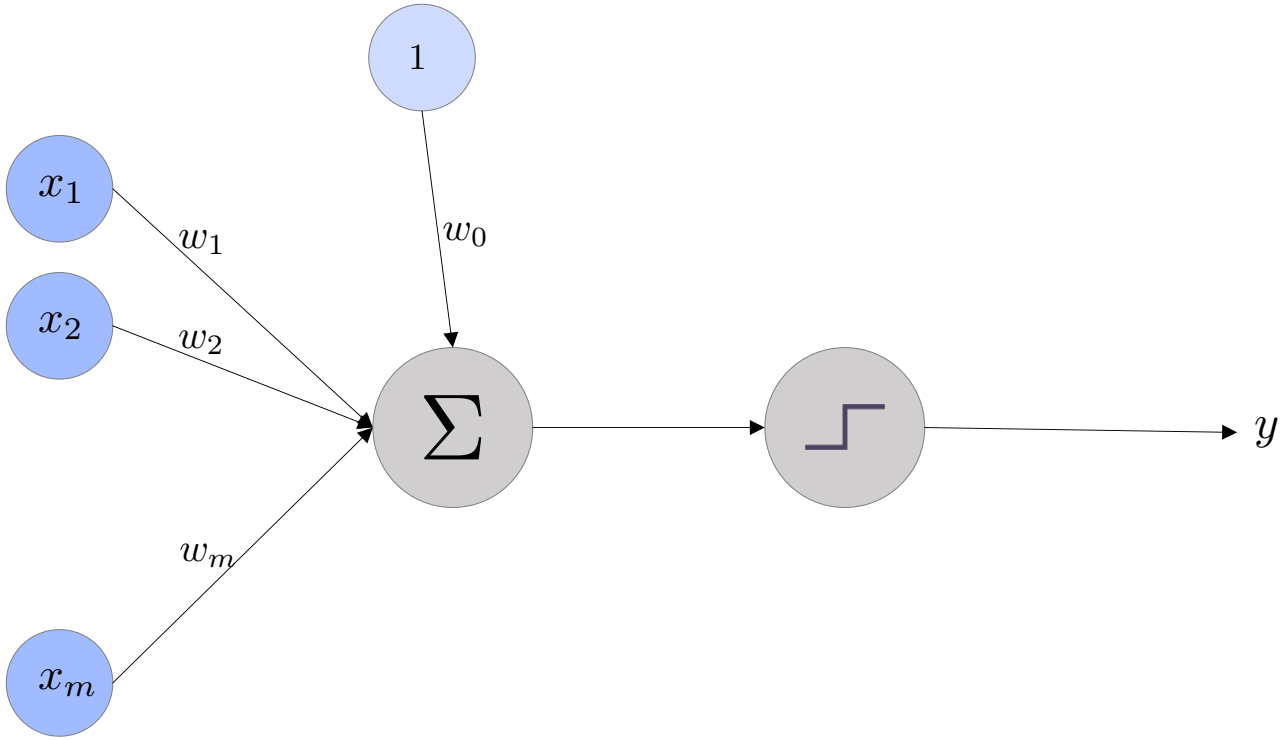
Towards the Single Layer Perceptron



$$f_{\mathbf{w},\theta} : \mathbb{R}^m \rightarrow \mathbb{R}$$

$$y = f_{\mathbf{w},\theta}(\mathbf{x}) = \begin{cases} 1 & \text{if } \mathbf{w}^\intercal \mathbf{x} > \theta \\ 0 & \text{otherwise} \end{cases}$$

Towards the Single Layer Perceptron



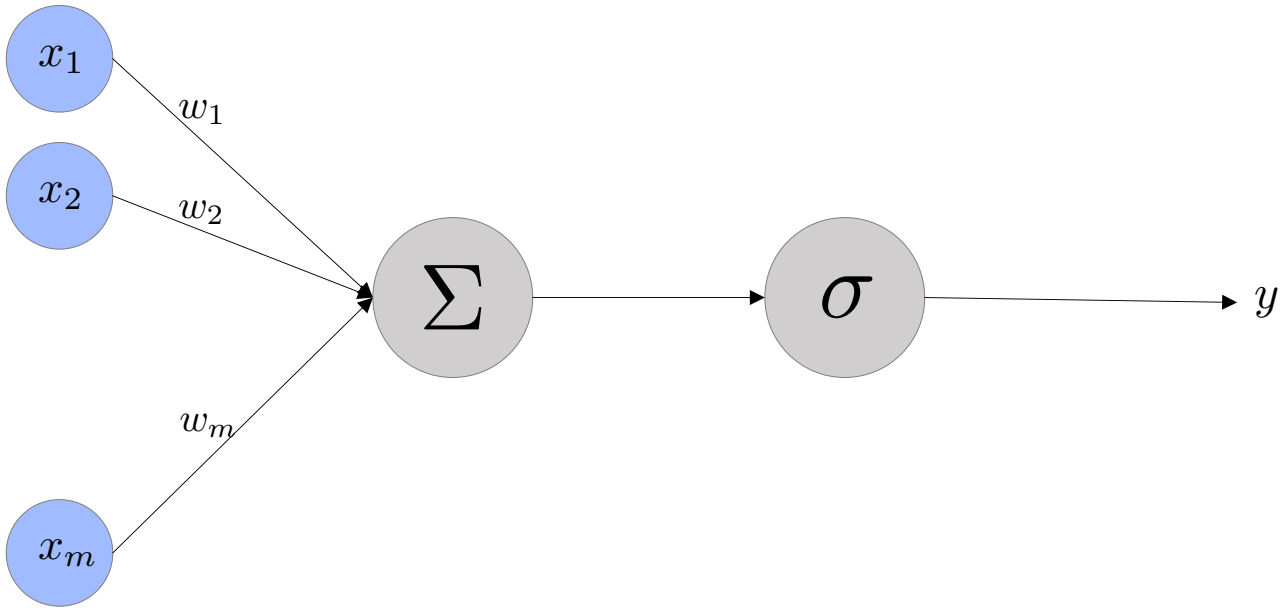
$$f_{\mathbf{w},\theta} : \mathbb{R}^m \rightarrow \mathbb{R}$$

$$y = f_{\mathbf{w},\theta}(\mathbf{x}) = \begin{cases} 1 & \text{if } \mathbf{w}^\intercal [1, \mathbf{x}] > \theta \\ 0 & \text{otherwise} \end{cases}$$

From now on we will use as standard the notation $\mathbf{w}^\intercal \mathbf{x}$

It means that we assume the presence of the bias term to be addressed

Towards the Single Layer Perceptron

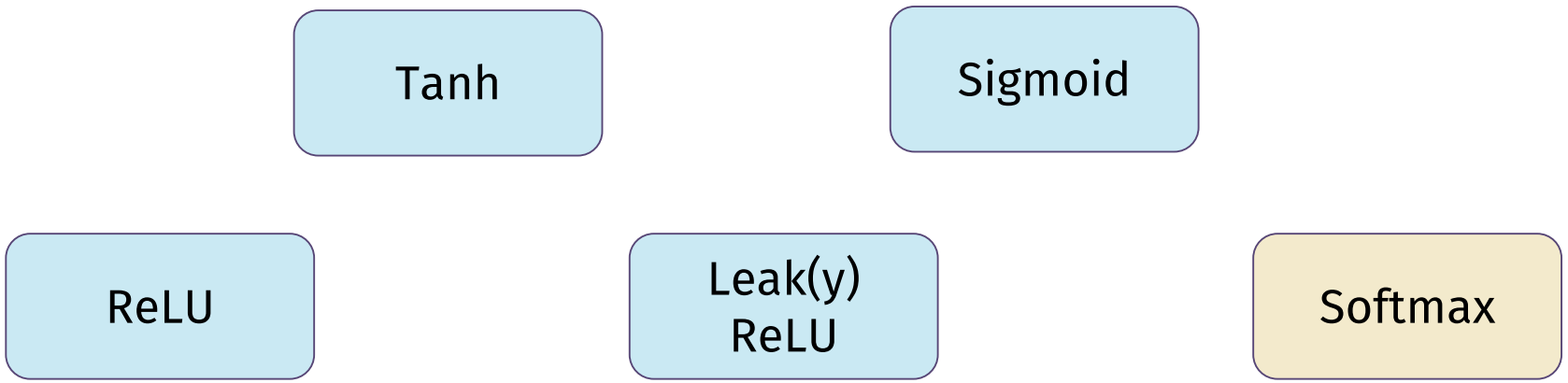


$$f_{\mathbf{w},\sigma} : \mathbb{R}^m \rightarrow \mathbb{R}$$

$$y = f_{\mathbf{w},\sigma}(\mathbf{x}) = \sigma(\mathbf{w}^\intercal \mathbf{x})$$

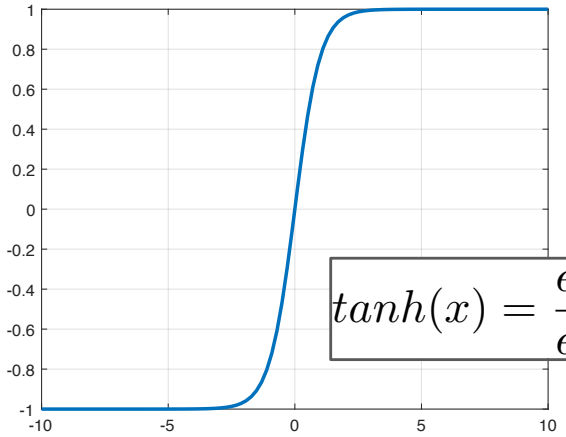
Non-Linear activation functions

- Nonlinear activation is key to achieving good function approximation
- It takes a single number and maps it to a different numerical value
- Popular functions



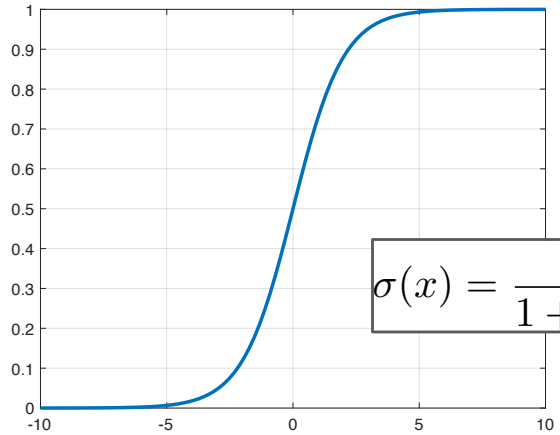
To practice with non-linear activation functions: https://playground.tensorflow.org/

