

Deep Equilibrium Nets for Solving Dynamic Stochastic Models

University of Lugano, 25-26 June 2024

Lecture 1: Introduction to deep neural nets

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This course is inspired by Simon Scheidegger and based on his various teaching materials that I was relying on as a student and those which came as a result of our scientific collaboration

Course information, day 1

Day 1, Tuesday, June 25th, 2024

Time	Main Topics
09:00 - 10:20	Introduction to Machine Learning
10:20 - 10:40	Coffee Break
10:40 - 12:00	Introduction to Machine Learning (part II)
12:00 - 13:30	Lunch Break
13:30 - 14:50	A hands-on session
14:50 - 15:10	Coffee Break
15:10 - 16:30	A hands-on session

Course information, day 2

Day 2, Wednesday, June 26th, 2024

Time	Main Topics
09:00 - 10:20	Introduction to Machine Learning
10:20 - 10:40	Coffee Break
10:40 - 12:00	Introduction to Machine Learning (part II)
12:00 - 13:30	Lunch Break
13:30 - 14:50	A hands-on session
14:50 - 15:10	Coffee Break
15:10 - 16:30	A hands-on session

Course information, day 3

Day 3, Thursday, August 8th, 2024

Time	Main Topics
09:00 - 10:20	Hands-on debugging session, Q&A, part I
10:20 - 10:40	Coffee Break
10:40 - 12:00	Hands-on debugging session, Q&A, Part II

Most recent info and course materials

- **GitHub:** https://github.com/alexmalova/DEQN_lectures
- **Nuvolos** enrollement key:
https://app.nuvolos.cloud/enroll/class/VCHjgGm_ovs

Info about me

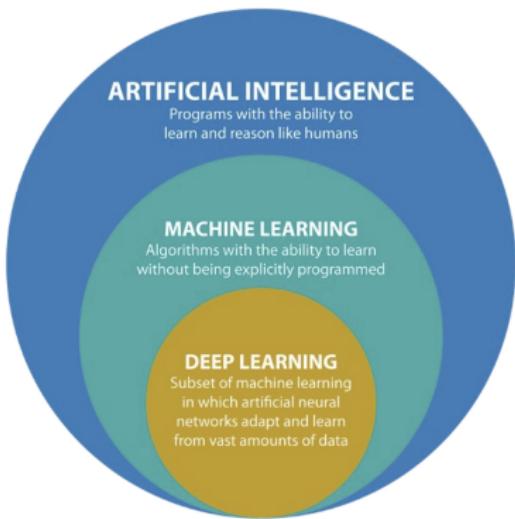
- **Assistant Professor** (non-tenure track) at the University of Munich,
Economist at ifo Institute
- **Ph.D. in Economics** from the University of Lausanne, 2023
(supervisors: *Simon Scheidegger, Kenza Benhima*)
- **Research interests:** macroeconomics of climate change, green energy transition, growth and development, applied quantitative economics
- **Webpage:** <https://sites.google.com/view/aleksandrafriedl>
- **Email:** friedl@ifo.de

Some terminology

- **Artificial Intelligence (AI)**: the effort to automate intellectual tasks normally performed by humans
- **Machine Learning (ML)**:



- **Deep Learning**: a particular example of an ML technique



figures from F. Chollet (2018)

Types of Machine Learning

- **Supervised learning:** the training data you feed to the algorithm includes the desired solutions, called labels
 - Classification: e.g. spam filter
 - Regression: e.g. car price based on car features
- **Unsupervised learning:** the training happens without labeling the data
 - Clustering: e.g. customer segmentation
- **Reinforcement learning:** the learning system, called an agent in this context, can observe the environment, select and perform actions, and get rewards in return

Building an ML algorithm I

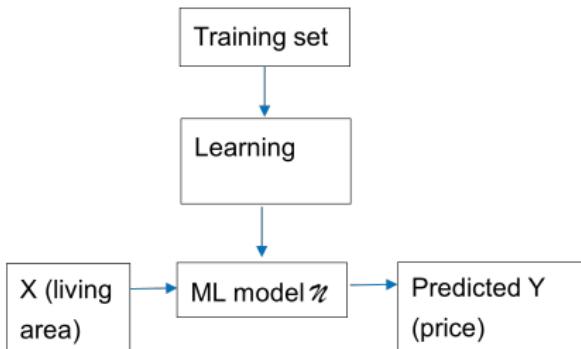
Living area (sq.feet)	Price (1000USD)
2104	400
1600	330
2400	369
1416	232
3000	540
...	...

