

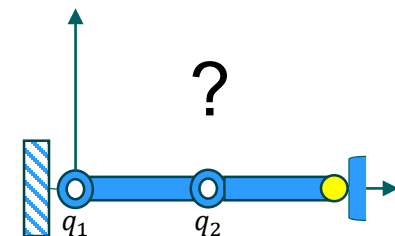
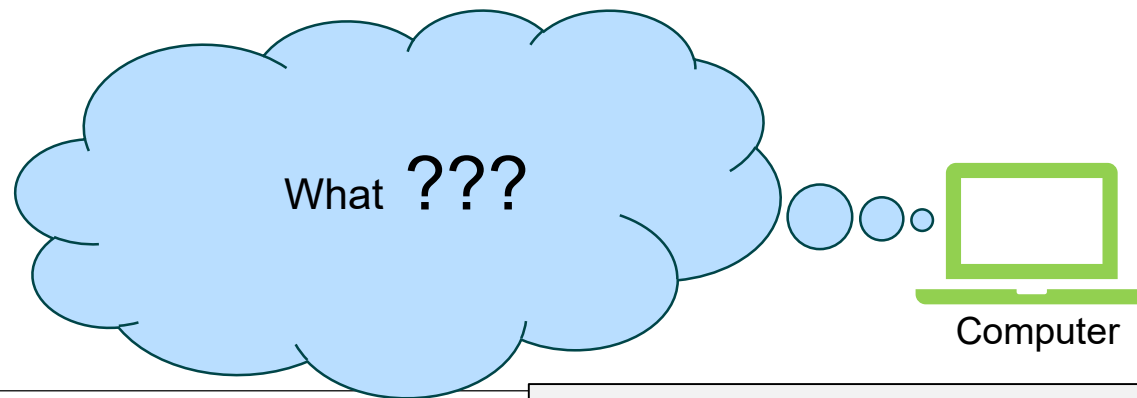
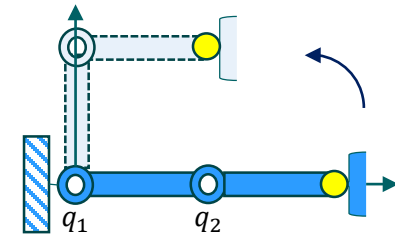
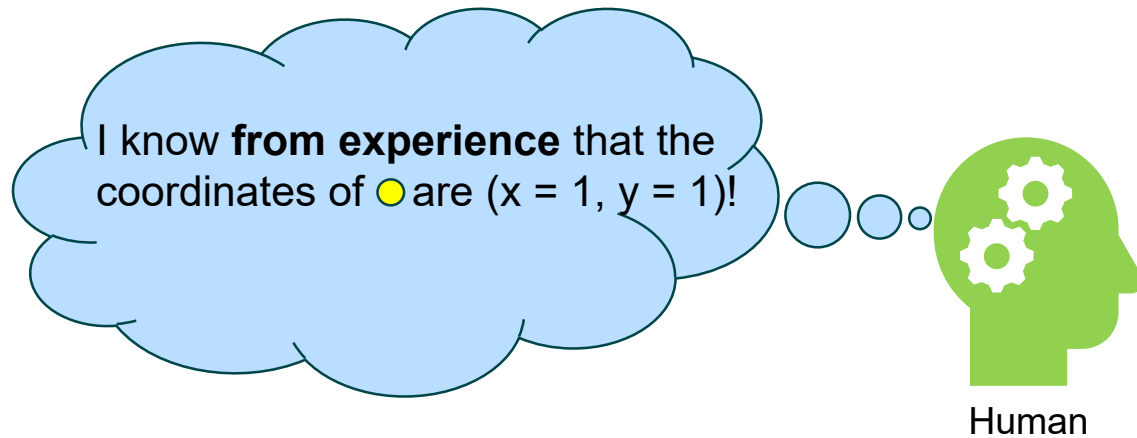


# Robotics und Machine Learning (ML)

Prof. Dr.-Ing. Eric Kaigom

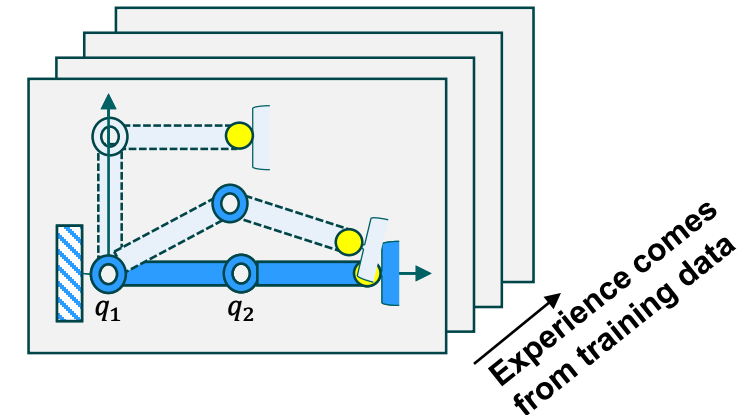
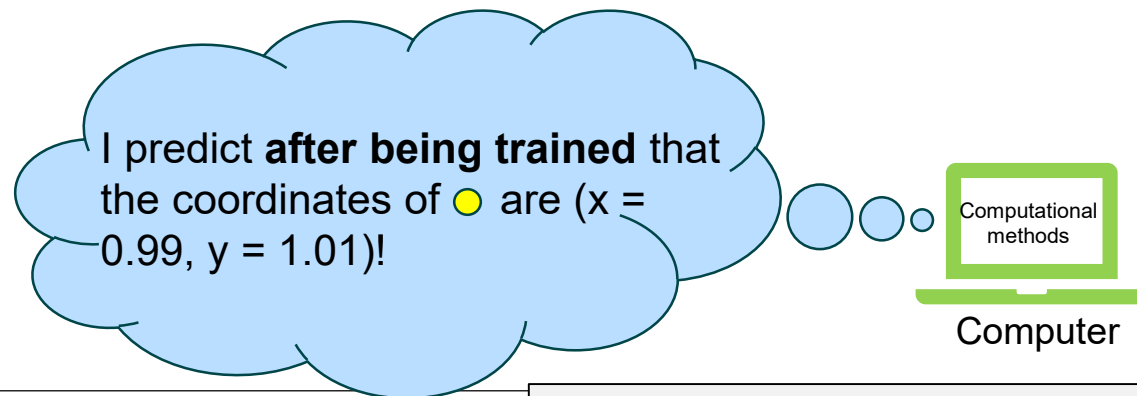
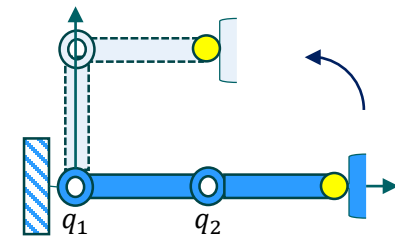
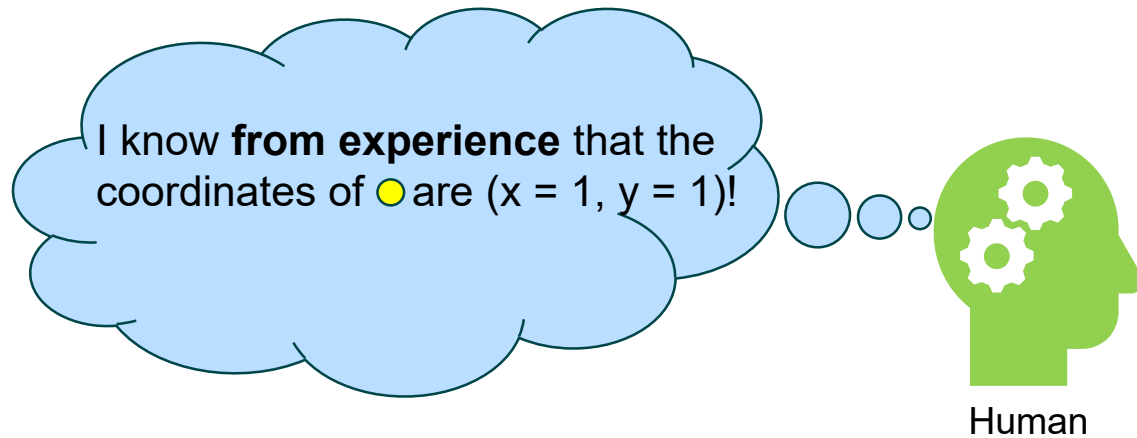
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Learning from experience – What are the coordinates of ● for  $q_1 = \frac{\pi}{2}$  and  $q_2 = -\frac{\pi}{2}$  ?



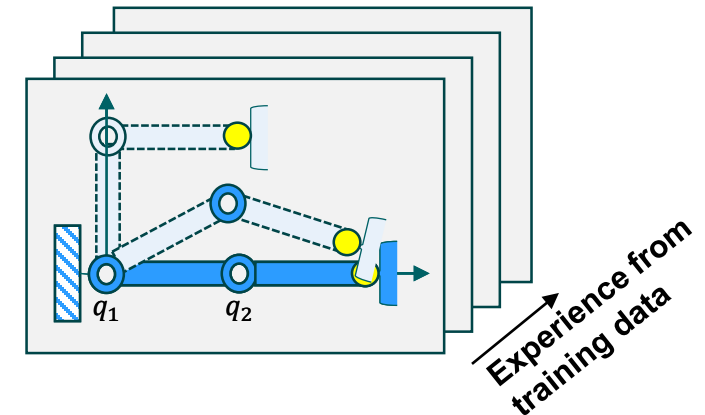
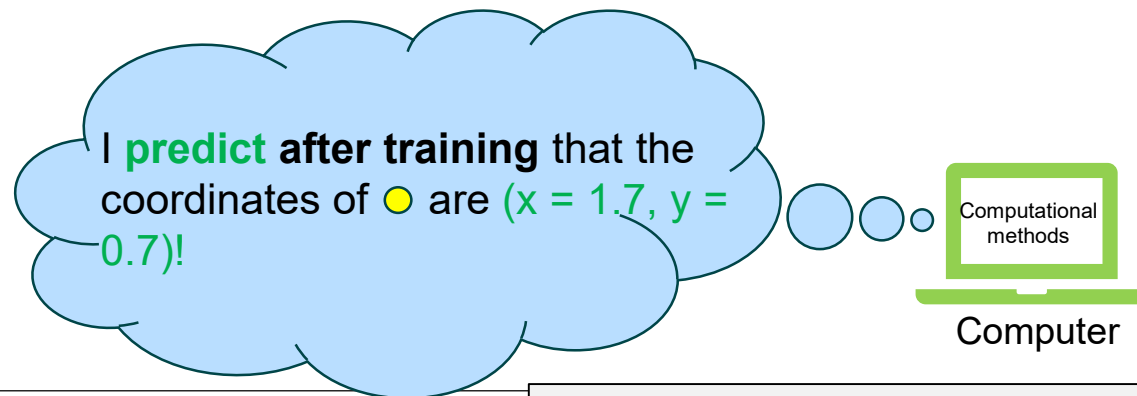
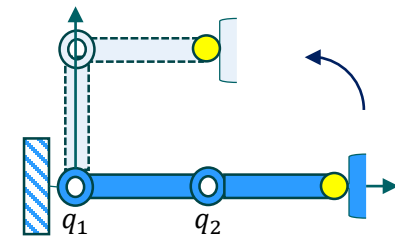
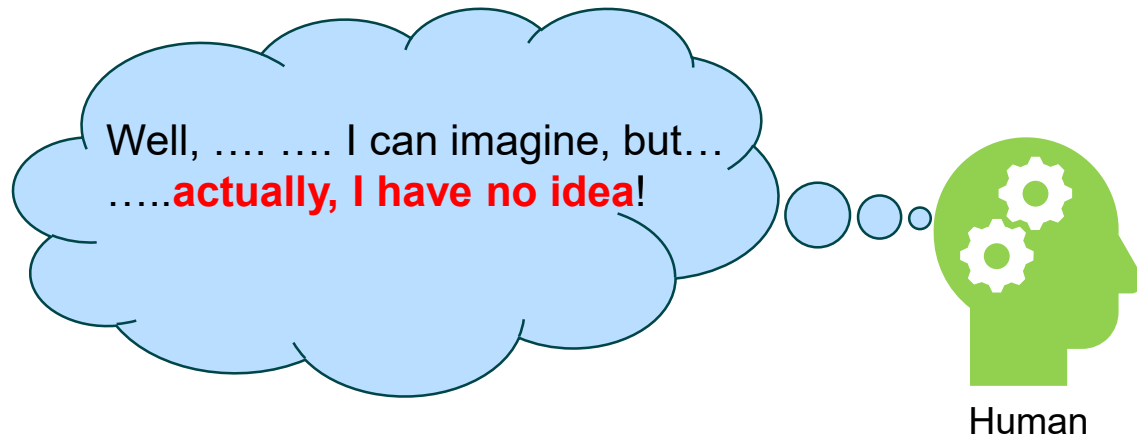
Can a computer (or in general a machine) do the same, i.e., **learn from experience** like a human?