Non-linear Activation functions



$$tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} = 2\sigma(2x) - 1$$

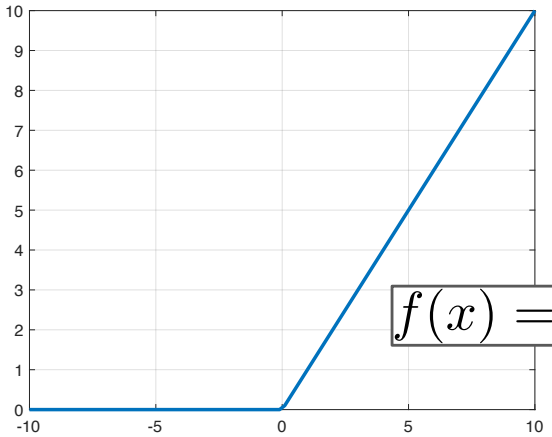
Tanh



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

Sigmoid

ReLU

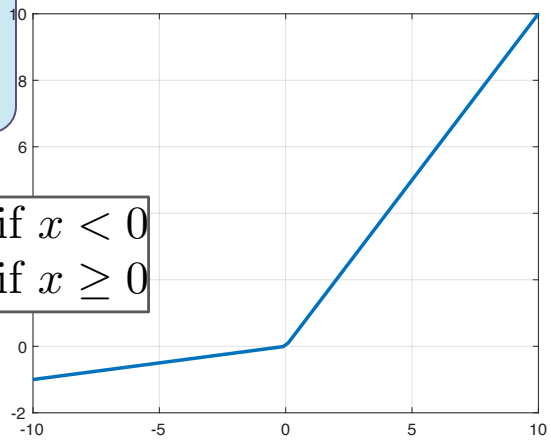


$$f(x) = max(0, x)$$

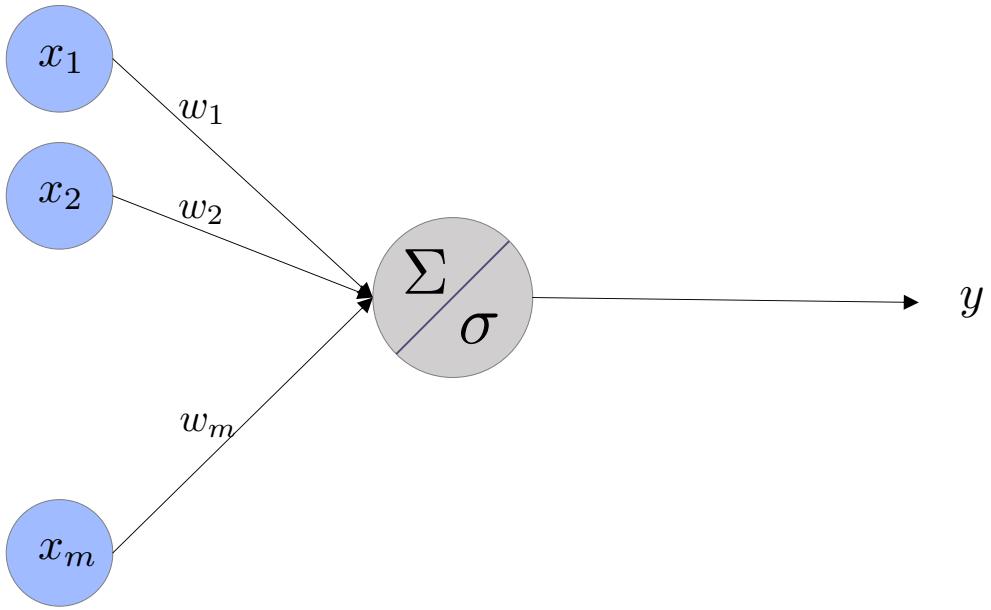
Leak(y) ReLU

$$f(x) = \begin{cases} \alpha x & \text{if } x < 0 \\ x & \text{if } x \geq 0 \end{cases}$$

$$\alpha = 0.1$$



Towards the Single Layer Perceptron



$$f_{\mathbf{w},\sigma} : \mathbb{R}^m \rightarrow \mathbb{R}$$

$$y = f_{\mathbf{w},\sigma}(\mathbf{x}) = \sigma(\mathbf{w}^\intercal \mathbf{x})$$

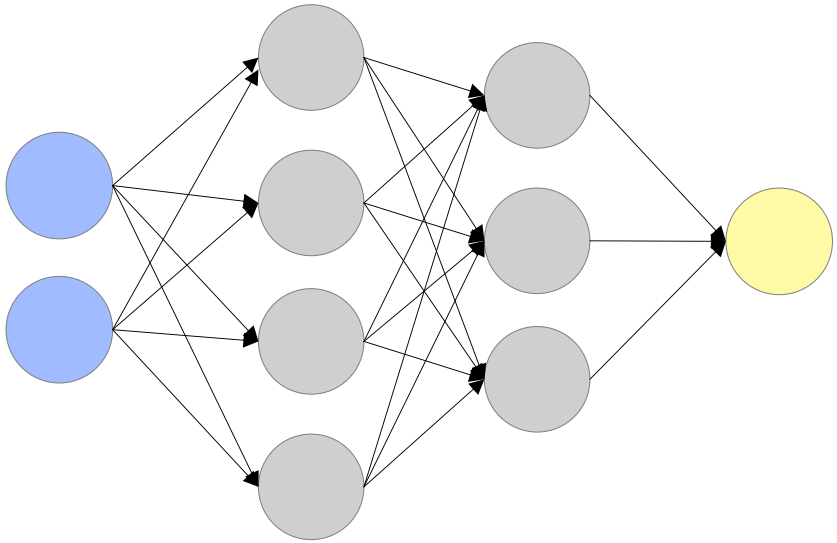
Basic Neural Networks

Neural Networks

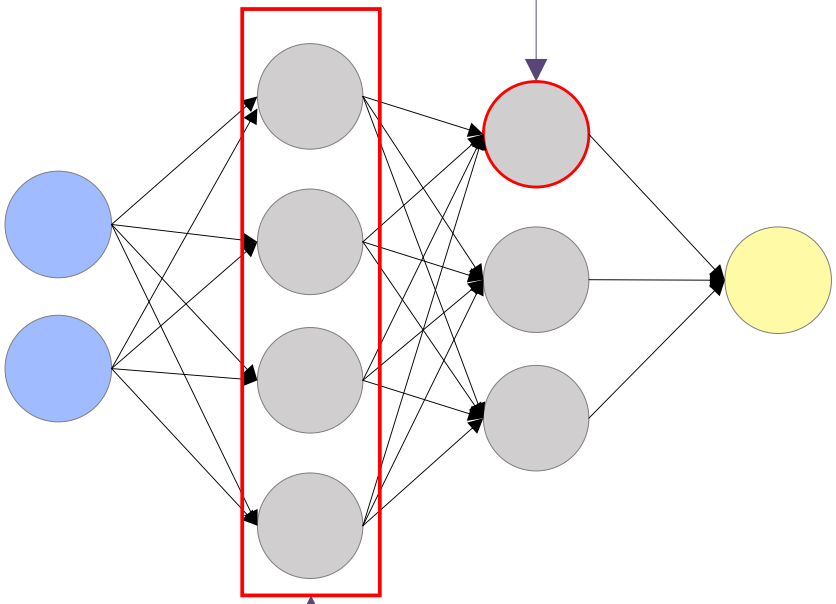
Neural Networks are composed of chains of layers that may be of three different types:

- INPUT LAYER
- (MULTIPLE) HIDDEN LAYER(S)
- OUTPUT LAYER

The layers are fully connected



Neural Networks



Each element of the layer plays the role of a neuron

The central layers are hidden. i.e. the intermediate output is not explicitly shown

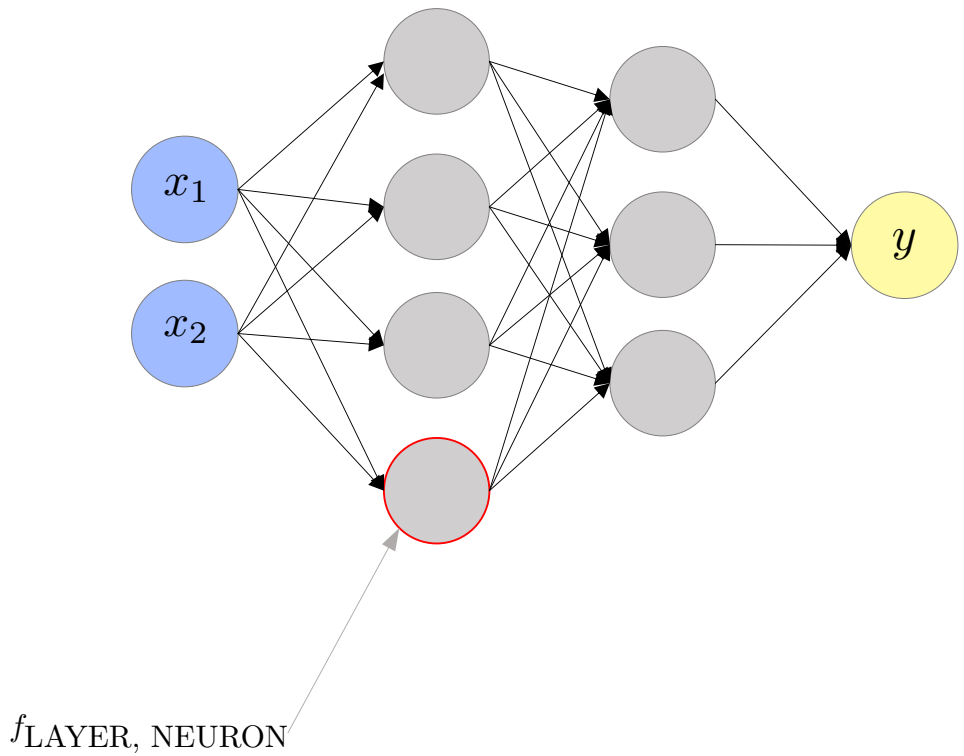
The dimensionality of the hidden layers determine the width