Question

Given data like this, how can we learn to predict the prices of other houses as a function of the size of their living areas?

Building an ML algorithm II

- x_i **input variables** (input features)
- y_i **output variable** (target variable)
- (x_i, y_i) **training example**
- $\{(x_i, y_i) : i = 1, 2, 3, \dots, m\}$ **training set**



Training model

To perform supervised learning, we must decide how we're going to represent functions/hypotheses/model \mathcal{H} in a computer.

Building an ML algorithm II

- **Model:** $N_{\rho}(x) = \rho_0 + \rho_1 x_1$, where $\rho = (\rho_0, \rho_1)$ are parameters of the model
- **Cost (loss) function:** $J(\rho) = \frac{1}{m} \sum_{i=1}^m (N_{\rho}(x^{(i)}) - y^{(i)})^2$
- We want to minimize $J(\rho)$ to obtain coefficients ρ

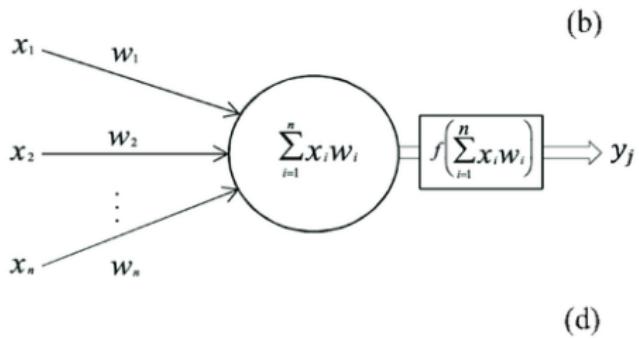
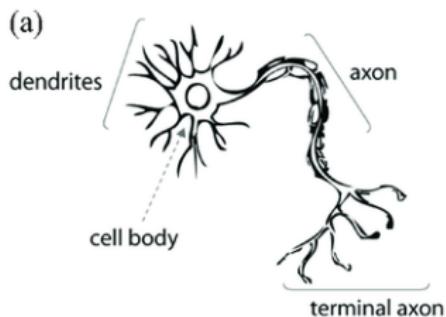
Available frameworks for ML

- Keras
- **Tensorflow**
- Pytorch
- Caffe
- Scikit-learn
- ... you name it

Outline of the presentation

- 1 Course information
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- 3 **Introduction to Artificial Neural Networks (ANNs)**
 - Building a NN
 - Loss function
 - (Stochastic) Gradient Descent
 - Backpropagation
- 4 Practical session

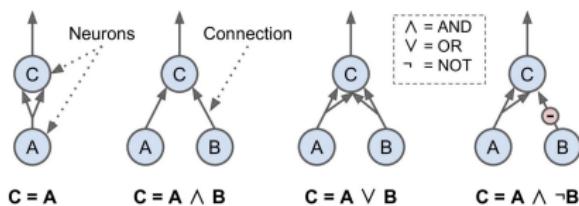
Artificial Neural Networks



[Meng, Hu, and Ancey(2020)]

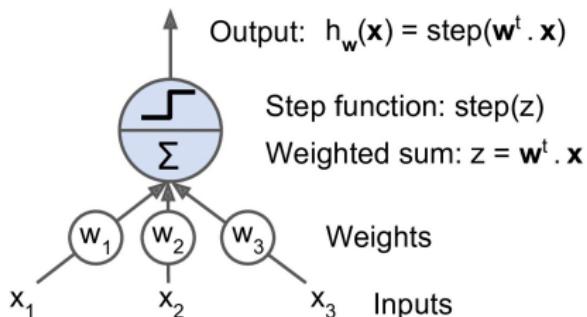
First artificial neuron (1943)

- McCulloch and Pitts' (1943) suggested a first mathematical model of a neuron:
 - one or more binary (on/off) inputs and one binary output
 - The artificial neuron simply activates its output when more than a certain number of its inputs are active.