Learning from experience – What are the coordinates of ● for  $q_1 = \frac{\pi}{2}$  and  $q_2 = -\frac{\pi}{2}$  ?



Can a computer (or in general a machine) do the same, i.e., **learn from experience** like a human?? **Yes!**

Learning from experience – What are the coordinates of ● for  $q_1 = \frac{\pi}{4}$  and  $q_2 = -\frac{\pi}{4}$  ?



A trained **machine** can **outperform** human capabilities in e.g. non-nominal cases by **learning from data** (entailing a rich and diversified experience).

# Machine Learning

## Machine Learning – A brief overview

**Machine learning** is the **process** of using **algorithms** to learn a **model** that helps **predict** the outcomes of previously **unseen events** (i.e., model input data) by using experiences condensed in **training data**.

What

Challenge and constraints understanding, selection of a learning approach

How

### Data management

- Collection
- Pre-processing
- etc

### Model development

- Hyperparameterization
- Optimization
- Validation, etc

### Applications

- Forward kinematics
- Backward kinematics
- etc

Our focus



## Understanding challenges, constraints, and opportunities - example



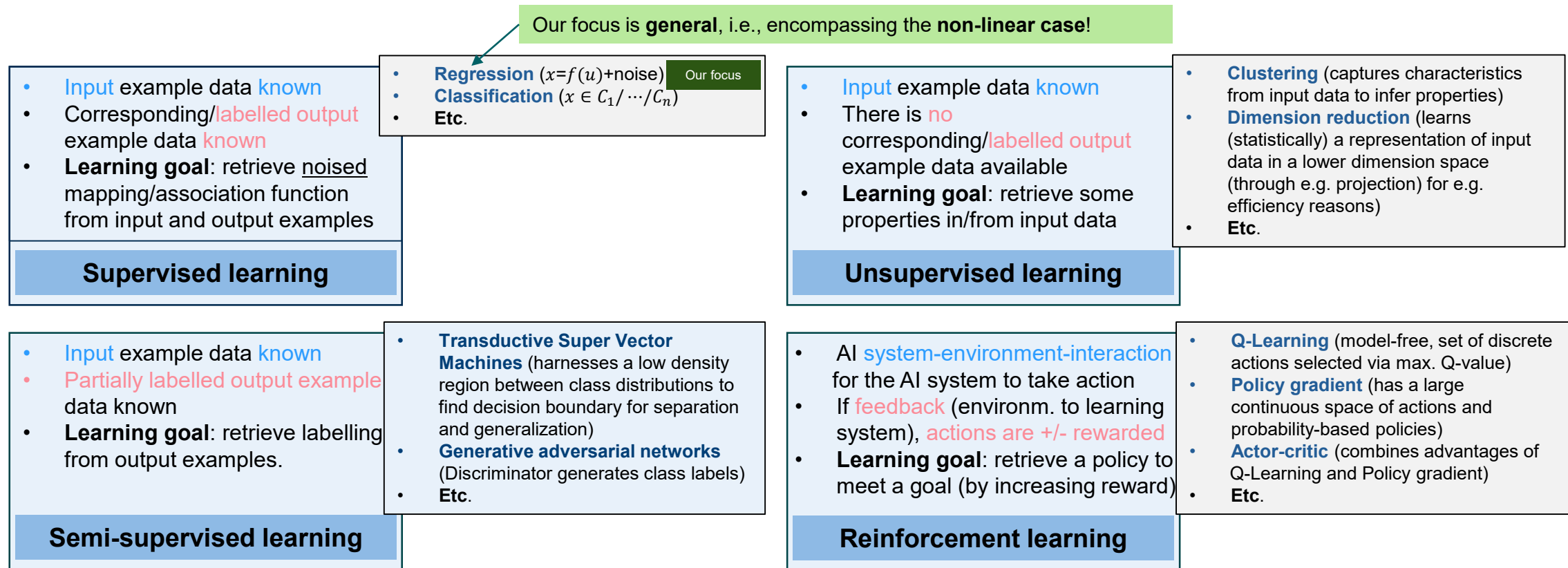
### Why and what

- Forward kinematics (FK) and backward kinematics (BK) not available in a closed form (e.g., refurbished robots)
- FK and BK prone to uncertainties (e.g., geometry, structural properties, noise, etc.)
- Access to input (e.g., joint pos.) and output (e.g., end-effector pos.) data via measurements and data acquisition

### How

- Instead of a **model-based** (i.e., analytical) derivation of the input-output or output-input mapping in closed form, **data** samples are **leveraged** to **capture** the **mapping model** (FK and BK)
- Captured models (FK and BK) can be used in **arbitrary** (e.g., physical or virtualized) **applications** and even **shared via mail** („FK and BK to go!“)

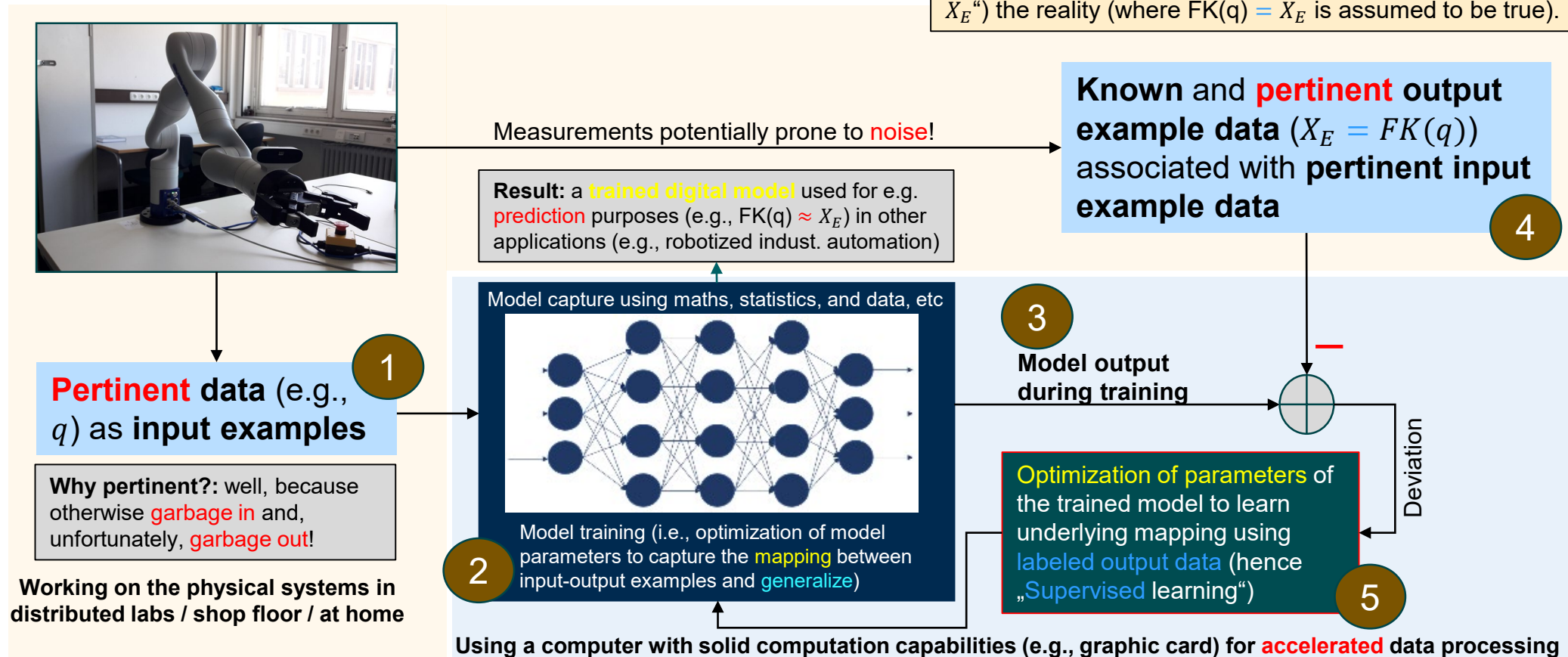
## Selecting a suitable machine learning approach





## Machine Learning – Supervised Learning (Big Picture)

**Hint:** The trained AI model predicts (i.e., approximates, hence „ $FK(q) \approx X_E$ “) the reality (where  $FK(q) = X_E$  is assumed to be true).



# Preparing data

## Why data preparation?

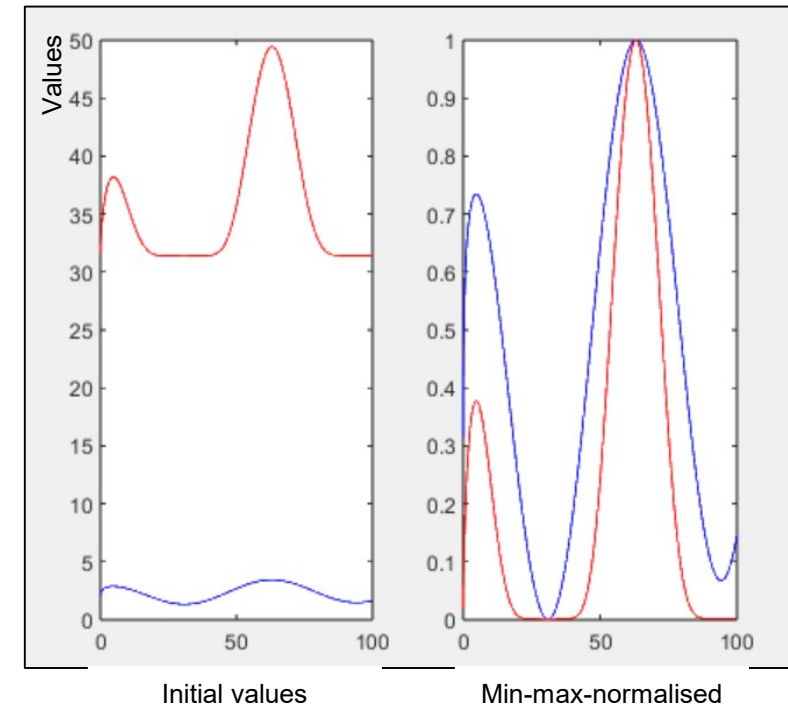
- An important step before data analysis (...in order to learn an unknown mapping or correspondence)
- Pivotal point in Machine Learning: How **features** are **distributed**
- **Implications:**
  - Preserve how the data samples (e.g., joint positions) relate to each other
  - Accommodate the impact of units
  - Avoid effects of relative scale (otherwise: learning performance can drop, i.e., convergence takes longer due to overshoot. More later on.)
- **Challenges:**
  - Impacts of outliers
  - etc

## Data preparation - Minimum-Maximum Normalization

- $x = [x_1 \ x_2 \ \dots \ x_n]$  the vector of  $n$  scalars
- $x_{min}$  and  $x_{max}$  is minimum and maximum value in  $x$
- $\hat{x}$  is the min-max-normalized value of  $x$ :

$$\hat{x} = \frac{x - x_{min}}{x_{max} - x_{min}}$$

- Values in  $\hat{x}$  are squeezed between 0 and 1, i.e., within [0 1]
- Is it possible to squeeze values between scalars  $z_0$  and  $z_1$  with  $z_0 < z_1$ ?