The depth is the number of hidden layers

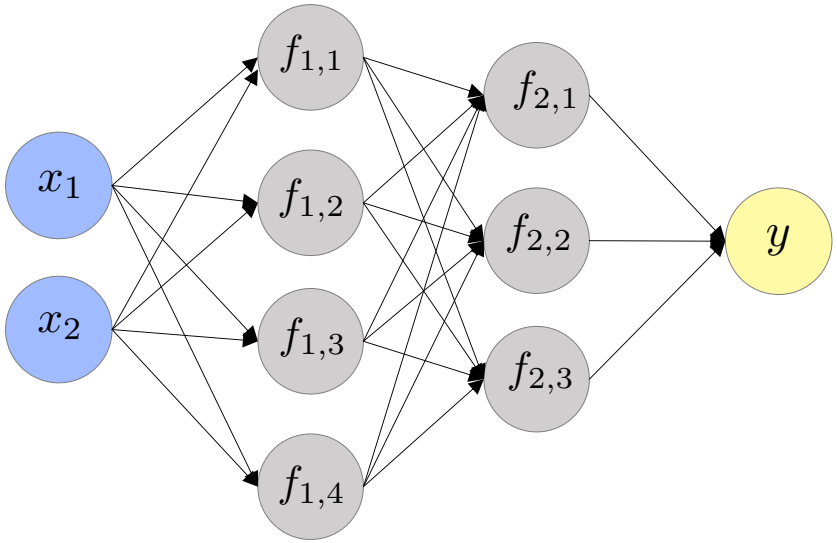
One network, two phases

- Forward propagation: the input flows into the network and produces a cost
- Backward propagation: allows the info to flow back into the net to compute the gradient (during the optimization)

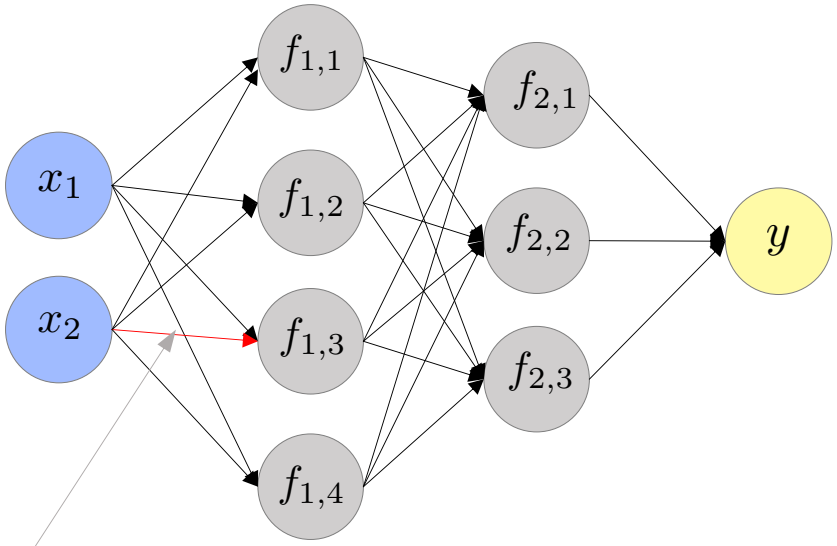
Forward propagation



Forward propagation

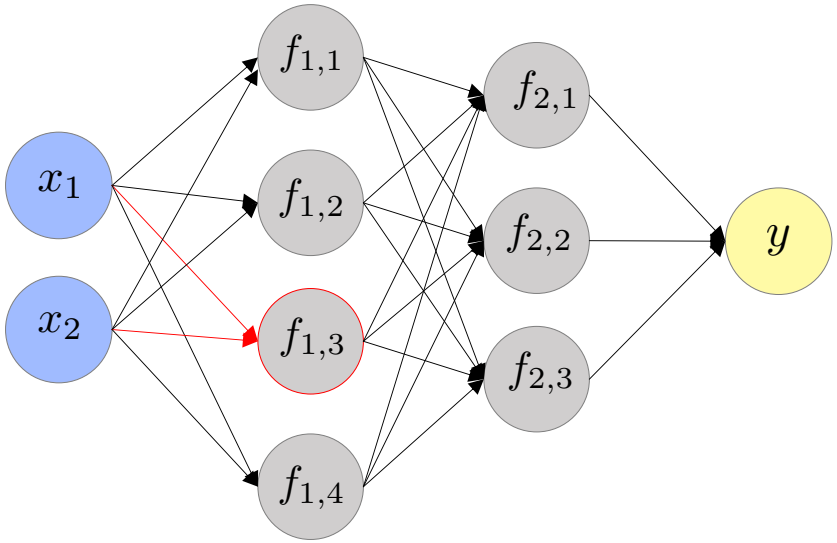


Forward propagation



$w_{(layer,In,Out)}$

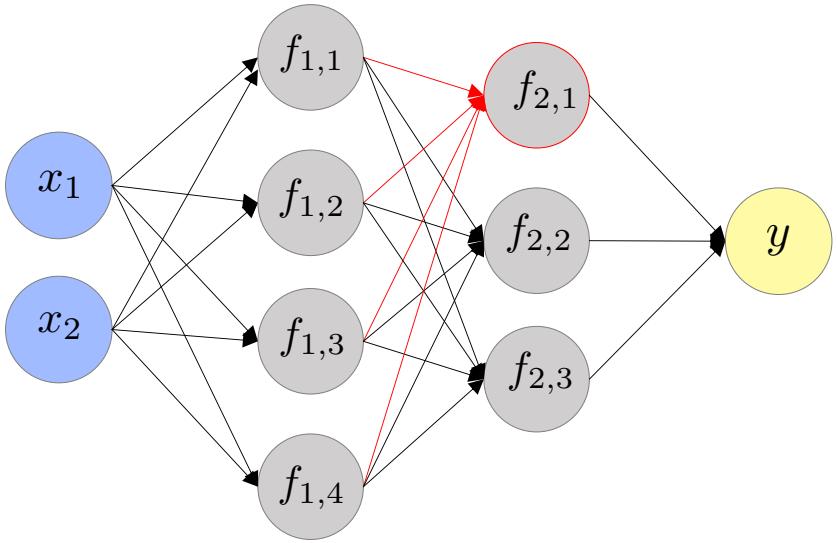
Forward propagation



$$f_{1,3}(\mathbf{x}) = \sigma(\mathbf{w}^{\intercal}_{(1,:,3)}\mathbf{x})$$

$$\mathbf{w}_{(1,:,3)} = [w_{(1,1,3)}w_{(1,2,3)}]$$

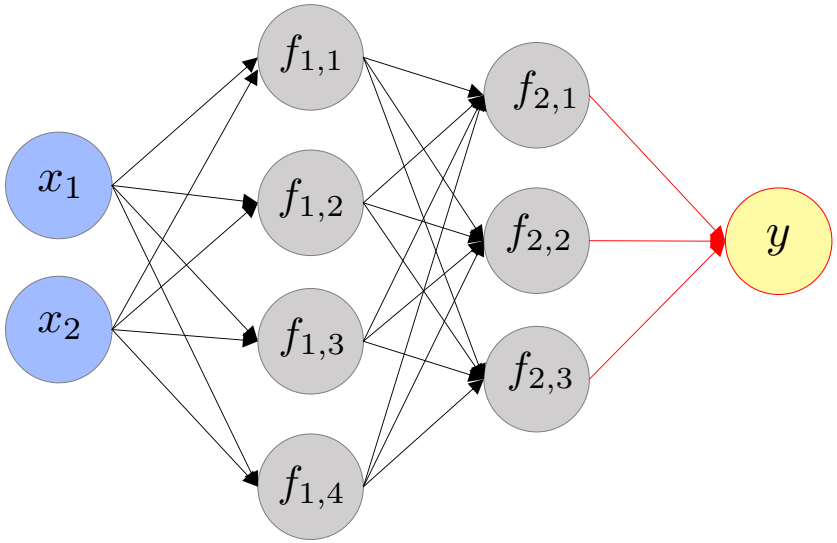
Forward propagation



$$f_{2,1}(\mathbf{f}_{(1,:)}) = \sigma(\mathbf{w}^{\mathsf{T}}_{(2,:,1)}\mathbf{f}_{(1,:)})$$

$$\mathbf{f}_{(1,:)} = [f_{1,1}f_{1,2}f_{1,3}f_{1,4}]$$

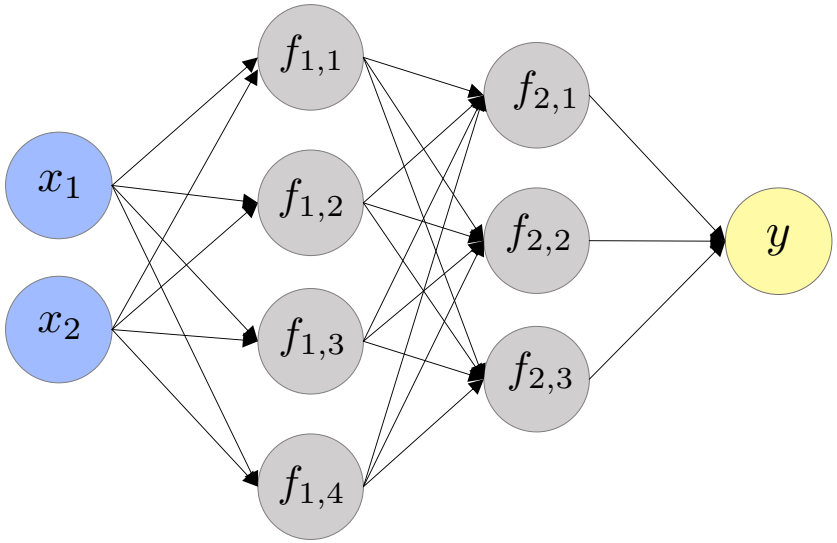
Forward propagation



$$y = \sigma(\mathbf{w}^{\intercal}_{(o,:)}\mathbf{f}_{(2,:)})$$

$$\mathbf{f}_{(2,:)} = [f_{2,1}f_{2,2}f_{2,3}]$$

Forward propagation



... hence, In this example... $f_{\mathbf{w}} : \mathbb{R}^2 \rightarrow \mathbb{R}$

$\mathbf{w} \in \mathbb{R}^{23+8}$

Bias terms

weights

How to train a [Deep] Neural Network

Training a Neural Network

- Training a (Deep) Neural Network means (as usual) learning the values for the model parameters (weights, bias terms) from the training set