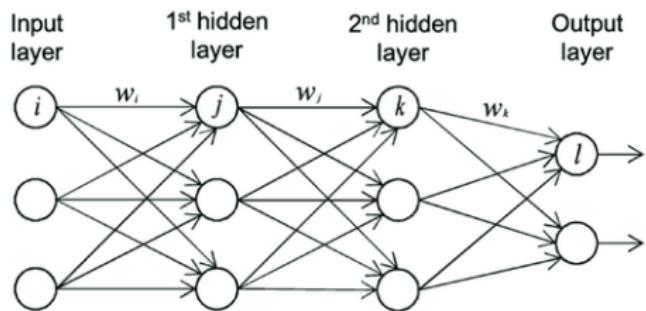
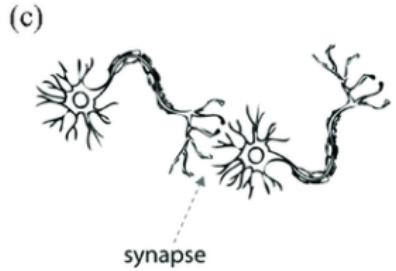
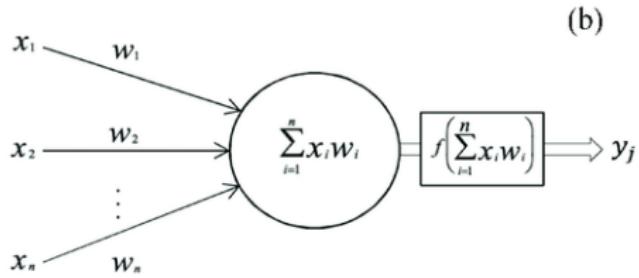
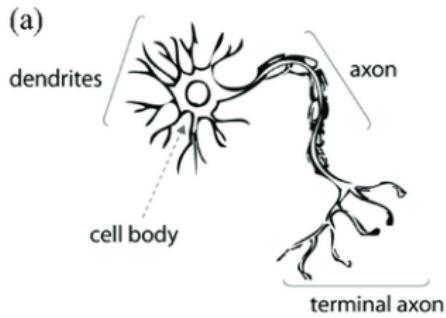


Perceptron (1957)

- Frank Rosenblatt (1957) suggested a simplest ANN architecture.
- The inputs x_i are multiplied by the weights w_i , and the neurons sum their values as z .
- If this sum is greater than the threshold ($\text{step}(z)$) then the neuron fires
- Neuron training:
 $w_{i,j}^{\text{next}} = w_{i,j} + \eta (\hat{y}_j - y_j) x_i$, where
 η - learning rate

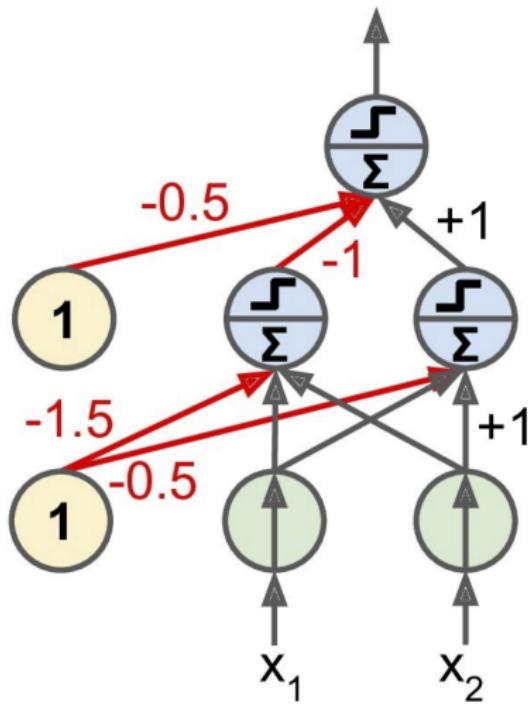
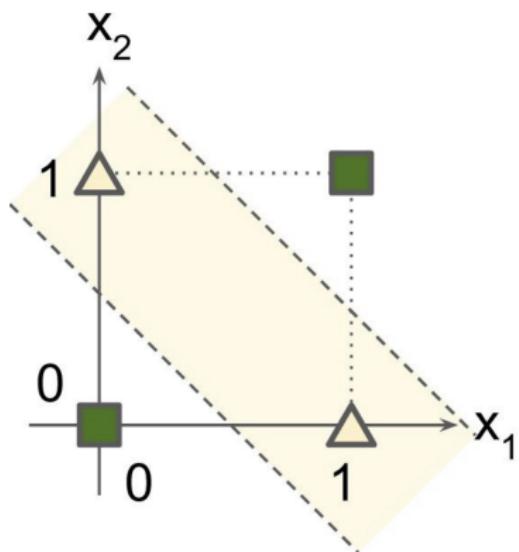