## Application #1

- 1) Use Matlab to randomly generate a vector  $V$  of 100 scalars between -100 and 100.
- 2) Carry out the min-max normalization of this vector and store the result in  $V_n$ .
- 3) Set the value at index 20 in  $V$  to 500. Store the result in  $V_o$ .
- 4) Carry out the min-max normalization of  $V_o$  and store the result in  $V_{on}$ .
- 5) Plot  $V$ ,  $V_n$  and  $V_{on}$  in three subplots. What do you observe?

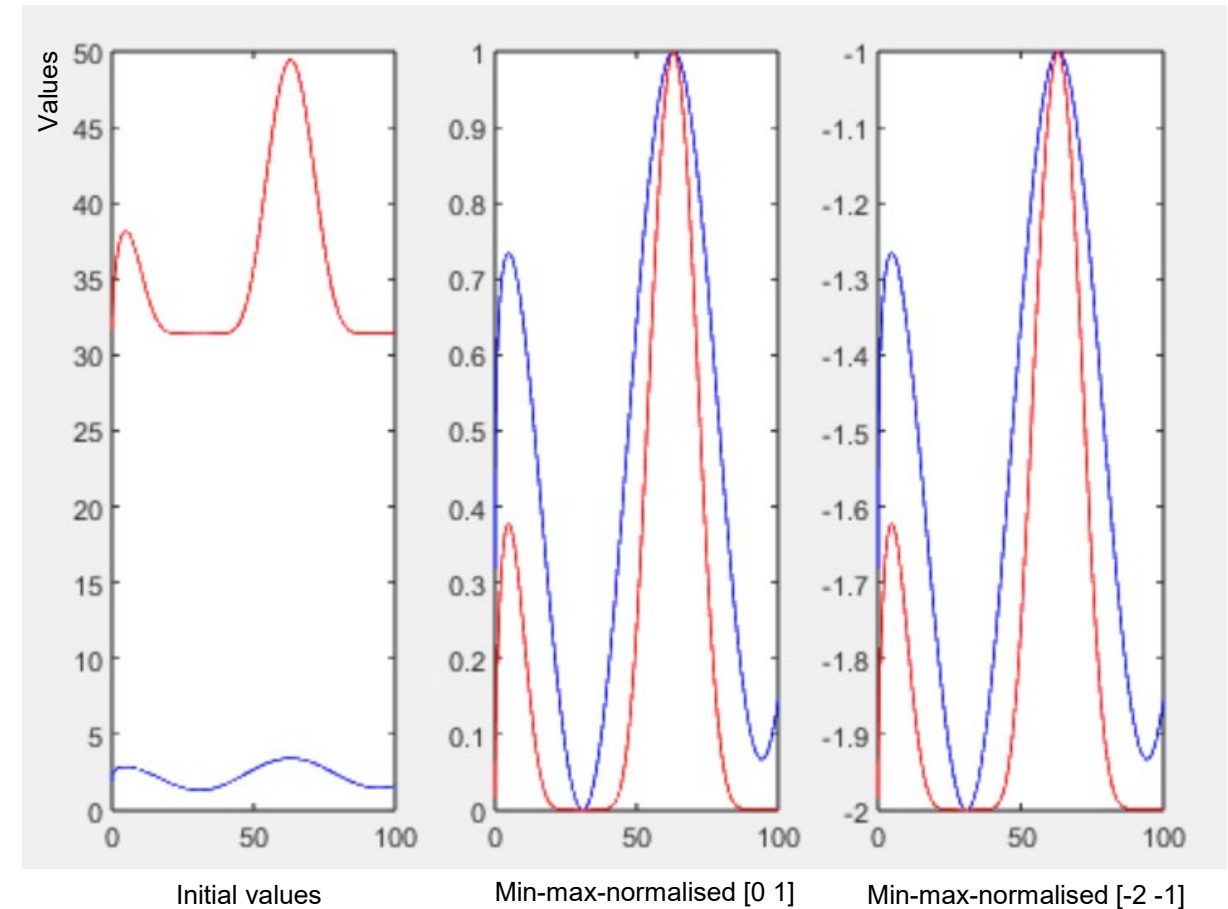
$$\hat{x} = \frac{x - x_{min}}{x_{max} - x_{min}}$$

## Data preparation - Minimum-Maximum Normalization

- $x = [x_1 \ x_2 \ \dots \ x_n]$  the vector of  $n$  scalar data
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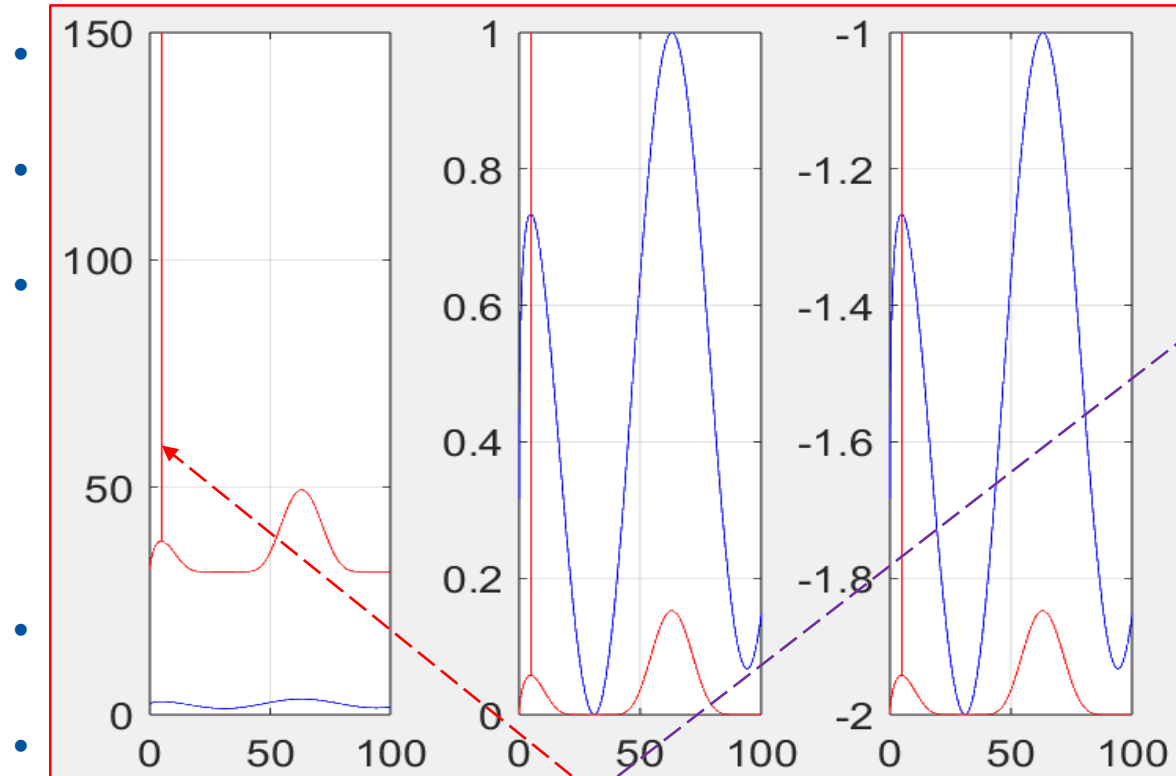
$$\hat{x} = z_0 + (z_1 - z_0) \frac{x - x_{min}}{x_{max} - x_{min}}$$

- Values in  $\hat{x}$  are squeezed between  $z_0$  and  $z_1$

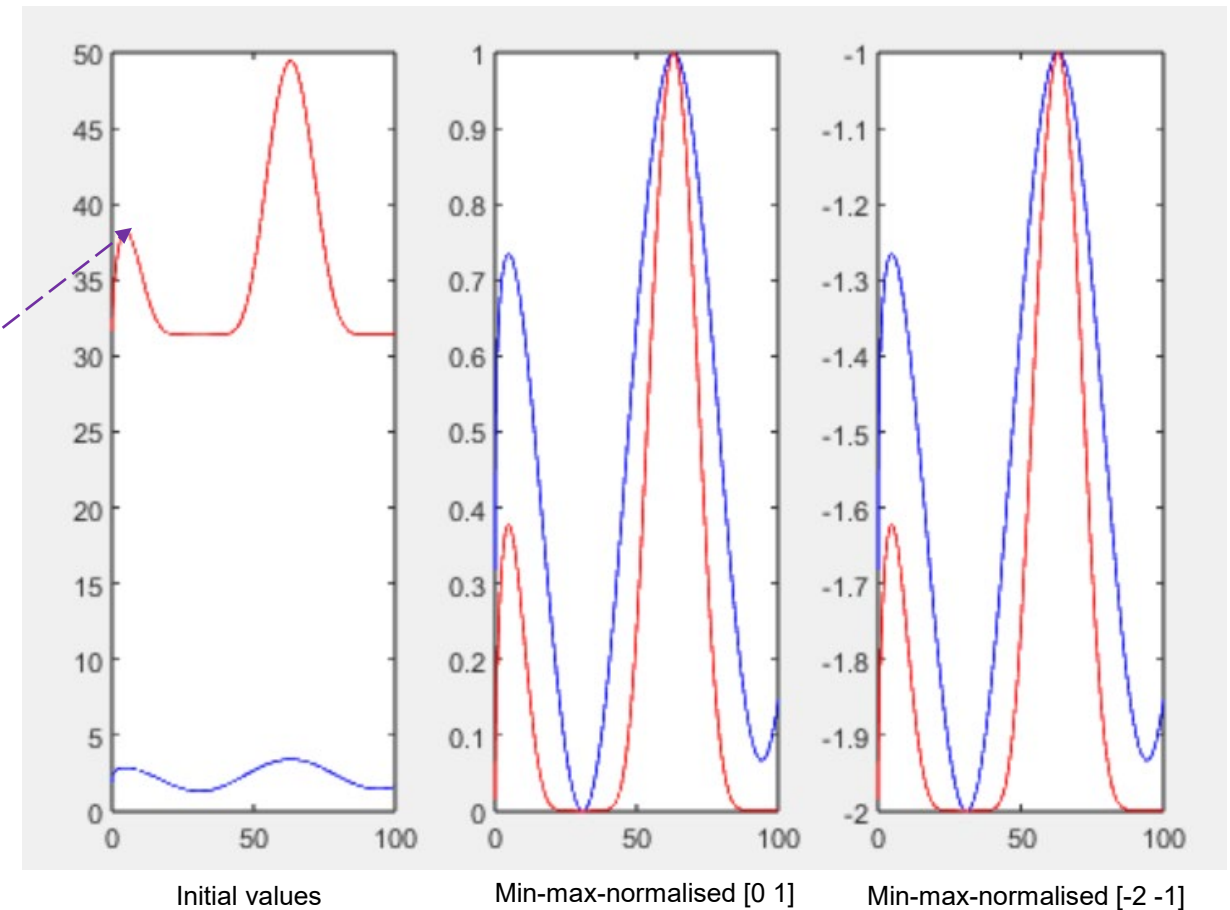




## Data preparation - Minimum-Maximum Normalization



- Min-max normalization faces **outliers** issues!
- Shape (of the **distribution**) is **preserved**
- How to influence **mean value** and **standard deviation**?