- An essential element of training is (as usual) the loss function, which estimates how much we lose with the prediction in place of the real output y

$$\ell : Y \times Y \rightarrow [0, +\infty]$$

where Y is the space of the output of the estimated function

$$f_{\mathbf{w}} : X \rightarrow Y$$

Training a Neural Network

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$$f_{\mathbf{w}} : X \rightarrow Y$$

Binary classification

$$f_{\mathbf{w}} : \mathbb{R}^m \rightarrow \{-1, 1\}$$

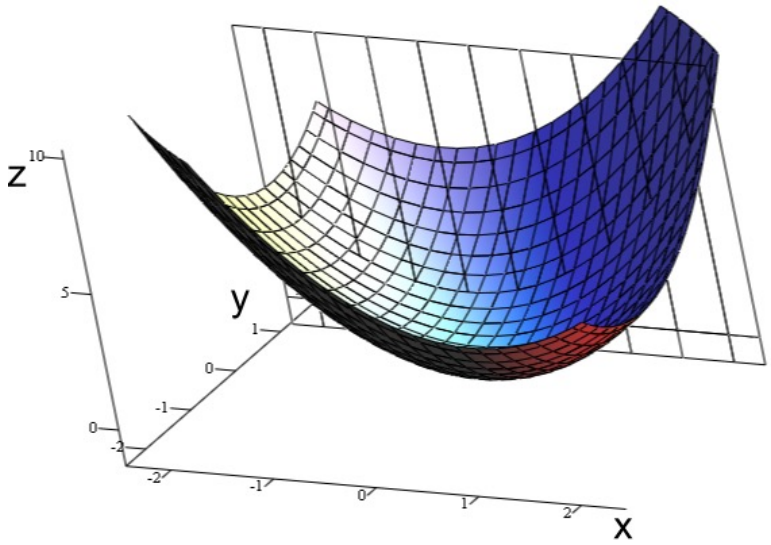
Multi-class classification (with M classes)

$$f_{\mathbf{w}} : \mathbb{R}^m \rightarrow \{0, \ldots, M-1\}$$

(Scalar) regression

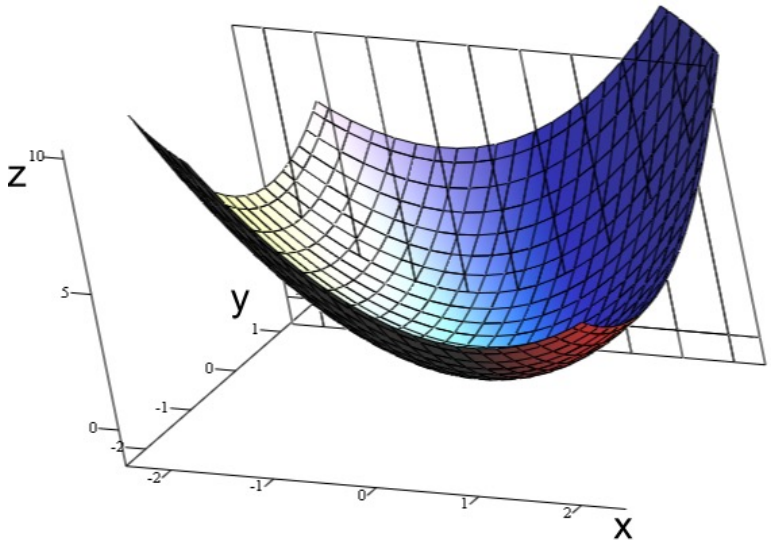
$$f_{\mathbf{w}} : \mathbb{R}^m \rightarrow \mathbb{R}$$

Training a deep NN is not...

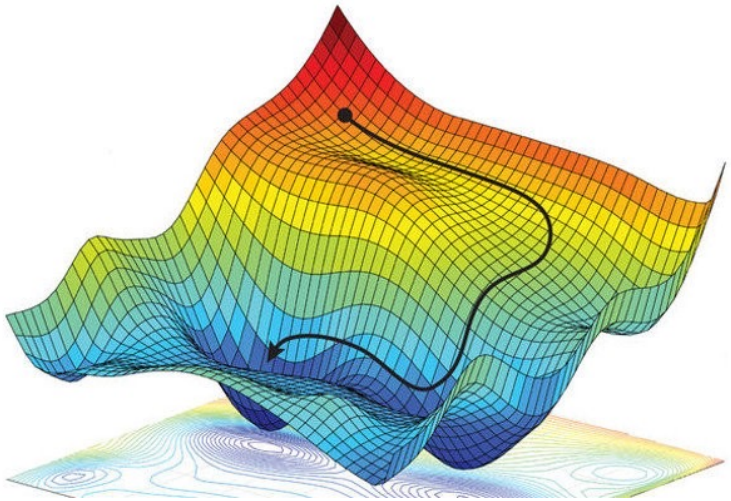


https://towardsdatascience.com/understand-convexity-in-optimization-db87653bf920?gi=b93b0698a062
https://medium.com/swlh/non-convex-optimization-in-deep-learning-26fa30a2b2b3

Training a deep NN is not...



...but more like...



https://towardsdatascience.com/understand-convexity-in-optimization-db87653bf920?gi=b93b0698a062
https://medium.com/swlh/non-convex-optimization-in-deep-learning-26fa30a2b2b3

Training a Neural Network

$$\mathbf{w}^* = \arg\min_{\mathbf{w}\in\mathbb{R}^P} \frac{1}{n}\sum_{i=1}^{n} \ell(f_{\mathbf{w}}(\mathbf{x}^i), y^i)$$

Total number of model parameters

$$\mathbf{x}^i \in X$$

$$y^i \in Y$$

Training set $S = \{\mathbf{x}^i, y^i\}_{i=1}^n$

Training a Neural Network

$$\mathbf{w}^* = \arg\min_{\mathbf{w}\in\mathbb{R}^P} \frac{1}{n}\sum_{i=1}^{n} \ell(f_{\mathbf{w}}(\mathbf{x}^i), y^i)[+\lambda\Psi(f_{\mathbf{w}})]$$

Total number of model parameters

Regularization term

$$\mathbf{x}^i \in X$$

$$y^i \in Y$$

Training set $S = \{\mathbf{x}^i, y^i\}_{i=1}^n$

Training a Neural Network

$$\mathbf{w}^* = \arg\min_{\mathbf{w}\in\mathbb{R}^P} \frac{1}{n}\sum_{i=1}^{n} \ell(f_{\mathbf{w}}(\mathbf{x}^i), y^i)[+\lambda\Psi(f_{\mathbf{w}})]$$

Total number of model parameters

$$\mathbf{x}^i \in X$$

$$y^i \in Y$$

Regularization term

Training set $S = \{\mathbf{x}^i, y^i\}_{i=1}^n$

$$\mathbf{w}^* = \arg\min_{\mathbf{w}\in\mathbb{R}^P} J(S; \mathbf{w})$$

To find the parameters we need an optimization strategy

Training a Neural Network

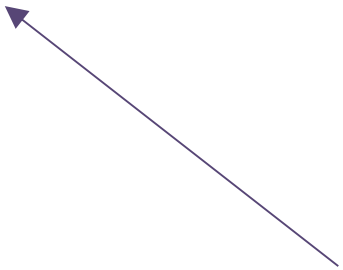
$$\mathbf{w}^* = \arg\min_{\mathbf{w} \in \mathbb{R}^P} J(S; \mathbf{w})$$

- We may resort to iterative approaches → Gradient Descent

$$\mathbf{w}_0 = 0$$

Or with random values

$$\mathbf{w}_t = \mathbf{w}_{t-1} - \gamma \nabla J(S; \mathbf{w}_{t-1})$$



- We need to compute the gradient of a possibly very complex function!

One network, two phases

- Forward propagation: the input flows into the network and produces a cost
- Backward propagation: allows the info to flow back into the net to compute the gradient (during the optimization)

Training a DNN

Back-propagation

- Backpropagation (1960s) aims to minimize the cost function by adjusting the weights and biases of the networks
- The level of adjustment is determined by the gradients of the cost function with respect to those parameters.
- The goal of backpropagation is to compute the partial derivatives of the cost function with respect to any parameter in the network.

Training a DNN

Back-propagation

- A key ingredient of back-propagation is the chain rule of derivation

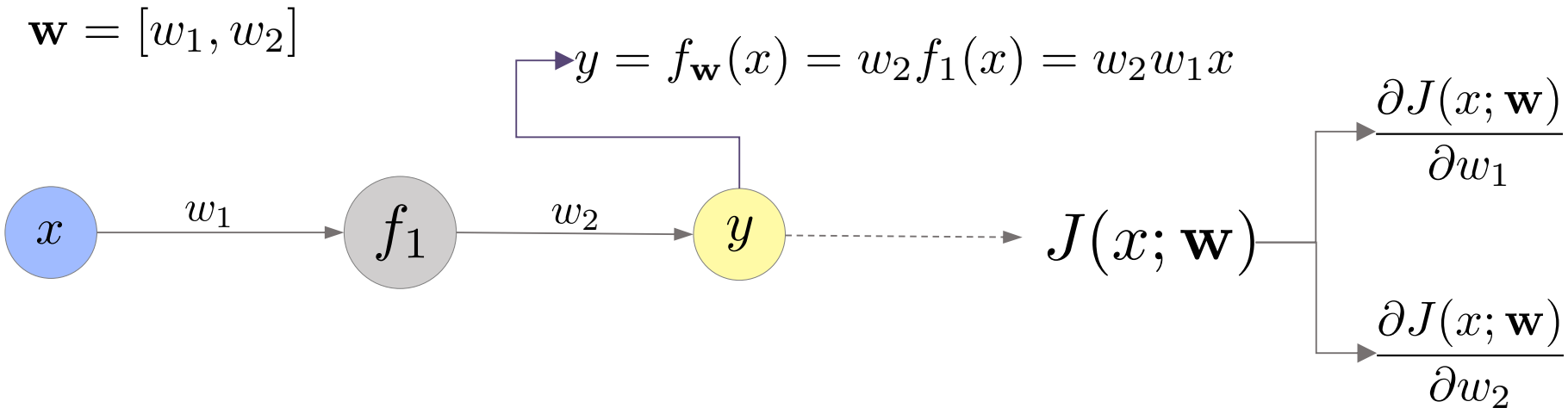
- Example: is F is a composite function such that

$$F = f \circ g \circ h \circ u \circ v$$

then

$$\frac{\partial F(x)}{\partial x} = \frac{\partial f(g(h(u(v(x)))))}{\partial x} = \frac{\partial f}{\partial g}\frac{\partial g}{\partial h}\frac{\partial h}{\partial u}\frac{\partial u}{\partial v}\frac{\partial v}{\partial x}$$