Artificial Neural Networks



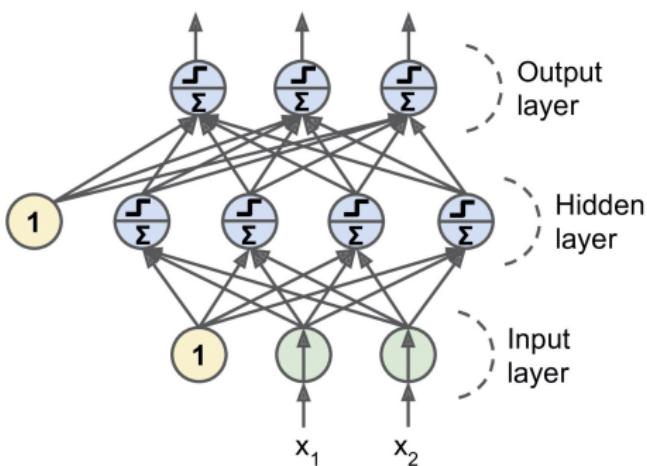
[Meng, Hu, and Ancey(2020)]

Multi-Layer Perceptron (example)

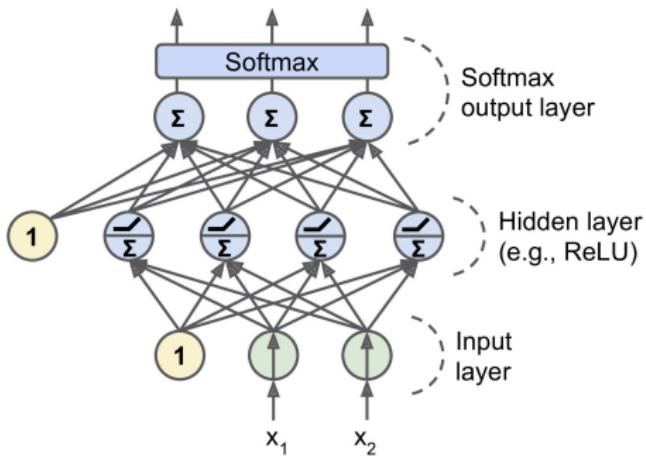


Activation function and backpropagation (1986)

In 1986, Rumelhart et al. suggested a modification to the ANN to enable backpropagation:



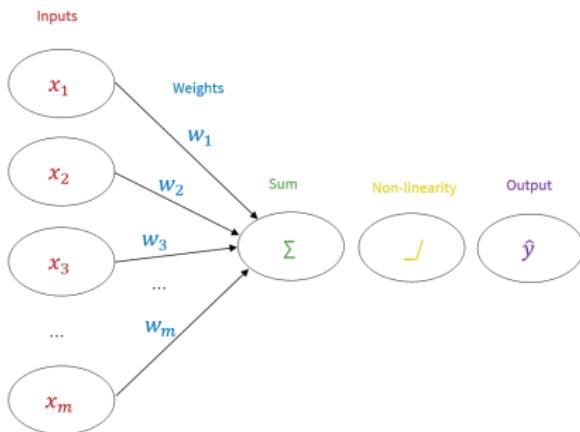
Step-function is flat - no gradients possible!



Introduce non-linear activation function which enables backpropagation

Perceptron: forward propagation

A modern neuron (perceptron) structure:



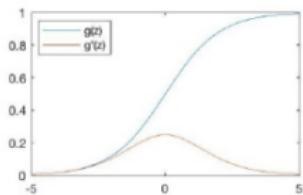
A way to get an output mathematically:

- $\hat{y} = g(w_0 + \sum_{i=1}^m x_i w_i)$
- Activation function $g(z)$
 - Sigmoid
 - tanH
 - ReLU
 - seLU
 - etc...

Activation functions

Here are some examples for the most popular activation functions:

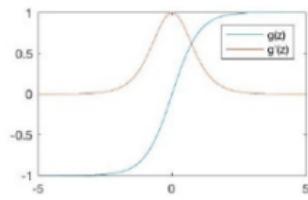
Sigmoid Function



$$g(z) = \frac{1}{1 + e^{-z}}$$

$$g'(z) = g(z)(1 - g(z))$$

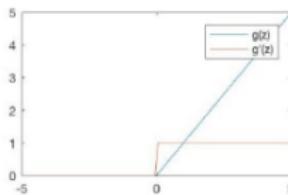
Hyperbolic Tangent



$$g(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$$

$$g'(z) = 1 - g(z)^2$$

Rectified Linear Unit (ReLU)



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

$$g'(z) = \begin{cases} 1, & z > 0 \\ 0, & \text{otherwise} \end{cases}$$

There is plenty of cheat sheets with activation functions and their properties...