## Data preparation - z-Score Normalization

- $x = [x_1 \ x_2 \ \dots \ x_n]$  the vector of  $n$  scalar data

- Mean value

$$\mu = \frac{1}{n} \sum_{i=1}^n x_i$$

- Standard deviation

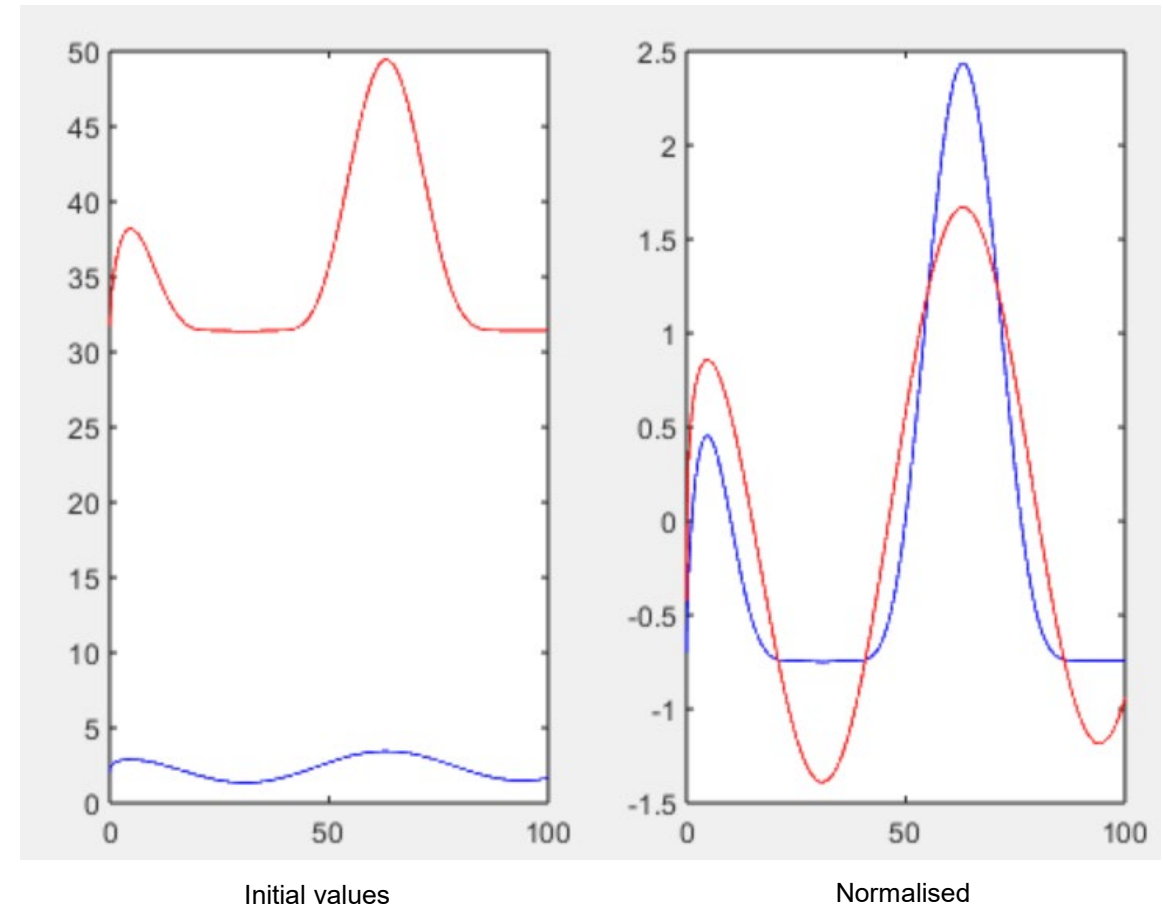
$$\sigma = \sqrt{\frac{1}{n-1} \sum_{i=1}^n (x_i - \mu)^2}$$

- Normalization:

$$\hat{x} = \frac{x - \mu}{\sigma}$$

- **Hints:**

- The feature  $\hat{x}$  hat mean  $\hat{\mu} = 0$  and standard dev.  $\hat{\sigma} = 1$
- Data are **not** necessary confined within  $[0 \ 1]$  (during training), which is helpful for robustness (w.r.t **new** test data outside  $[-1 \ 1]$ )!



## Data preparation - z-Score Normalization

- $x = [x_1 \ x_2 \ \dots \ x_n]$  the vector of  $n$  scalar data

- Mean value

$$\mu = \frac{1}{n} \sum_{i=1}^n x_i$$

- Standard deviation

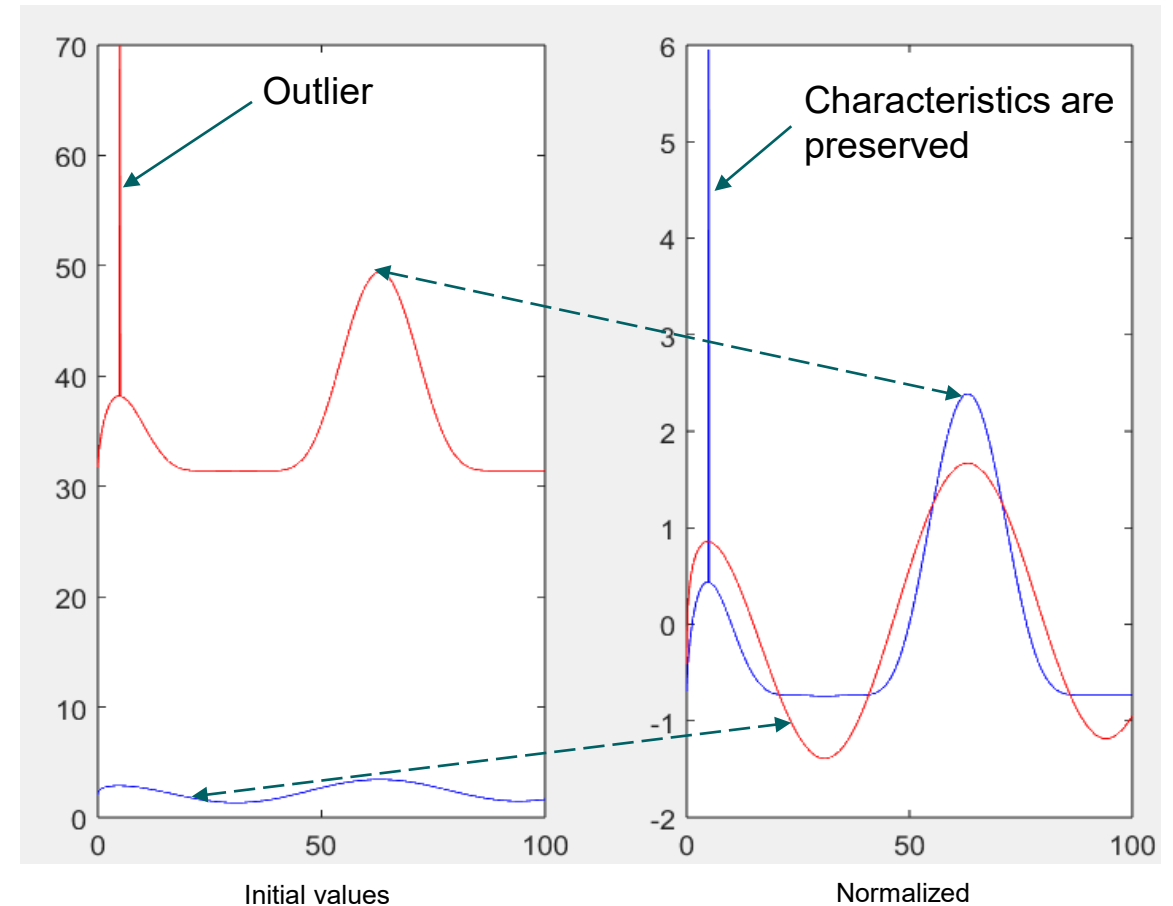
$$\sigma = \sqrt{\frac{1}{n-1} \sum_{i=1}^n (x_i - \mu)^2}$$

- Normalisation:

$$\hat{x} = \frac{x - \mu}{\sigma}$$

- **Hints:**

- Useful properties about outliers are kept!
- Impact of outliers on normalized data is mitigated (hence robustness!)



## Application #2:

- Assume that  $u = [x_1, \dots, x_n]^T$  is a dataset
- Calculate Min-Max(z-Score(x))

## Solution:

$$\hat{x} = \frac{x - x_{\min}}{x_{\max} - x_{\min}} = \frac{\frac{x - \mu}{\sigma} - \frac{x_{\min} - \mu}{\sigma}}{\frac{x_{\max} - \mu}{\sigma} - \frac{x_{\min} - \mu}{\sigma}} = \frac{x - x_{\min}}{x_{\max} - x_{\min}}$$