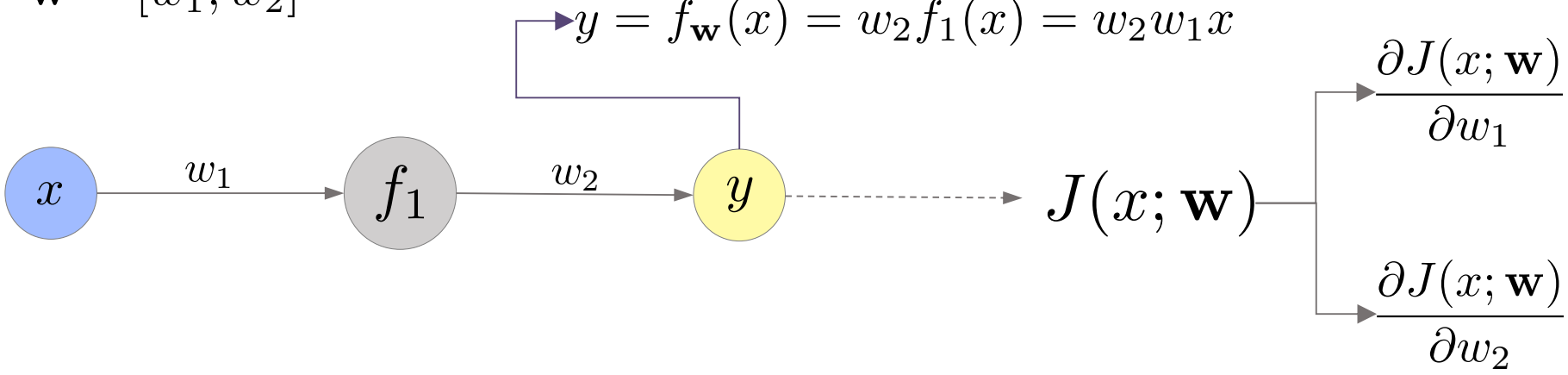
Backpropagation: example 1



From http://introtodeeplearning.com/slides/6S191_MIT_DeepLearning_L1.pdf

Backpropagation: example 1

$$\mathbf{w} = [w_1, w_2]$$



$$\frac{\partial J(x; \mathbf{w})}{\partial w_1}$$

$$\frac{\partial J(x; \mathbf{w})}{\partial w_2}$$

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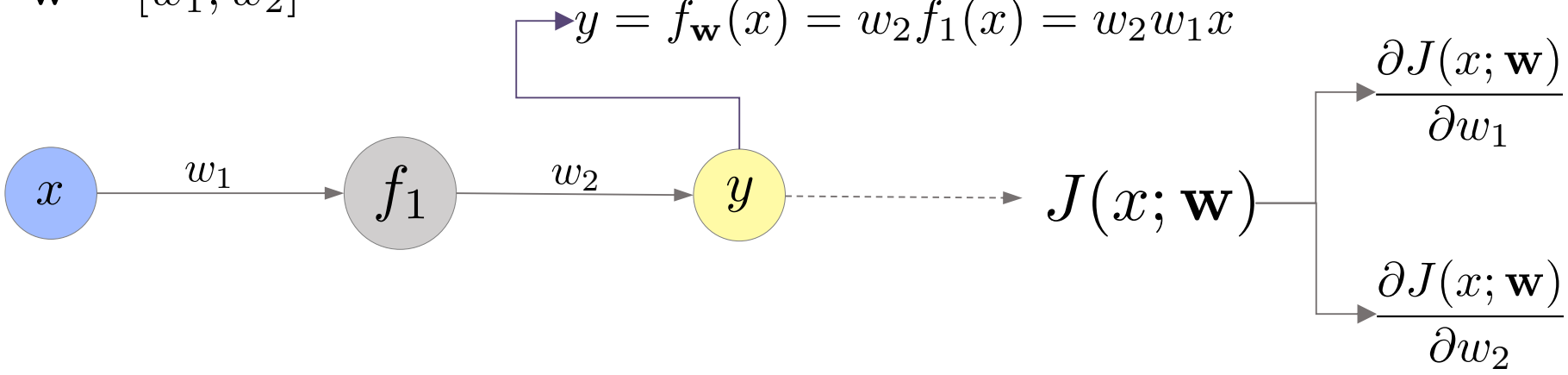
Backpropagation: example 1

$$\mathbf{w} = [w_1, w_2]$$



$$\frac{\partial J(x; \mathbf{w})}{\partial w_2} = \frac{\partial J(x; \mathbf{w})}{\partial f_{\mathbf{w}}(x)} \frac{\partial f_{\mathbf{w}}(x)}{\partial w_2}$$

$$\frac{\partial J(x; \mathbf{w})}{\partial w_2}$$

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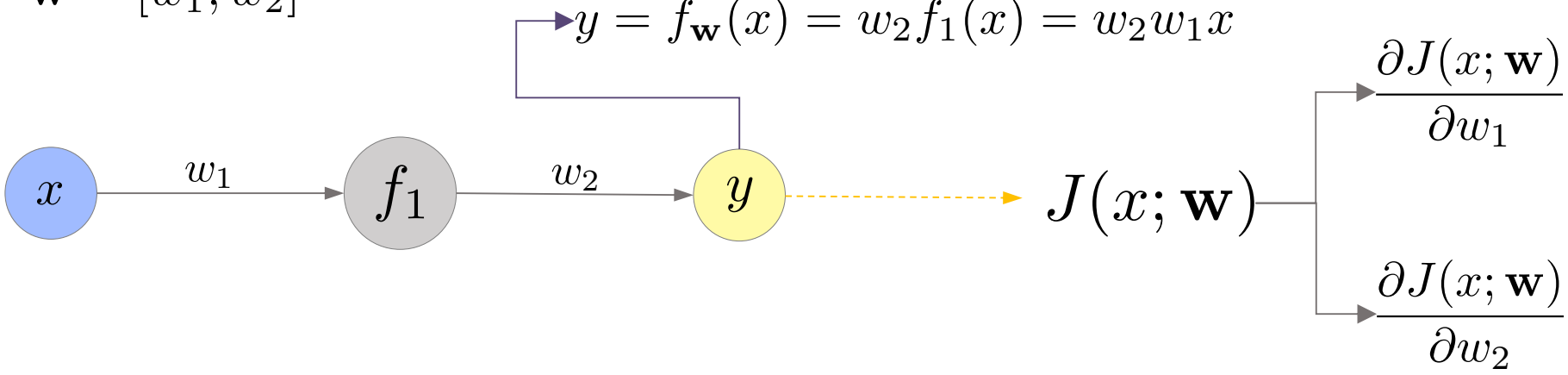

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From http://introtodeeplearning.com/slides/6S191_MIT_DeepLearning_L1.pdf

Backpropagation: example 1

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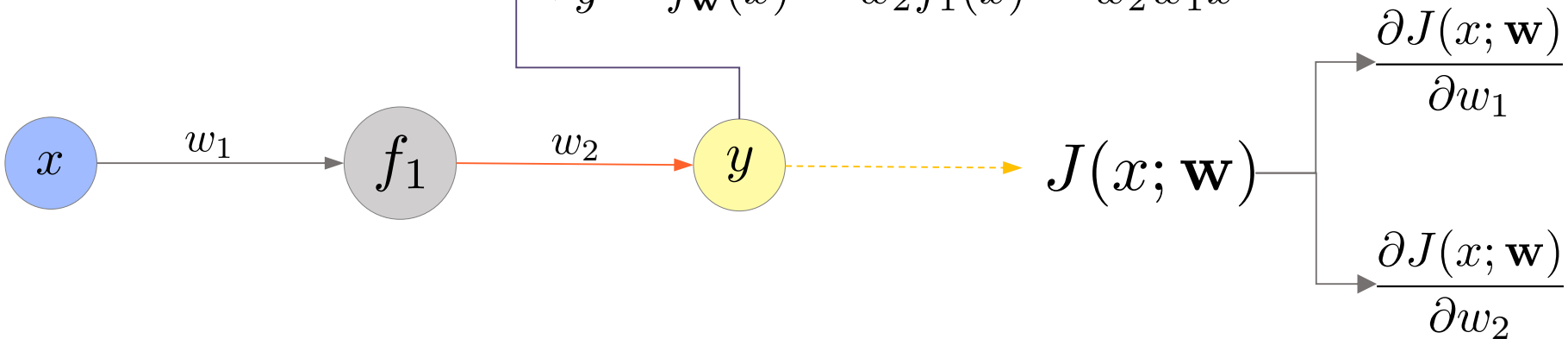

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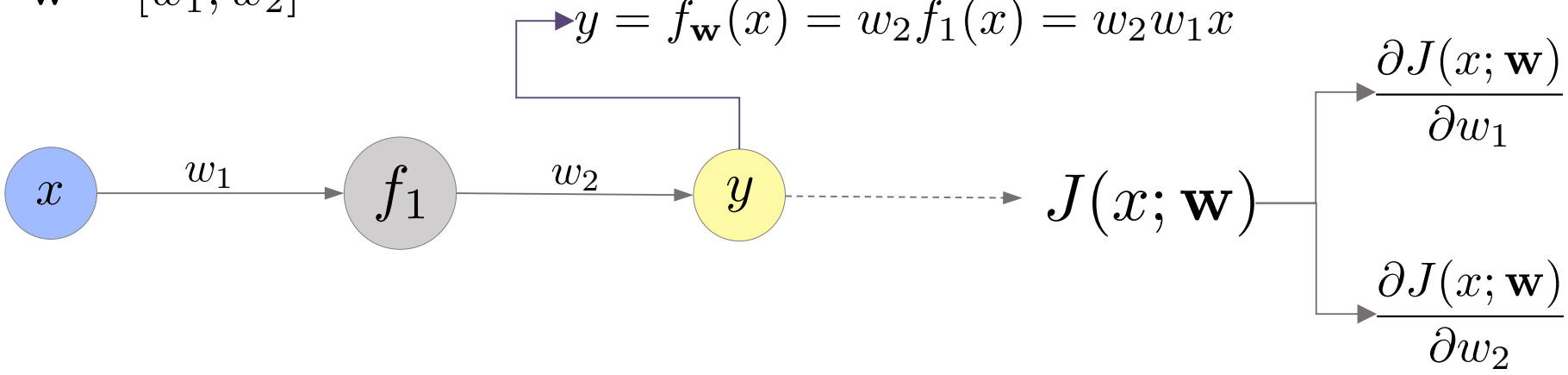