Building a FNN: multioutput perceptron

An FNN stands for Feed-Forward Neural Network (our focus during the course). Let's start with a single neuron (perceptron) with multiple outputs:



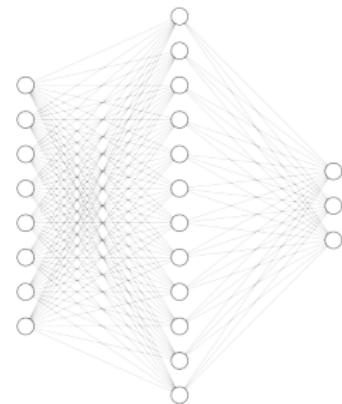
Input Layer $\in \mathbb{R}^n$

Output Layer $\in \mathbb{R}^3$

- $\hat{y}_1 = g\left(w_{0,1} + \sum_{j=1}^m x_j w_{j,1}\right)$
- $\hat{y}_2 = g\left(w_{0,2} + \sum_{j=1}^m x_j w_{j,2}\right)$
- $\hat{y}_3 = g\left(w_{0,3} + \sum_{j=1}^m x_j w_{j,3}\right)$

Building a FNN: single hidden layer NN

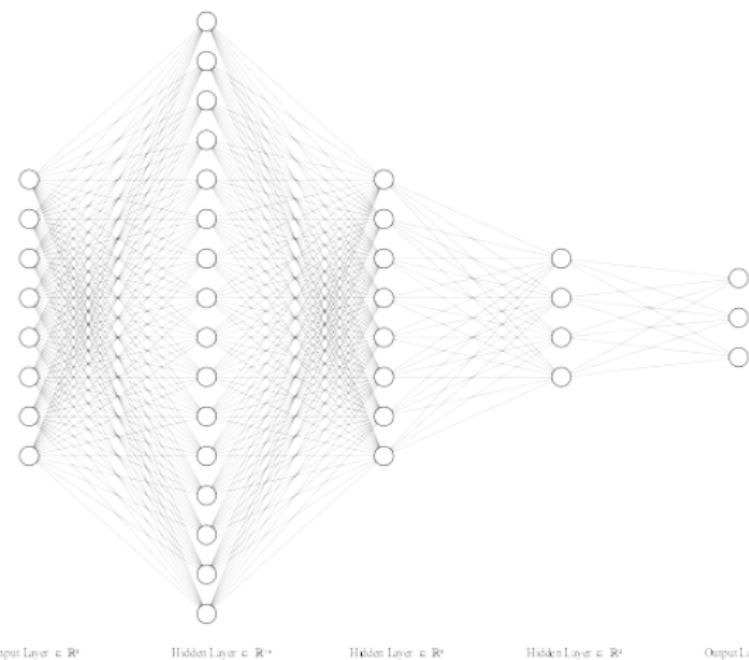
Let's take a look at with a single hidden layer NN:



- **Hidden layer:**
 $y_1 = g(w_{0,1}^{(1)} + \sum_{j=1}^m x_j w_{j,1}^{(1)})$
- **Output layer:**
 $\hat{y}_1 = f(w_{0,1}^{(2)} + \sum_{j=1}^m x_j w_{j,1}^{(2)})$
- Activation functions $g(z)$ and $f(z)$ can (and probably should) be different

Building a FNN: deep fully connected NN

Let's wrap up a deep fully connected NN:



Capabilities of ANNs

- **Boolean functions:**

- Every Boolean function can be represented by a network with a single hidden layer.
- Might require exponential (in number of inputs) hidden units.

- **Continuous functions:**

- Every bounded continuous function can be approximated with arbitrarily small error, by network with one hidden layer [Cybenko 1989; Hornik et al. 1989].