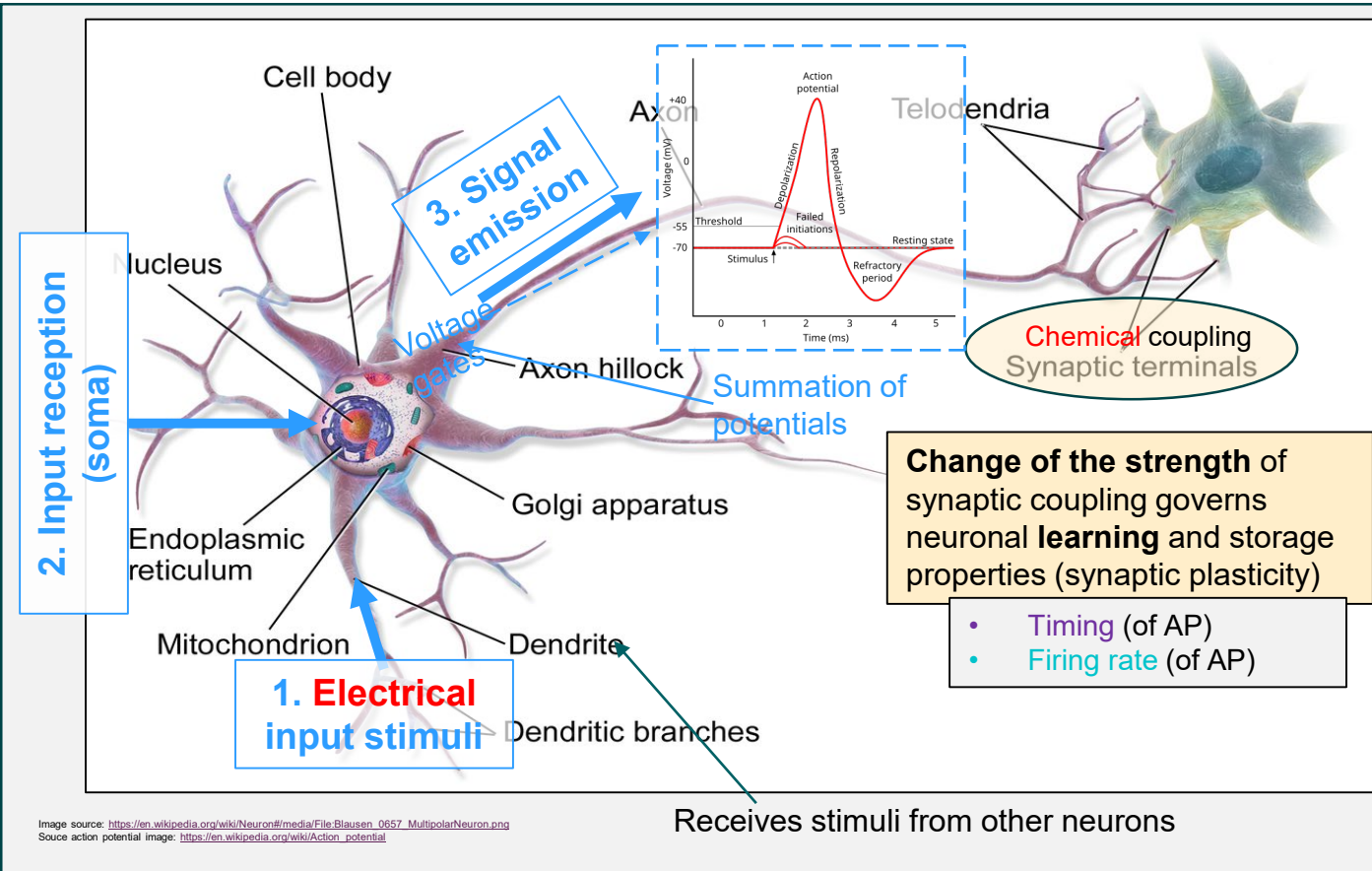
```
>> n=10; a=rand(n,1)'; zm = normalize(a, 'range') - normalize(normalize(a), 'range')
zm =
    1.0e-15 *
    -0.1110  -0.0555      0      0      0      0      0      0      0  -0.1110
```

Min-max  
Between [0 1]

Z-score  
Between [0 1]

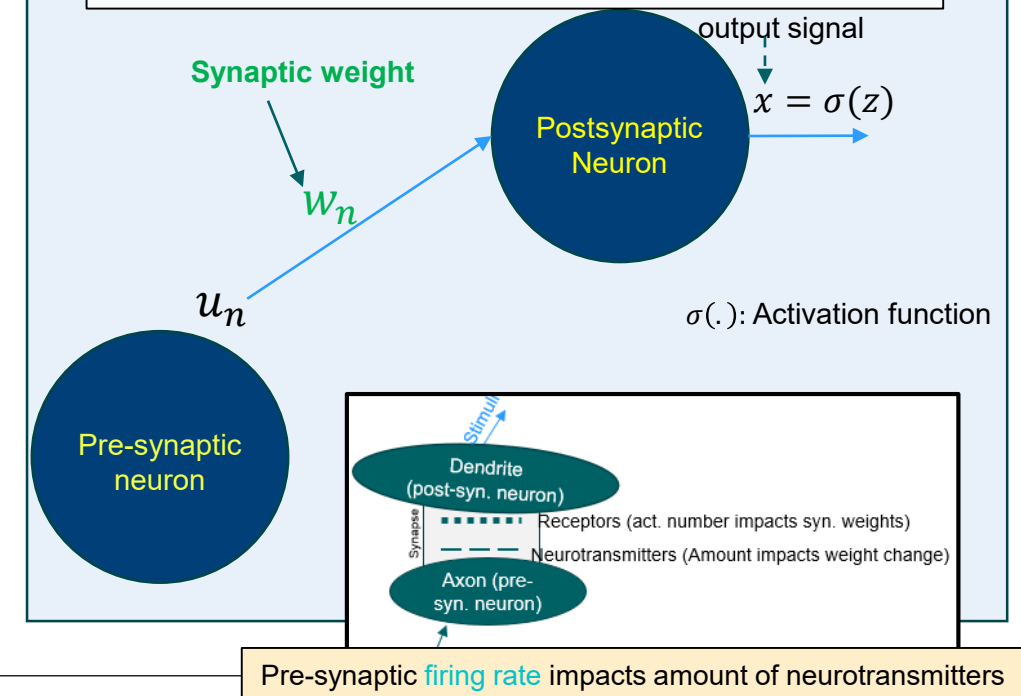
# Using neurons to reason

## Neuron model – Synapse dynamics



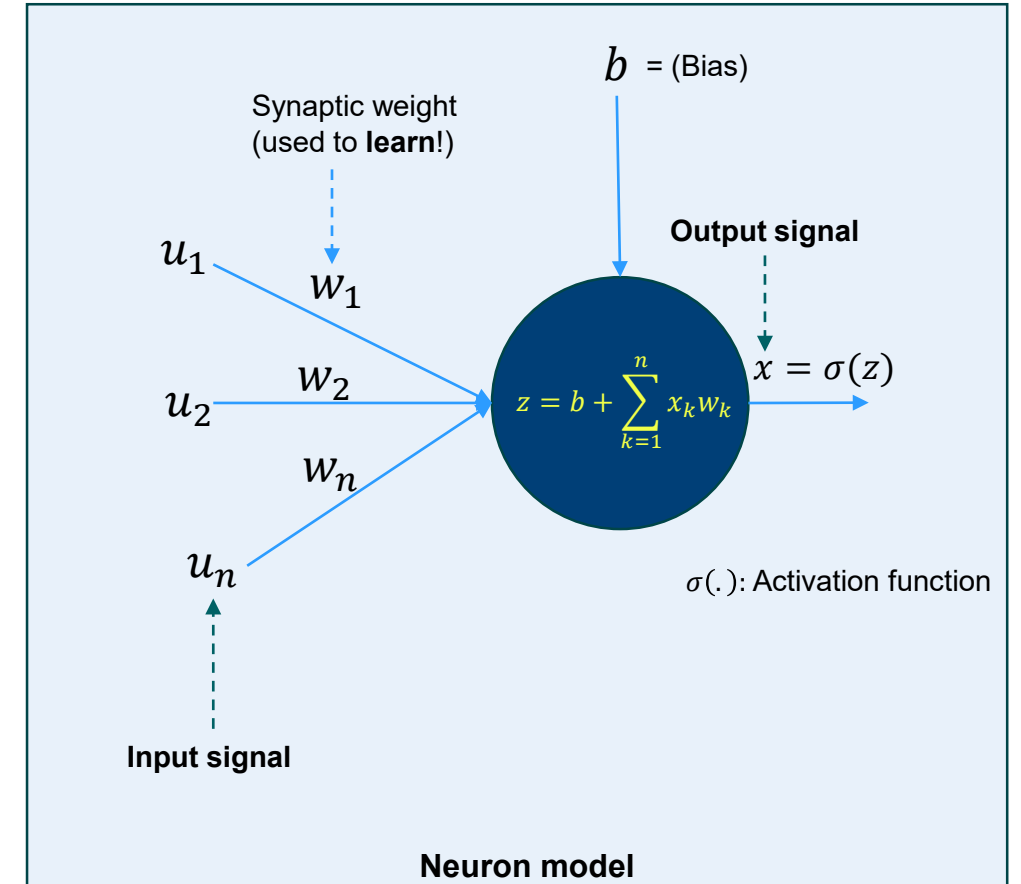
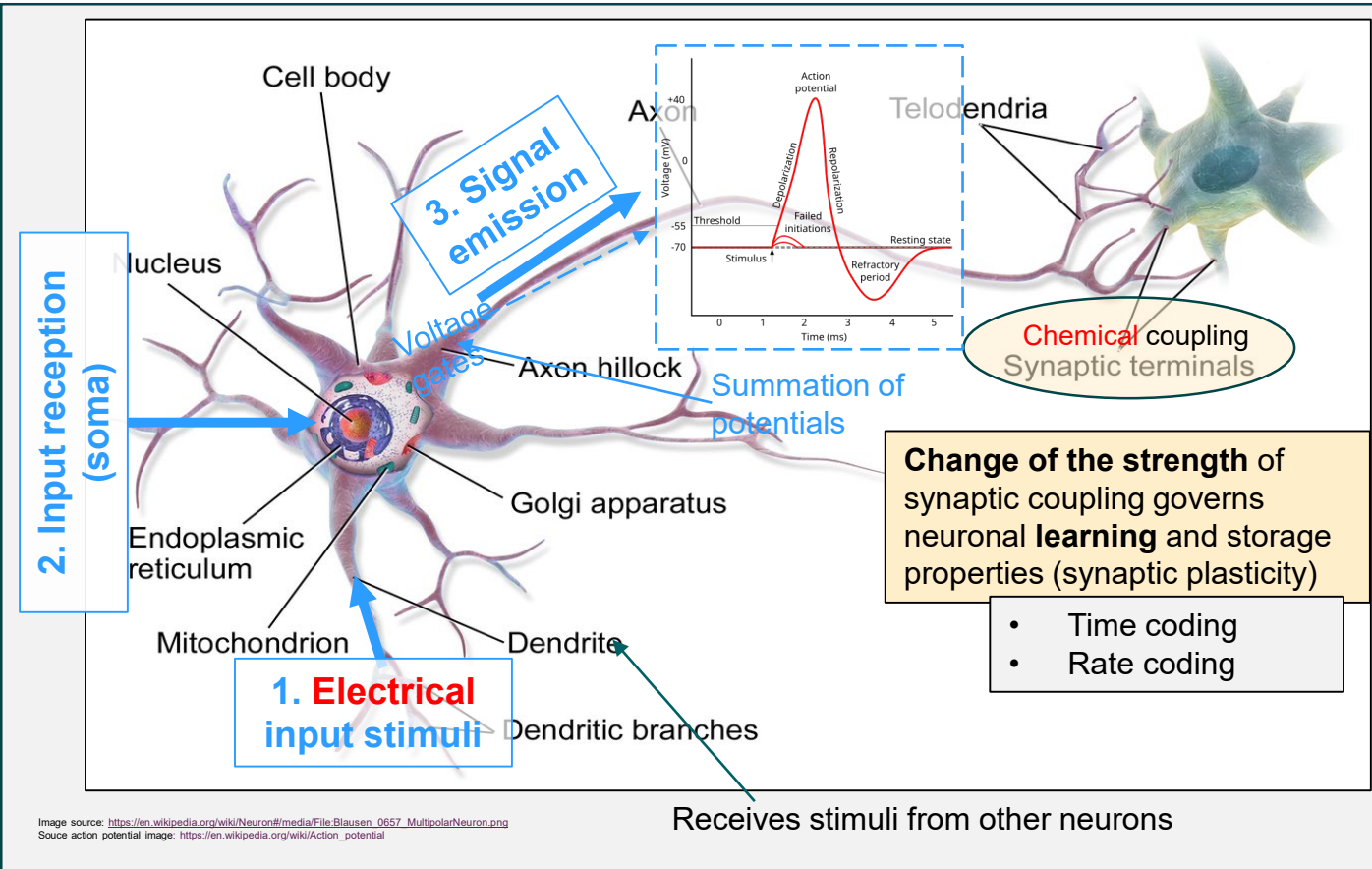
### Spike-timing-dependent plasticity