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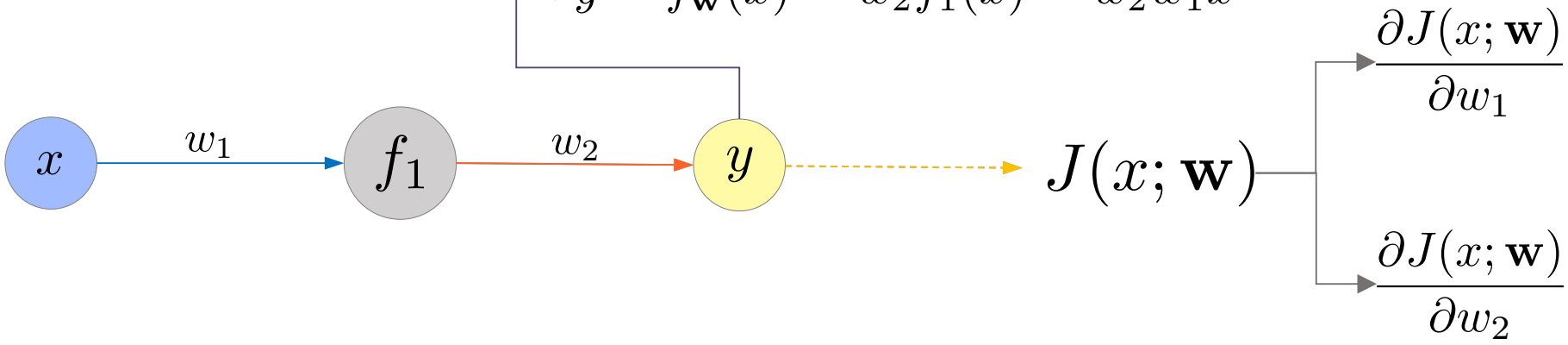

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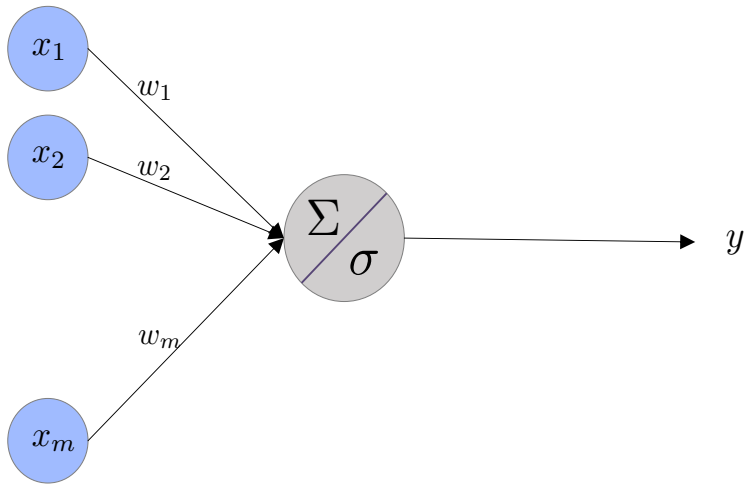
Backpropagation: example 2

- Let's consider the case where we have only one neuron, this time with a non-linearity
- Let's also assume we are using the square loss

$$\mathbf{x}^i \in X$$

$$y^i \in Y$$

Training set $S = \{\mathbf{x}^i, y^i\}_{i=1}^n$



$$J(S;\mathbf{w}) = \frac{1}{n}\sum_{i=1}^{n}(y^i - f_{\mathbf{w}}(\mathbf{x}^i))^2 =$$

$$= \frac{1}{n}\sum_{i=1}^{n}(y^i - f_{\sigma}(\mathbf{w}^\intercal \mathbf{x}^i))^2 =$$

$$= \frac{1}{n}\sum_{i=1}^{n}(y^i - \sigma(\mathbf{w}^\intercal \mathbf{x}^i))^2$$

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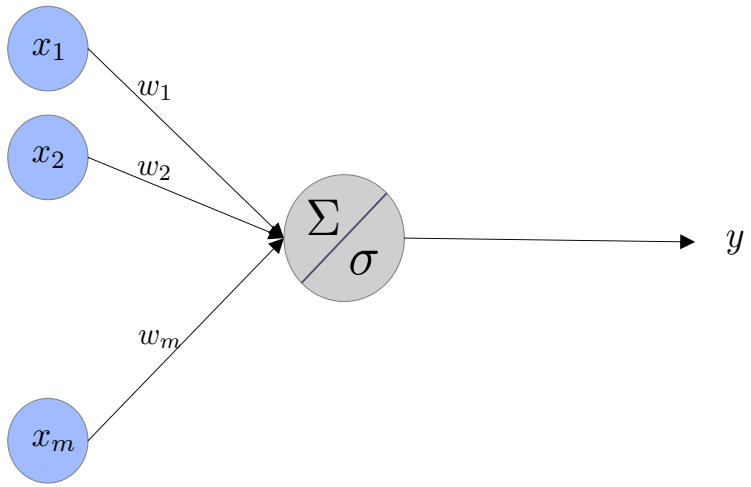

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For simplicity, we consider the cost function restricted to sample i

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$$J^i(\mathbf{w})$$

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We apply the chain rule of derivation

$$\frac{\partial J^i(\mathbf{w})}{\partial w_k} = \frac{\partial J^i(\mathbf{w})}{\partial f_\sigma(\mathbf{w}^\intercal \mathbf{x}^i)} \frac{\partial f_\sigma(\mathbf{w}^\intercal \mathbf{x}^i)}{\partial \mathbf{w}^\intercal \mathbf{x}^i} \frac{\partial \mathbf{w}^\intercal \mathbf{x}^i}{\partial w_k}$$

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Backpropagation: example 2

$$\frac{\partial J^i(\mathbf{w})}{\partial w_k} = \frac{\partial J^i(\mathbf{w})}{\partial f_\sigma(\mathbf{w}^\intercal \mathbf{x}^i)} \frac{\partial f_\sigma(\mathbf{w}^\intercal \mathbf{x}^i)}{\partial \mathbf{w}^\intercal \mathbf{x}^i} \frac{\partial \mathbf{w}^\intercal \mathbf{x}^i}{\partial w_k}$$

$$\frac{\partial \mathbf{w}^\intercal \mathbf{x}^i}{\partial w_k} = x_k$$

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Backpropagation: example 2

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This was for a single unit and a single sample

What to do for using all the samples?

What to do when we have multiple units?

Training a [Deep] Neural Network

A parenthesis on Gradient Descent algorithms

$$\mathbf{w}^* = \arg \min_{\mathbf{w} \in \mathbb{R}^P} J(S; \mathbf{w})$$

$$\mathbf{w}_0 = 0$$

$$\mathbf{w}_t = \mathbf{w}_{t-1} - \gamma \nabla J(S; \mathbf{w}_{t-1})$$

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Batch Gradient Descent (GD)

Smoothly converging towards the optimum, but computationally demanding

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known to converge well in practice: empirically, it provides a better exploration of the space

May require many iterations

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$$\mathbf{w}_t = \mathbf{w}_{t-1} - \gamma\nabla J(x^{[i:i+B]};\mathbf{w}_{t-1})$$

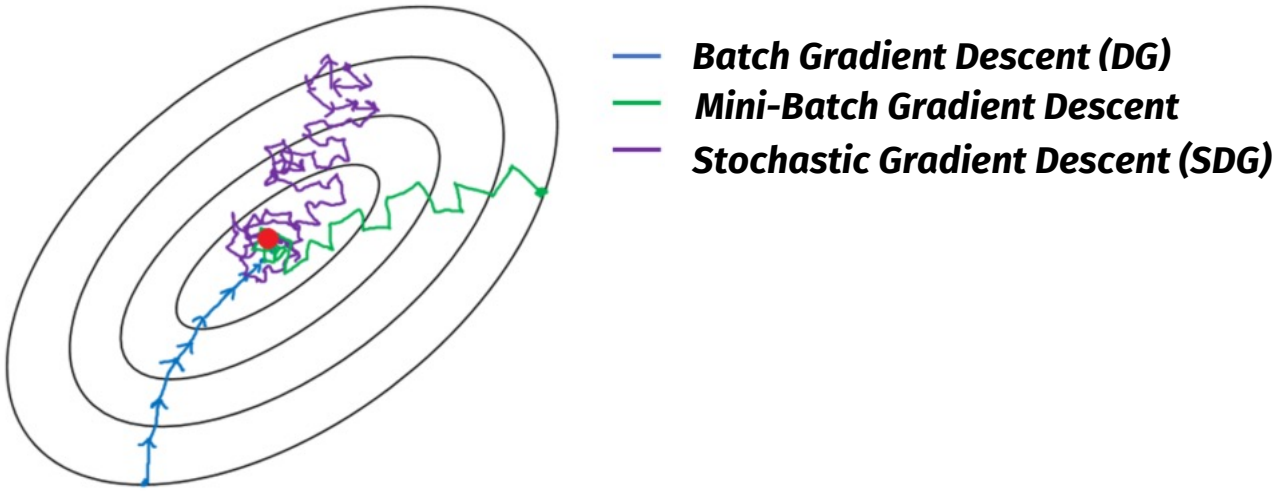
Mini-batch Gradient Descent

A good compromise

B is the mini-batch size (when B=1 you go back to SGD)

Training a [Deep] Neural Network

A parenthesis on Gradient Descent algorithms



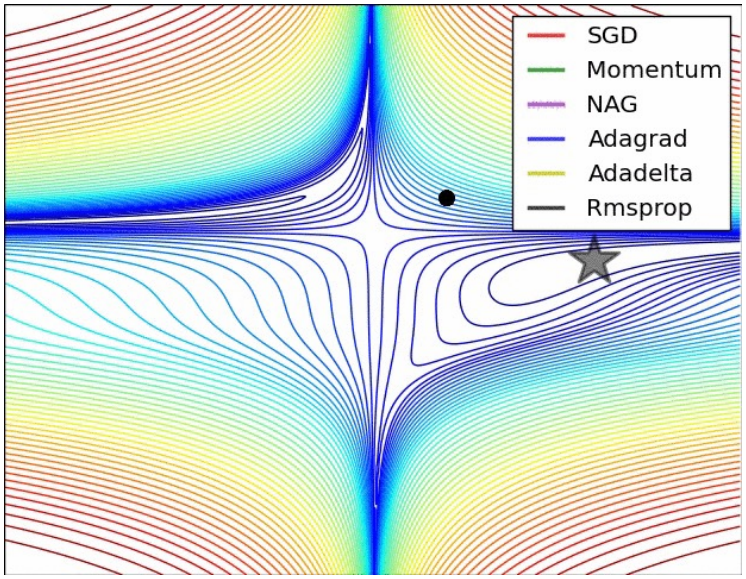
Picture from https://towardsdatascience.com/gradient-descent-algorithm-and-its-variants-10f652806a3

Training a [Deep] Neural Network

A parenthesis on Gradient Descent algorithms

Batch Gradient Descent (DG)
Mini-Batch Gradient Descent
Stochastic Gradient Descent (SDG)

There are also alternative optimization strategies…



Picture from https://towardsdatascience.com/gradient-descent-algorithm-and-its-variants-10f652806a3

Training a [Deep] Neural Network

A parenthesis on terminology

Given the complexity of deep models, it is necessary to go through the entire training set more than once at training time

One **epoch** is when the dataset is entirely passed forward and backwards through the architecture

The **[mini-]batch** size is the number of training samples in a mini-batch

An **iteration** is the number of batches needed to complete one epoch

→ Number of epochs and batch size are hyper-parameters of the model, usually set a priori

Training a [Deep] Neural Network

Model selection

What does it mean to perform model selection with this family of methods?