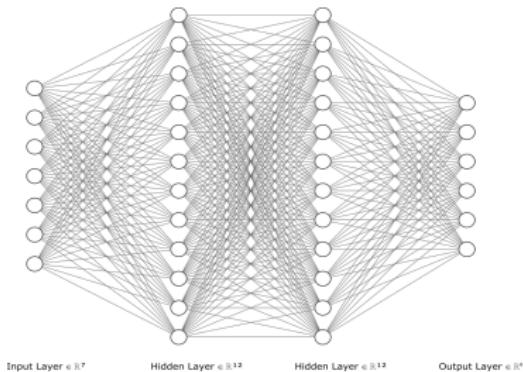
- **Deep NN are in practice superior to other ML methods in presence of large data sets.**

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Loss function: MSE

Training a model consists of minimizing a loss \mathcal{L}_w which reflects the performance of the predictor $N_w(x)$ on a training data set.



- Empirical loss:

$$\mathcal{L}_w = \frac{1}{m} \sum_{i=1}^m \mathcal{L}(N_w(x^{(i)}), \hat{y}^{(i)})$$

- Mean Squared Error:

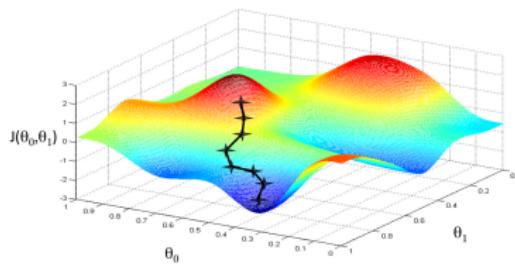
$$J(\rho) = \frac{1}{m} \sum_{i=1}^m (N_w(x^{(i)}) - \hat{y}^{(i)})^2$$

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Gradient descent: general idea

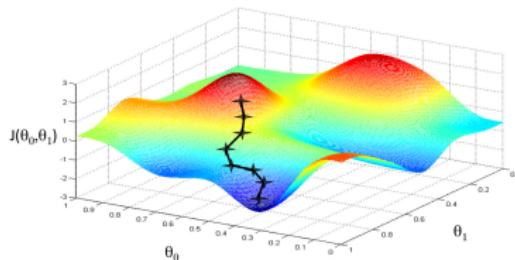
We want to find the network weights θ^* that achieve the lowest loss \mathcal{L}_θ :
$$\theta^* = \arg \min_\theta \mathcal{L}_\theta$$



- Randomly pick initial weights (θ_0, θ_1)
- Compute gradient
- Take small steps in the opposite direction of gradient
- Repeat until convergence

Gradient descent: more specific

We want to find the network weights θ^* that achieve the lowest loss \mathcal{L}_θ :

$$\theta^* = \arg \min_\theta \mathcal{L}_\theta$$


- Initialize weights randomly \mathcal{N}_θ
- Repeat until convergence
 - 1 Compute gradient: $\frac{\partial \mathcal{L}_\theta}{\partial \theta}$
 - 2 Update weights: $\theta^{new} = \theta^{old} - \eta \frac{\partial \mathcal{L}_\theta}{\partial \theta}$, where η is a learning rate
 - 3 Return new weights

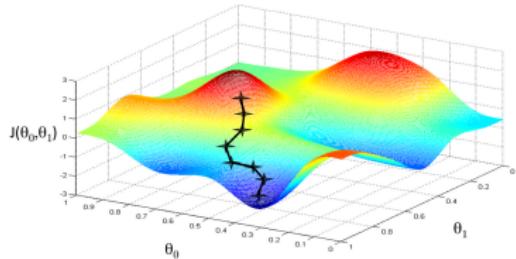
Problem with gradient descent

Taking gradients can be computationally expensive

Stochastic gradient descent

We want to find the network weights θ^* that achieve the lowest loss \mathcal{L}_θ :

$$\theta^* = \arg \min_{\theta} \mathcal{L}_\theta$$



- Initialize weights randomly \mathcal{N}_θ
- Repeat until convergence
 - ➊ Pick a single data point *i*
 - ➋ Compute gradient: $\frac{\partial \mathcal{L}_\theta^i}{\partial \theta}$
 - ➌ Update weights:
$$\theta^{new} = \theta^{old} - \eta \frac{\partial \mathcal{L}_\theta^i}{\partial \theta}, \text{ where } \eta \text{ is a learning rate}$$
 - ➍ Return new weights