- Process associated with the modification (optimization) of the synaptic weights
- Depends upon temporal dynamics (e.g., latency) between action potential (AP) in pre- and postsynaptic neurons (+/- strength of long-term potentiation resp. depression)

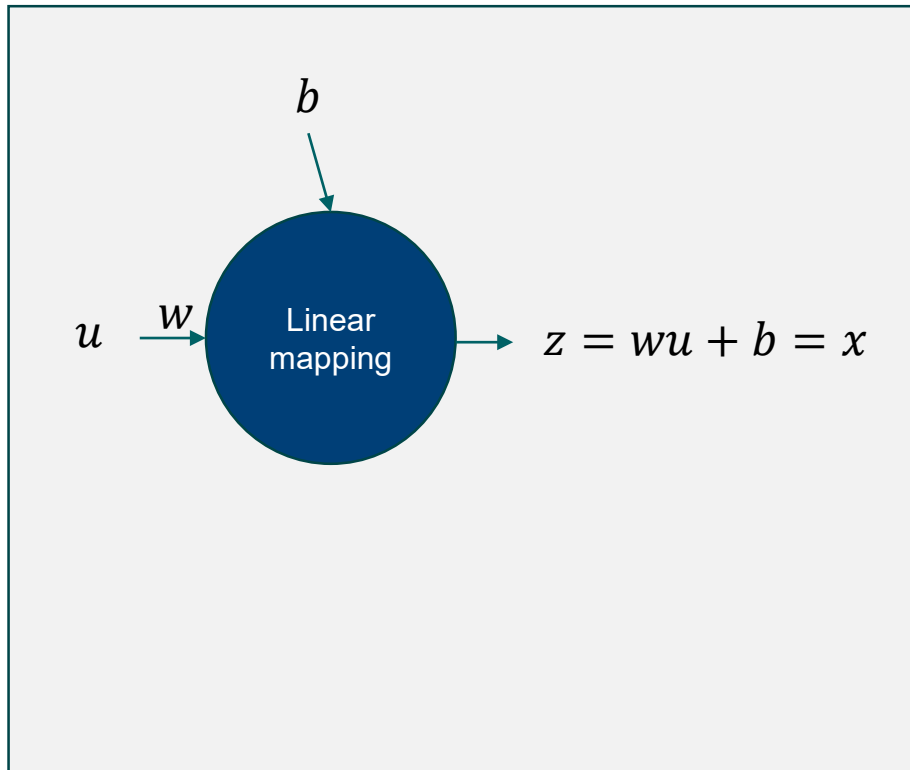




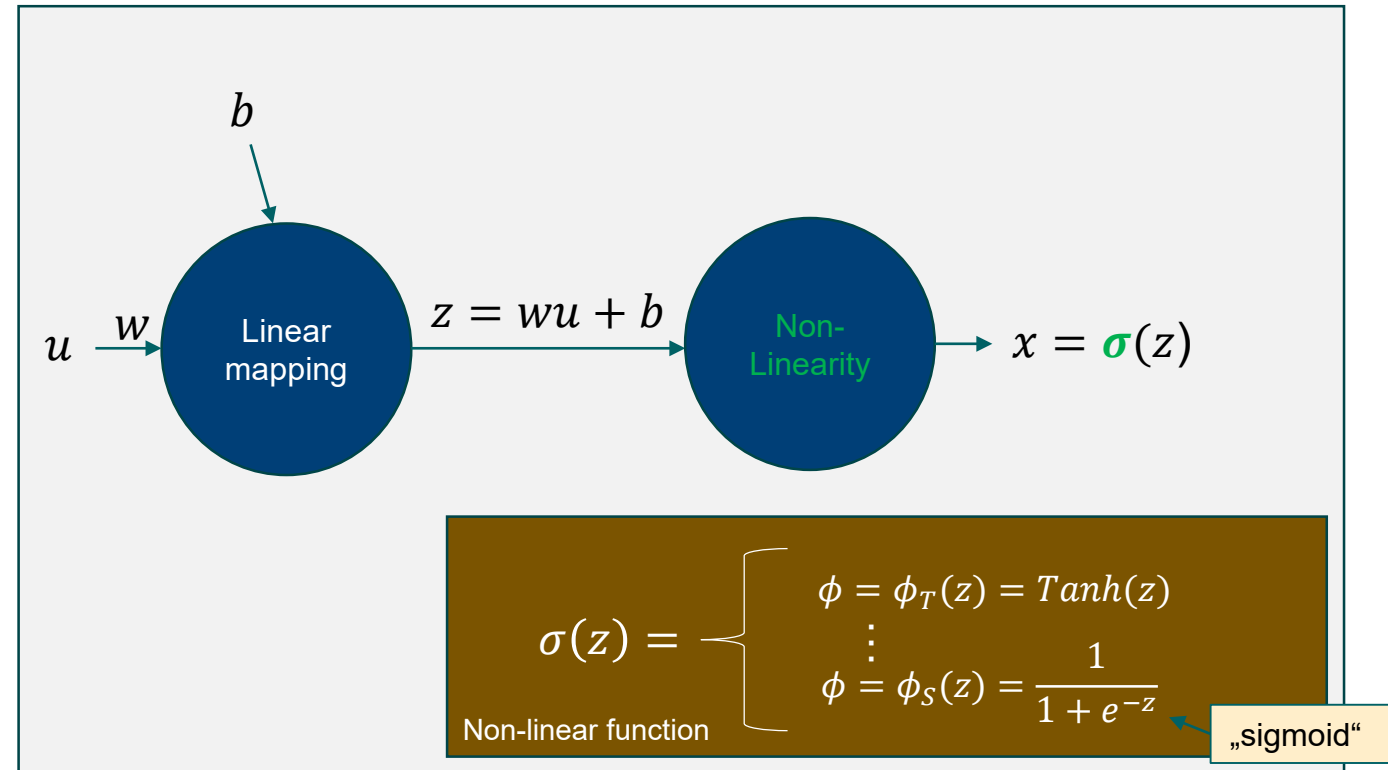
## Neuron model – Synapse dynamics



## Artificial neuron

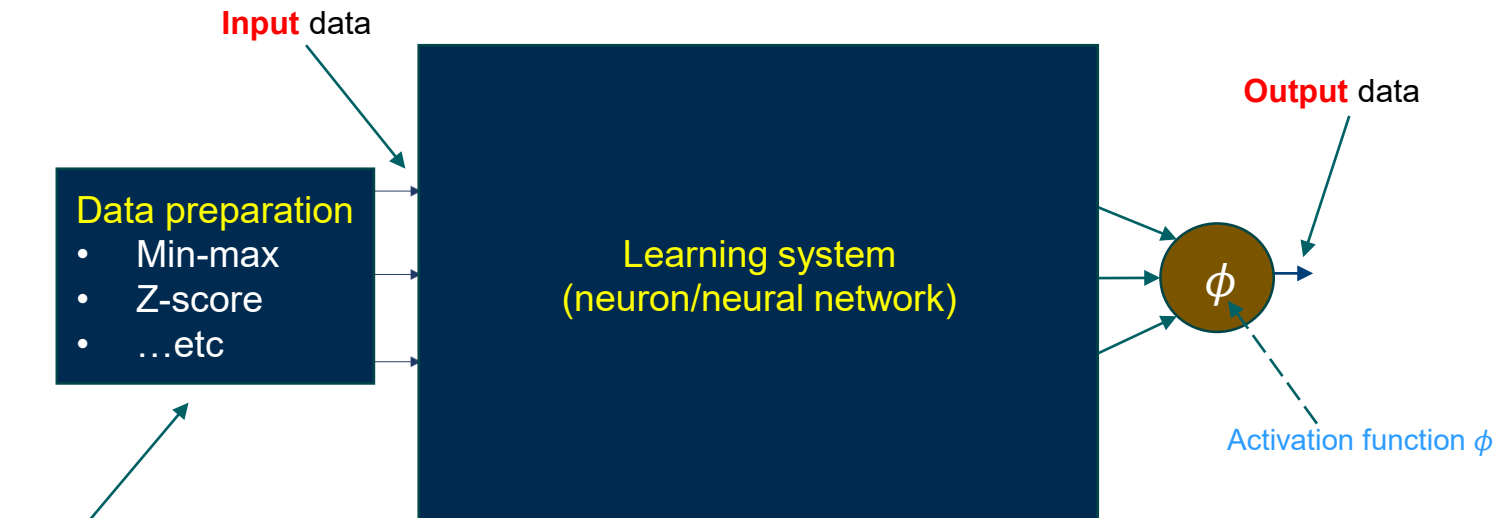


Identity activation



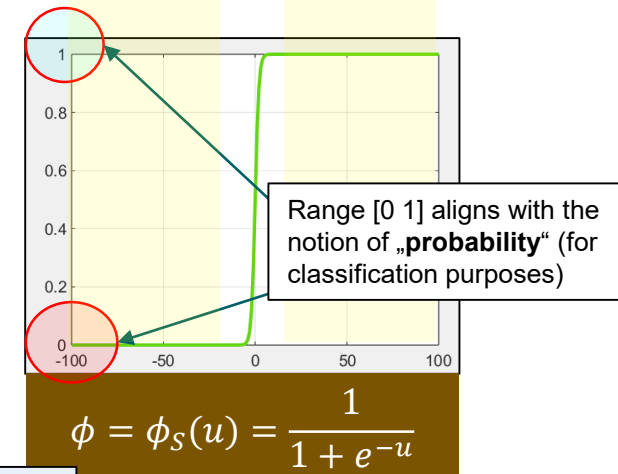
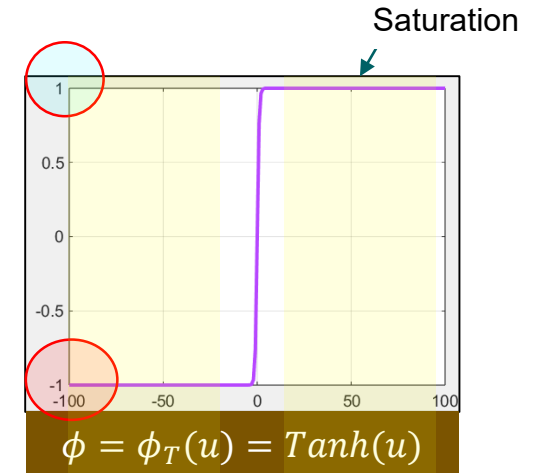
From identity activation to **non-linear** activation