Training a [Deep] Neural Network

Model selection

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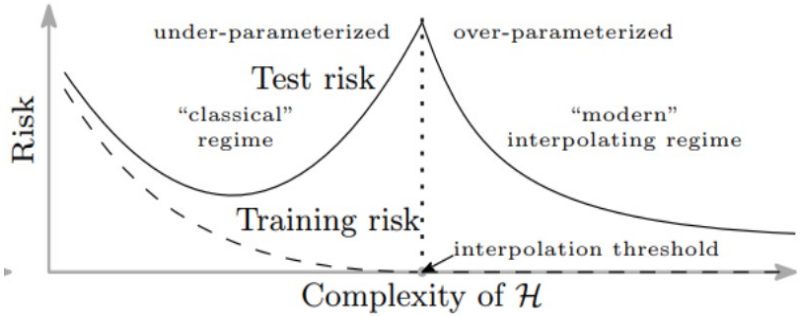
In principle, one could apply the same protocol adopted for more classical methods



What's the complexity here?

Training a [Deep] Neural Network

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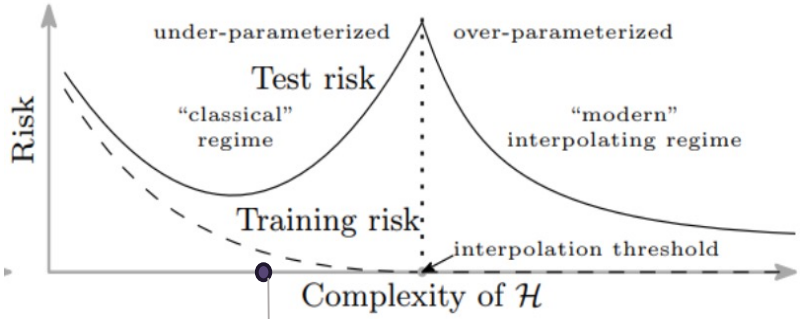
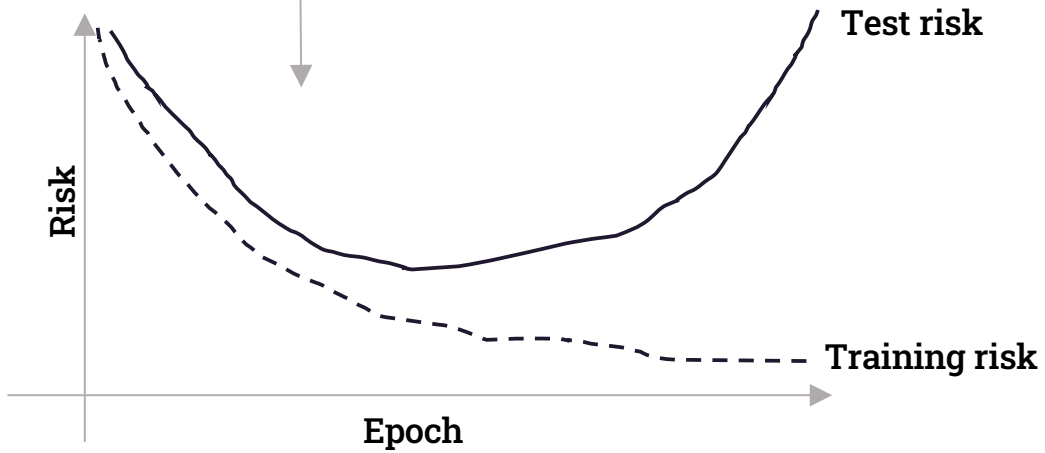


What's the complexity here?

In practice, we fix the model (i.e. a certain complexity) and, often, also the values of many (if not all) hyper-parameters; we reason on the training-validation error vs the number of epochs



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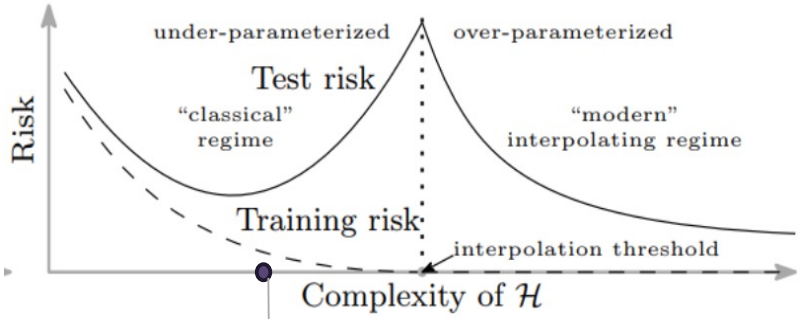

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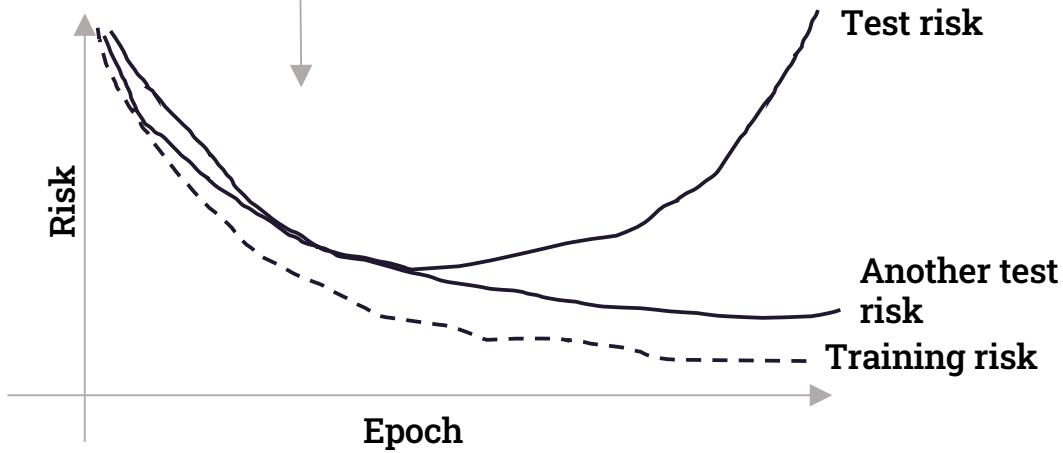


Training a [Deep] Neural Network

How to prevent overfitting

- Classical approaches can still be adopted:
  - Adding regularization terms
  - Using Early Stopping criterion

- One alternative (popular) option: Dropout

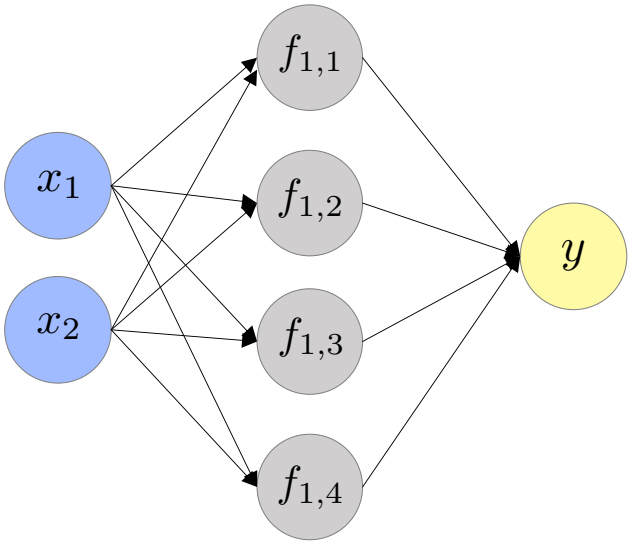
Training a [Deep] Neural Network

Dropout

- Overfitted DNN models tend to suffer from a problem of co-adaptation: models weights are adjusted co-linearly to learn the model training data too well… so the model doesn't generalize
- With limited training data weights likely become adapted to them, and the model doesn't generalize
- Bagging and Dropout are ways to break this co-adaptation

Training a [Deep] Neural Network

Bagging: intuition



P = 0.5

Training a [Deep] Neural Network

Bagging: intuition

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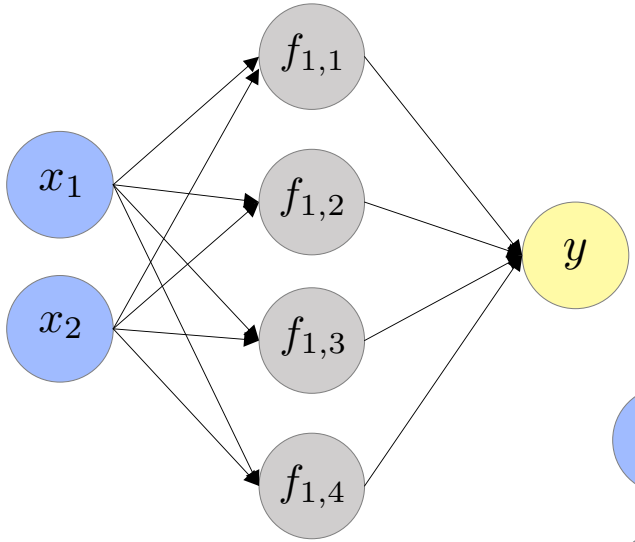