Problem with stochastic gradient descent based on a single data point

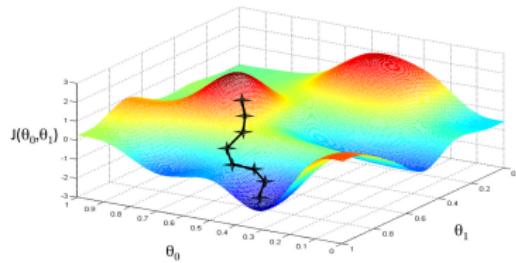
Taking gradients base don the single data point can be noisy

Stochastic gradient descent with batches

We want to find the network weights θ^* that achieve the lowest loss \mathcal{L}_θ :

$$\theta^* = \arg \min_{\theta} \mathcal{L}_\theta$$

- Initialize weights randomly \mathcal{N}_θ
- Repeat until convergence



- ➊ Pick a batch of data points B
- ➋ Compute gradient:
$$\frac{\partial \mathcal{L}_\theta}{\partial \theta} = \frac{1}{B} \sum_{k=1}^B \frac{\partial \mathcal{L}_\theta^k}{\partial \theta}$$
- ➌ Update weights:
$$\theta^{new} = \theta^{old} - \eta \frac{\partial \mathcal{L}_\theta}{\partial \theta}, \text{ where } \eta \text{ is a learning rate}$$
- ➍ Return new weights

Stochastic gradient descent with batches: justification

Justification

From Deisenroth et al. (2021) Mathematics for Machine learning, Sec. 7.1.3.: *"The key insight about why taking a subset of data is a sensible is to realize that for gradient descent to converge, we only require that the gradient is an unbiased estimate of the true gradient."*

Training: some terminology

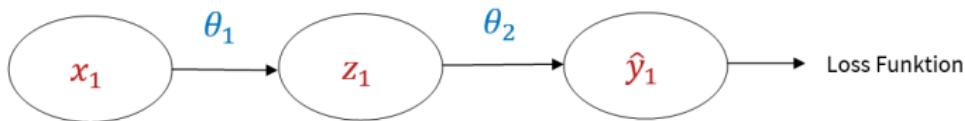
- The batch used for a SGD is called **mini-batch**
- An **epoch** refers to a complete pass through the entire dataset, where the algorithm has iterated over all the mini-batches once.

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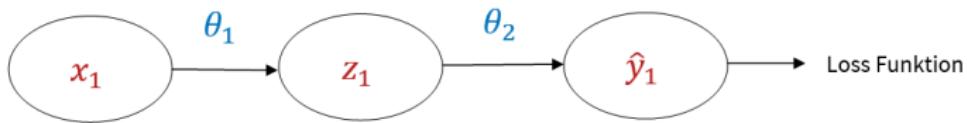
Computing gradients: error backpropagation

- How does a small change in one weight (e.g., θ_2) affect the final loss function \mathcal{L}_θ ?



Computing gradients: error backpropagation

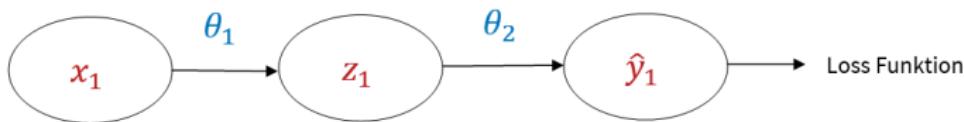
- How does a small change in one weight (e.g., θ_2) affect the final loss function \mathcal{L}_θ ?



- Chain rule: $\frac{\partial \mathcal{L}_\theta}{\partial \theta_2} = \frac{\partial \mathcal{L}_\theta}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial \theta_2}$

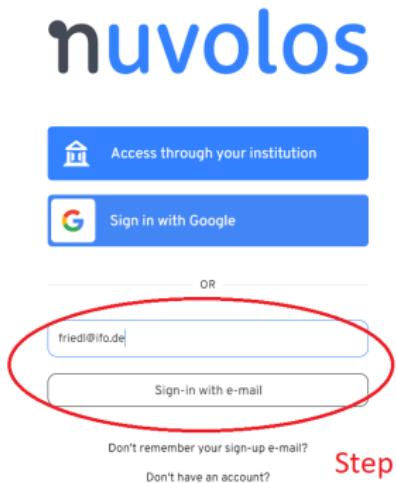
Computing gradients: error backpropagation

- How does a small change in one weight (e.g., θ_2) affect the final loss function \mathcal{L}_θ ?