## Data preparation and activation function



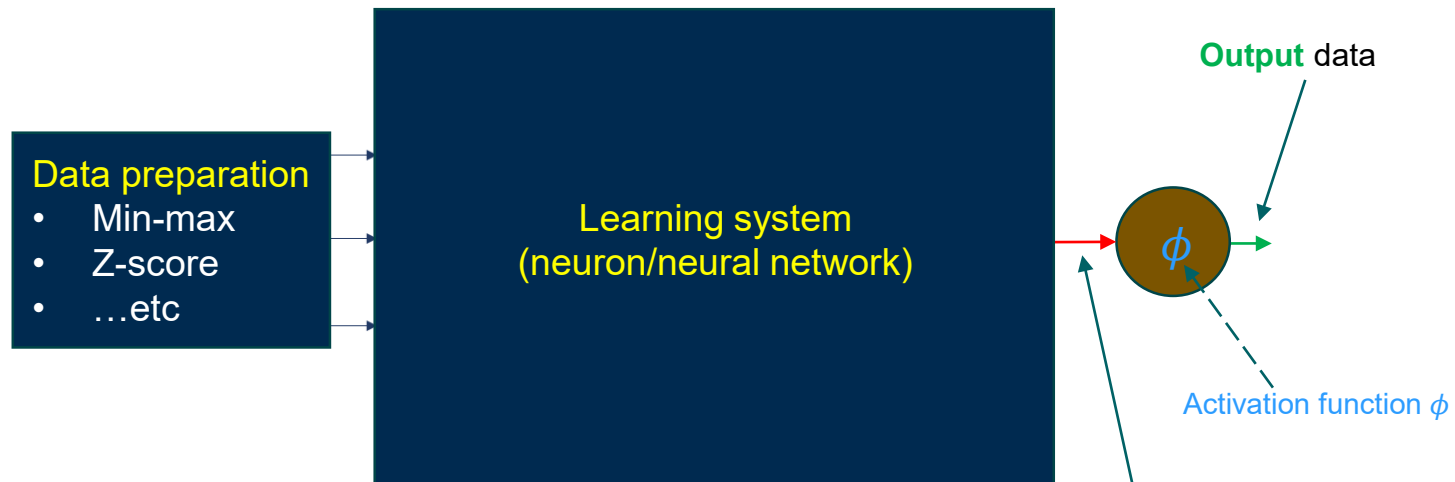
### Data preparation helps

- keep the input training data in the **range** of the **activation function  $\phi$**
- **accelerate** the training process



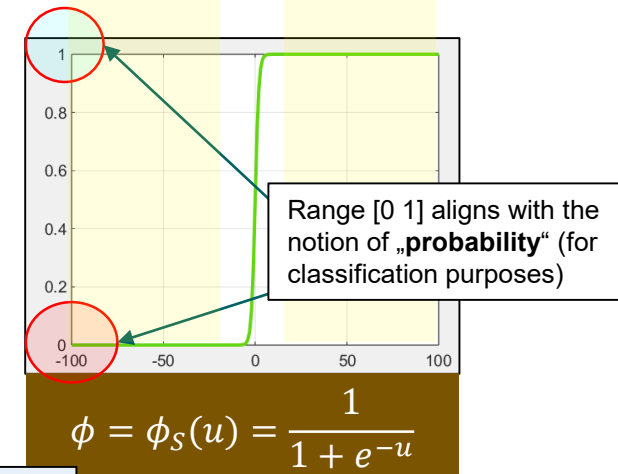
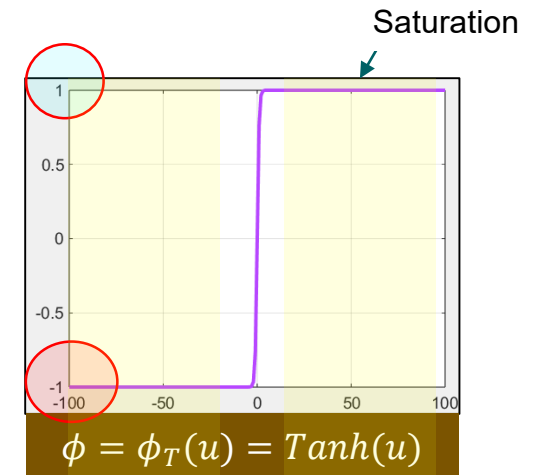
Called  
„Sigmoid“

## Activation function - Saturation



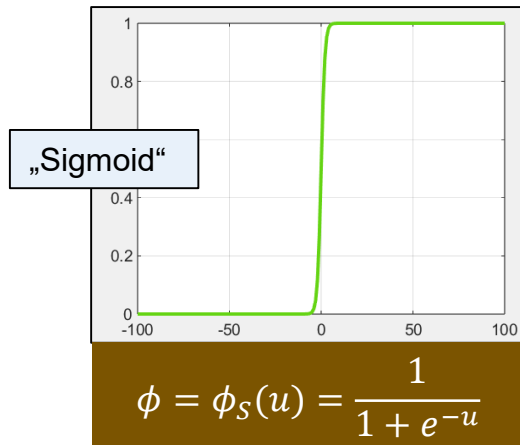
### When saturated

- **Output** of the **activation function  $\phi$**  does not respond to variations of its **input**
- learning capabilities drop, as potentially captured non-linear mappings are limited



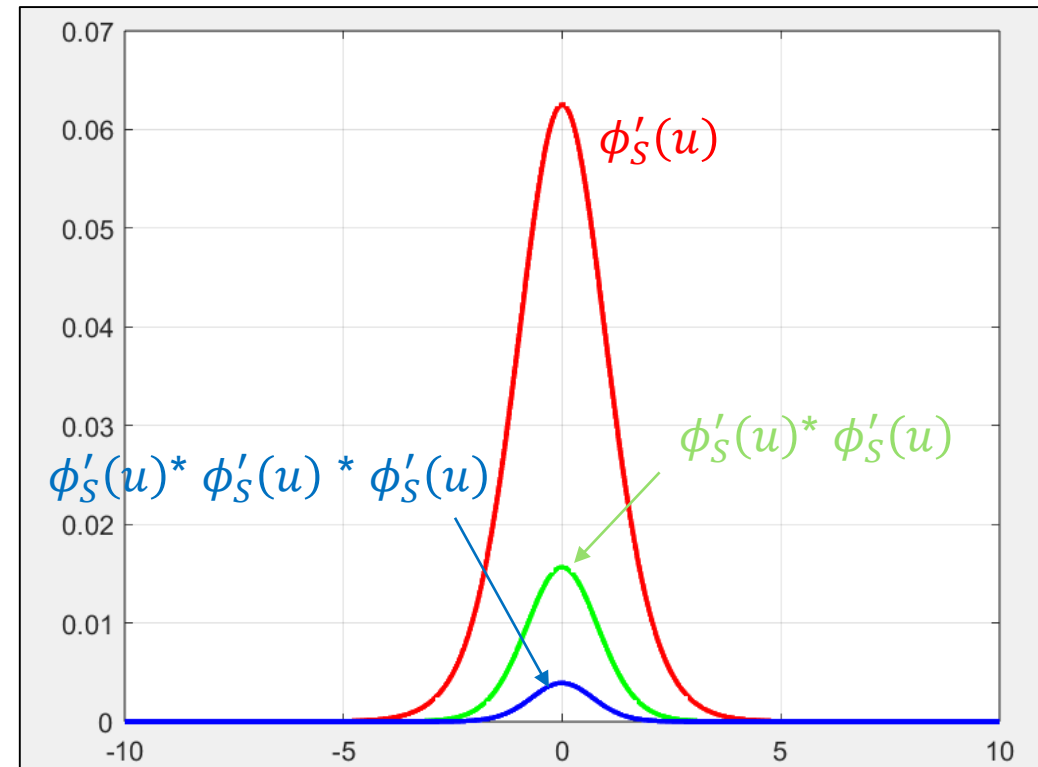
Called  
„Sigmoid“

## Activation function – Product of derivatives



„Sigmoid derivative“

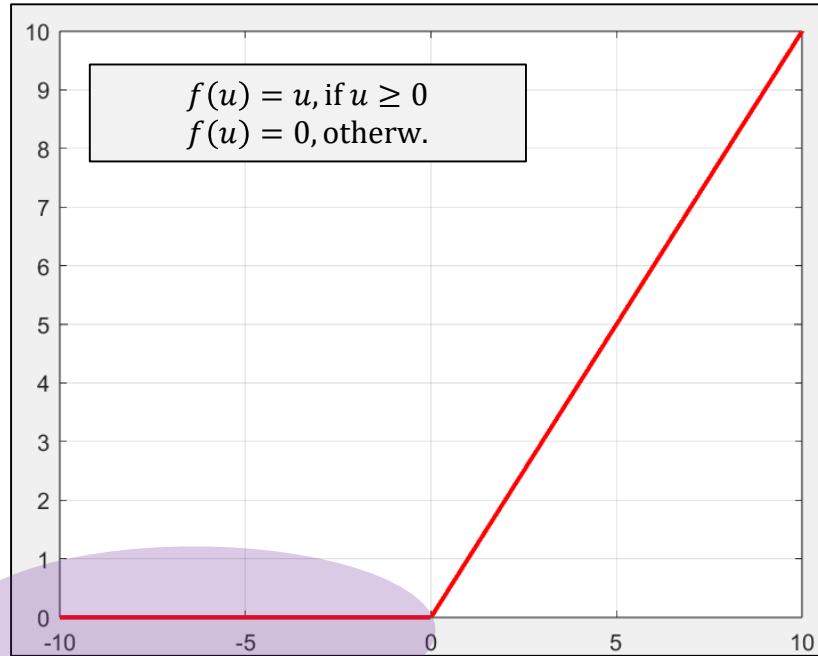
$$\phi'_S(u) = (1 - \phi_S(u))\phi_S(u)$$



**Observation:** The amplitude of the product of the derivative  $\phi'_S(u)$  by itself decreases with the increasing number of product terms.

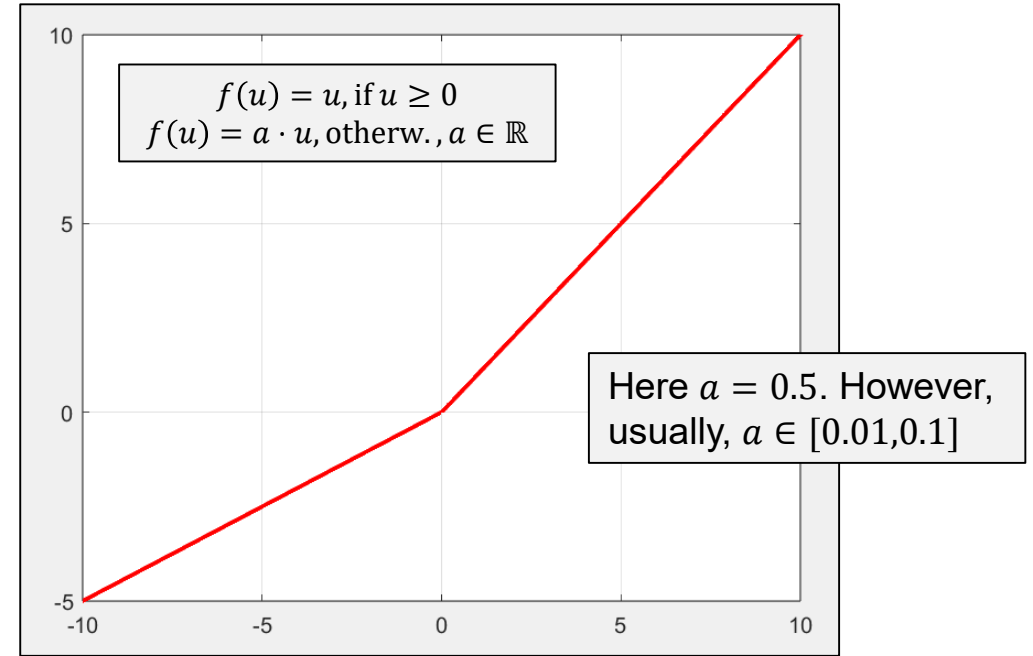
**Application#3:** verify above-mentioned behavior ( $\phi'_S(u) * \dots * \phi'_S(u)$ ) of the sigmoid by writing and executing a matlab code for three product terms.