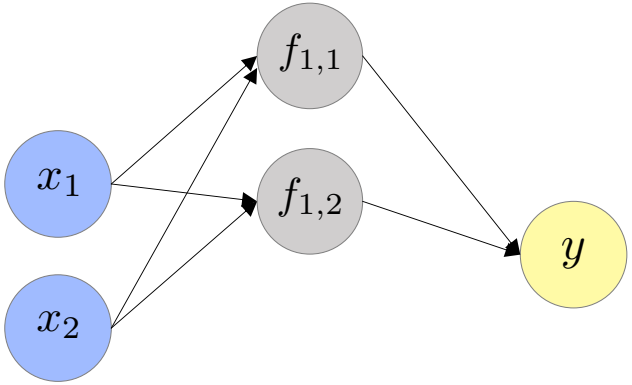

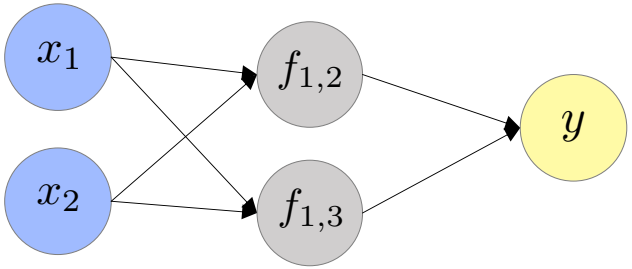

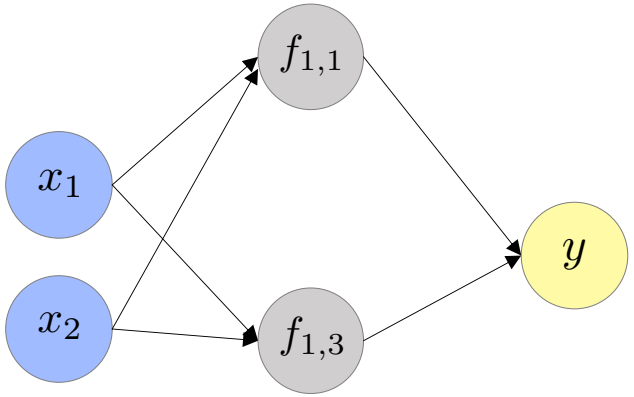

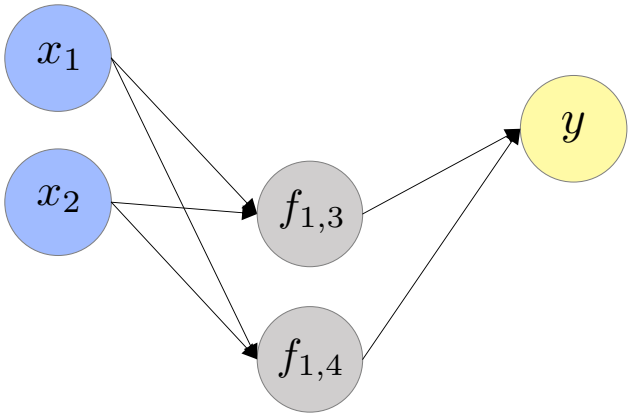

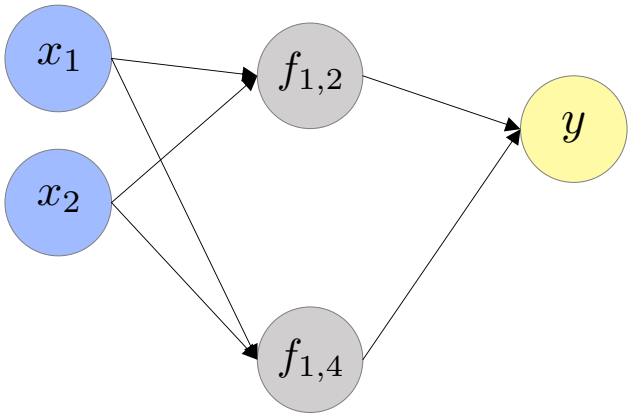

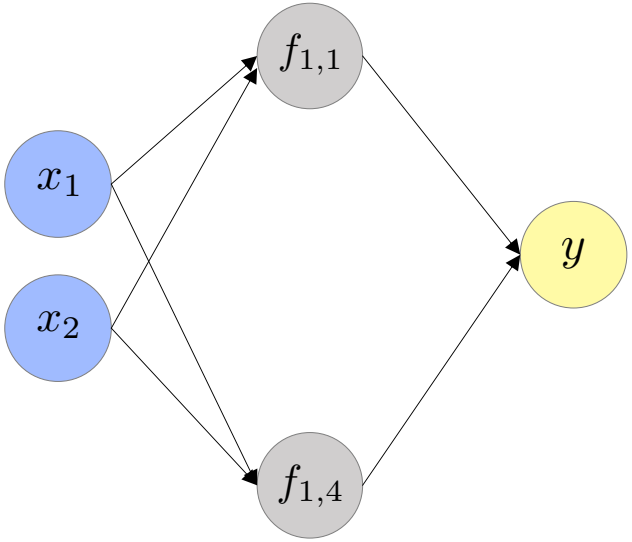

Training a [Deep] Neural Network

Bagging and Dropout

With Bagging

- Each sub-network is trained and evaluated on each test sample
- The final prediction is given by the votes of all models

Bagging may be computationally very expensive

Dropout is a way to approximate the same behaviour

→ At each step of the optimisation, some fraction of weights are dropped out of each layer (=set to 0)

UniGe | MaLGa

Some final considerations

Success with a price

- **Lots of parameters → REQUIRE → lots of data… Some important observations, among the others:**
  - Deep Networks are strongly computationally demanding
  - In many applications, it's not easy to have data
  - In general, it's not easy to have labelled data

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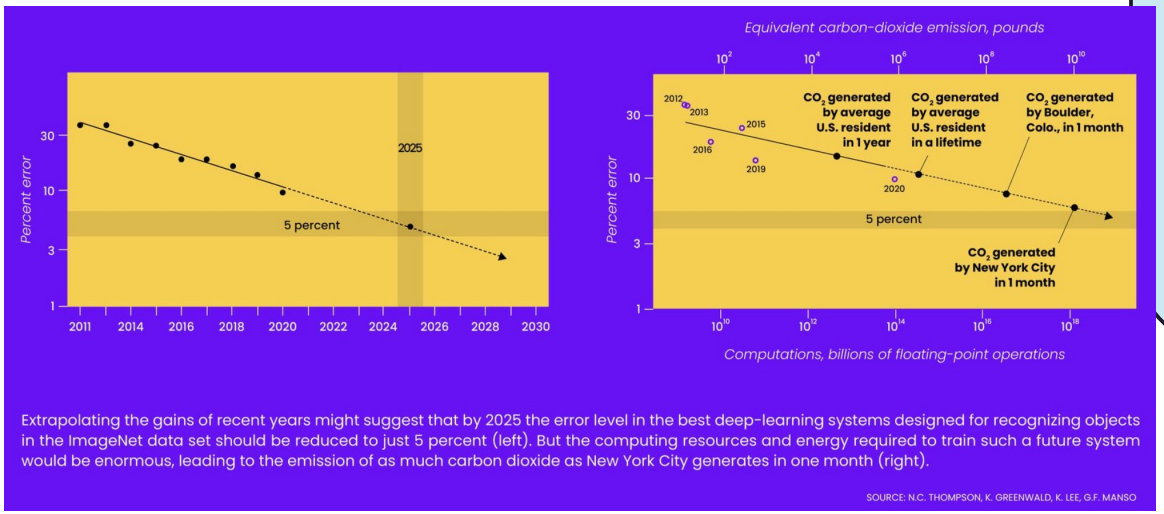

Extrapolating the gains of recent years might suggest that by 2025 the error level in the best deep-learning systems designed for recognizing objects in the ImageNet data set should be reduced to just 5 percent (left). But the computing resources and energy required to train such a future system would be enormous, leading to the emission of as much carbon dioxide as New York City generates in one month (right).

SOURCE: N.C. THOMPSON, K. GREENWALD, K. LEE, G.F. MANSO

Very well-established research directions aim at

- devising strategies for re-using knowledge
- synthetically augment the data
- Improving the efficiency of deep networks
- …

Success with a price

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  - Deep Networks are strongly computationally demanding
  - In many applications, it's not easy to have data
  - In general, it's not easy to have labelled data
- **Deep architectures are often designed and used as black-boxes**
  - Difficult to interpret the models
  - Difficult to explain their behaviours

Success with a price

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  - In general, it's not easy to have labelled data
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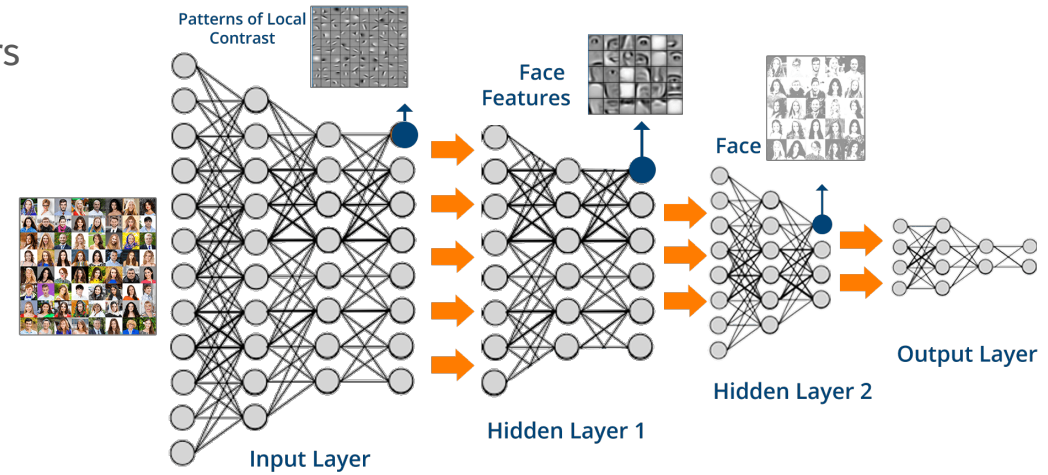

Success with a price

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- **Hard to encode prior knowledge**
- **A fully reliable theory is still largely missing… they work but sometimes we don't know exactly why**

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