- Chain rule: $\frac{\partial \mathcal{L}_\theta}{\partial \theta_2} = \frac{\partial \mathcal{L}_\theta}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial \theta_2}$
- Repeat this for every weight in the network using gradients from later layers: $\frac{\partial \mathcal{L}_\theta}{\partial \theta_1} = \frac{\partial \mathcal{L}_\theta}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial \theta_1} = \frac{\partial \mathcal{L}_\theta}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z_1} \frac{\partial z_1}{\partial \theta_1}$

Login to Nuvolos: step 1



Step 1. Sign-up here



Login to Nuvolos: step 2

The screenshot shows the Nuvolos application interface. On the left, there is a vertical sidebar with icons for navigation: a house (Dashboard), a grid (Courses), a document (Course details), a gear (Settings), a folder (File manager), a camera (Media), and a link (Share). A red circle highlights the camera icon. A red arrow points from the text "Step 2. Press here" to the camera icon. The main content area displays the "DEQN PhD course" details, including its description: "A Ph.D. course on the application of deep neural networks as a global solution method". Below this, there is a section titled "Getting Started with Nuvolos" which lists useful features like "Objects" and "Snapshots". The "Objects" section contains a note about receiving objects from instructors and creating your own. It also mentions that files can be downloaded. The "Snapshots" section explains how saved versions of objects can be restored if deleted or modified. The "Navigation" section provides information on using the top toolbar to switch between organizations, courses, instances, and snapshots. To the right, there is a "Course checklist" panel with several items: "Upload files" (green icon), "Invite students" (blue icon, note: No students have joined yet), "Distribute material" (blue icon, note: No material has been shared yet), "Create assignment" (blue icon, note: No assignments have been created yet), and "Add application startup schedule" (blue icon, note: Define class times when applications are prestarted). At the bottom, there is a footer bar with various icons for navigation and search.

INFO INSTITUT > DEQN PHD COURSE > MASTER > CURRENT STATE

DEQN PhD course ⓘ

A Ph.D. course on the application of deep neural networks as a global solution method ⓘ

Getting Started with Nuvolos

Below are useful features of Nuvolos to maximize productivity.

Objects

Nuvolos can store files, applications (with pre-installed packages / libraries) and tables. You can receive objects from the instructor or create your own (only files and tables).

Step 2. Press here

Files (multiple - even complete folders) can be downloaded to your local computer if needed. [Learn more](#)

Snapshots

You should save your work always in the applications you use. Different saved versions of objects can be stored in snapshots. If you accidentally delete or modify an object, you can restore past versions from snapshots. We recommend to make snapshots often to be able to reverse accidental changes. [Learn more](#)

Navigation

Use the top toolbar to navigate. The house icon takes you back to the dashboard. The first selector can be used to switch organizations. The second selector can be used to switch spaces (courses). The third selector switches instances. The last selector can be used to switch snapshots.

DEMONSTRATION > DEMONSTRATION RESEARCH PROJECT > MASTER > CURRENT STATE

Login to Nuvolos: step 3

The screenshot shows the Nuvolos web interface with the following navigation path: IFO INSTITUT > DEQN PHD COURSE > MASTER > CURRENT STATE. On the left, there is a sidebar with icons for Applications, Schedules, and Settings. The main content area is titled 'Applications' and contains a table with one row. The row has columns for Type (Jupyter), Name (deqn_phd_course), Size (1 CU), Status (green circle with power icon), Description (JupyterLab 4.1.2 + Python 3.11 + TexLive), Space usage (21.7 kB), and Actions (three dots). A red oval highlights the 'deqn_phd_course' name. Below the table, a red box contains the text 'Step 3. Press here'. The bottom section is titled 'Schedules' and shows a table with one row, indicating 'No scheduled applications found.' There are also sections for 'Show past schedules too' and 'Actions'.

Type	Name	Size	Credit/hour	Status	Description	Space usage	Actions
Jupyter	deqn_phd_course	1 CU	-	Green circle with power icon	JupyterLab 4.1.2 + Python 3.11 + TexLive	21.7 kB	...

Step 3. Press here

Type	Name	Date	Custom resources	Session length [min]	Actions
No scheduled applications found. Consider scheduling a new application via the "Schedule for start" button in actions.					

Let's look at SGD closer

- Let's look at this notebook on Nuvolos.cloud:
01_GradientDescent_and_StochasticGradientDescent.ipynb

Questions?