## Activation function – Fixing saturation issues



Rectified Linear Unit (ReLU) Activation

- Not sensitive to negative inputs (might lead to dead neuron!)
- Unbounded for positive inputs



Leaky Rectified Linear Unit (LReLU)

- Customized response (via  $a$ ) to negative inputs (helps control the amplitude of derivative for negative inputs)
- Unbounded and no saturation hazard (thus: enhances learning rate during (optimization-based) learning)



## Activation function – Fixing derivative issues

### Data preparation

- Min-max
- Z-score
- ...etc

Learning system  
(via parameter optimization)

$\phi$

Activation function  $\phi$

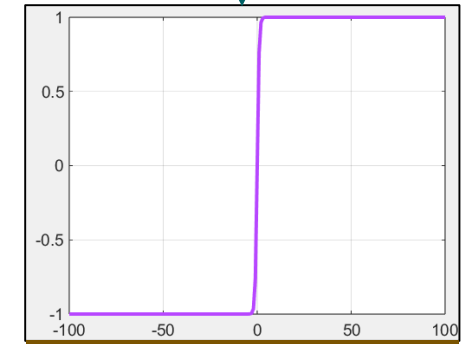
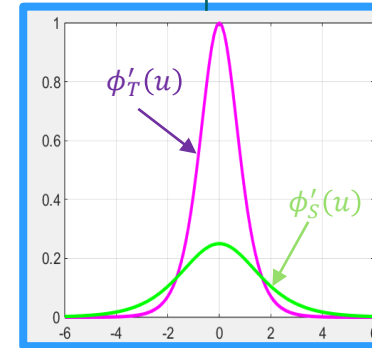
### Derivative of $\phi_T$ and $\phi_S$ :

$$\phi'_T(u) = 1 - \tanh^2(u)$$

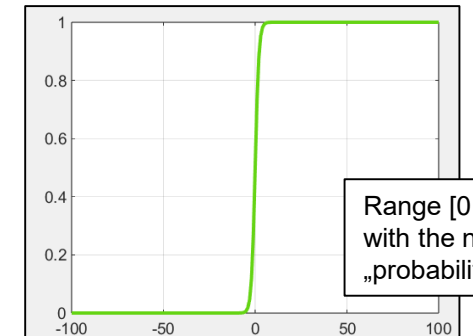
„Sigmoid derivative“

$$\phi'_S(u) = (1 - \phi_S(u))\phi_S(u)$$

$\phi_T(u)$  provides a  
larger derivative  
(i.e., “gradient”,  
more in short)



$$\phi = \phi_T(u) = \tanh(u)$$

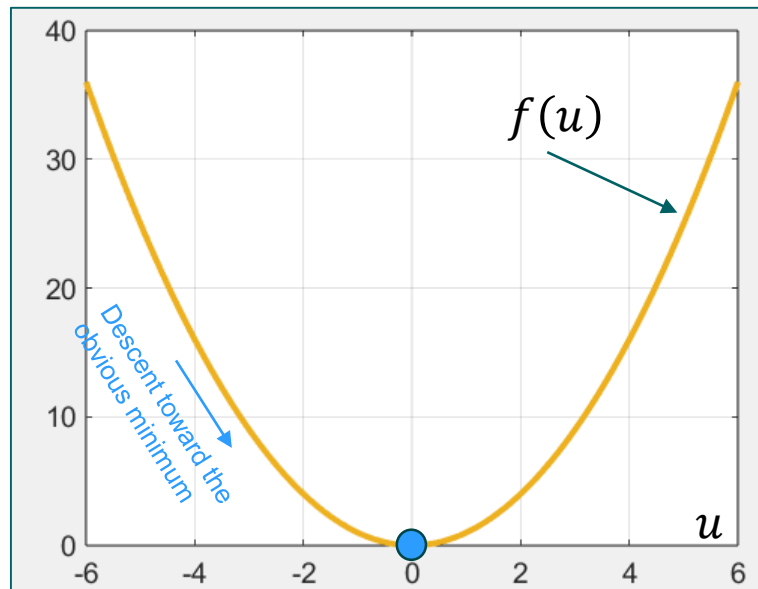


Range [0 1] aligns  
with the notion of  
„probability“

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

## What is an „optimization“ and how does it work?

**Goal:** looking for a location with „maximum“ or „minimum“ function value



**Optimization goal:** find  $u^*$  that e.g. minimizes the 1D (or n-D) loss function  $f(u)$ .

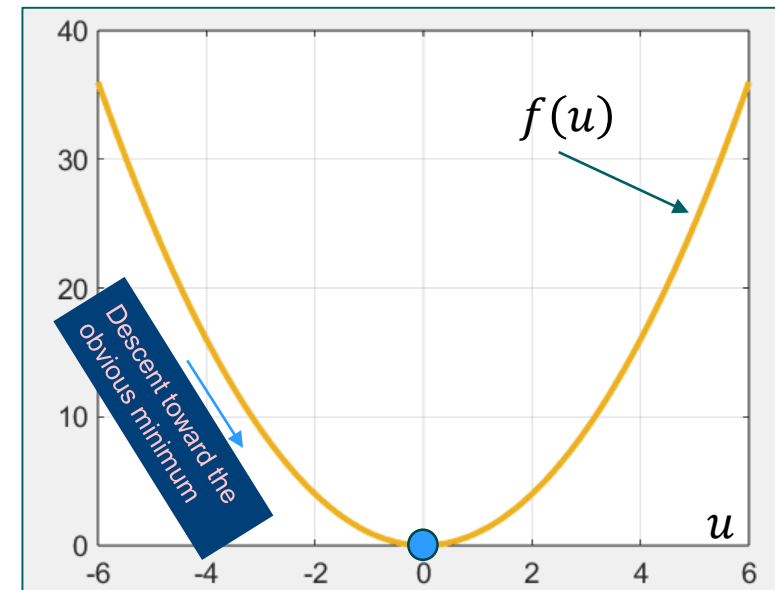
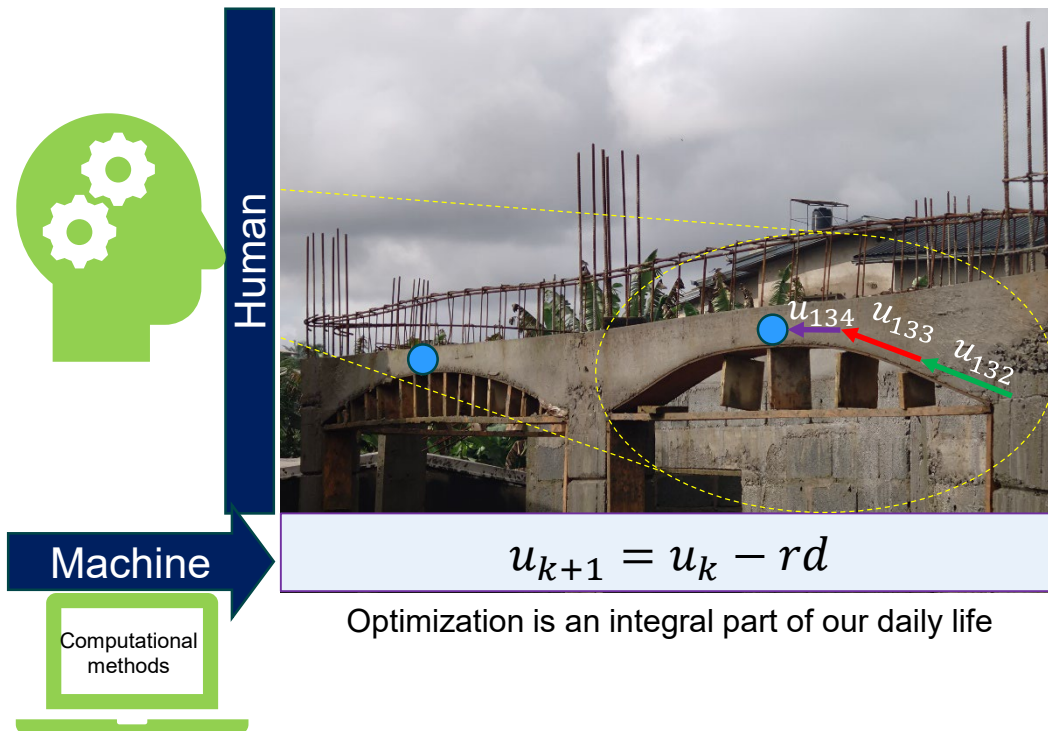


$$u_{k+1} = u_k - rd$$

Optimization is an integral part of our daily life

Whereas **humans** tend to perceive optimum in some cases **from experiences** (see, e.g., r.h.s), the **gradient** can help **machines** do so in a systematic way!

## What is an „optimization“ and how does it work?



**Optimization goal:** find  $u^*$  that e.g. minimizes the 1D (or n-D) loss function  $f(u)$ .

While humans tend to perceive an optimum in some cases (see, e.g., l.h.s), the gradient  $d$  can help machines do so in a systematic way with rate  $r$ !

## What is a gradient?

- Preliminary:  $x = f(u)$  is a real function of a real variable  $u$ .
- Gradient  $\nabla f(u)_{u_0}$  of  $f(u)$  w.r.t  $u$  at position  $u = u_0$  is given by

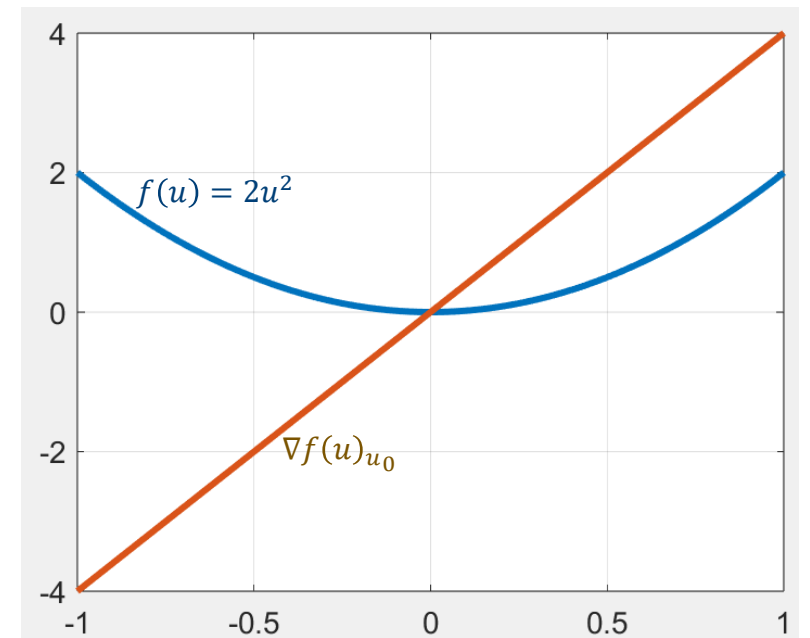
$$\nabla f(u)_{u_0} = \left. \frac{\partial f(u)}{\partial u} \right|_{u=u_0}$$

$f$  is differentiable at  $u_0$

1. Order derivative w.r.t  $u$  at  $u = u_0$

In the  $n$ -dimensional space:  $f: \mathbb{R}^n \rightarrow \mathbb{R}$

- $u = (u_1, \dots, u_n)$
- $\nabla f(u)_{u_0} = \left[ \frac{\partial f(u)}{\partial u_1}, \dots, \frac{\partial f(u)}{\partial u_n} \right]_{u=u_0}^T$



Gradient example

## What is a gradient?

- Preliminary:  $x = f(u)$  is a real function of a real variable  $u$ .
- Gradient  $\nabla f(u)_{u_0}$  of  $f(u)$  w.r.t  $u$  at position  $u = u_0$  is given by

$$\nabla f(u)_{u_0} = \left. \frac{\partial f(u)}{\partial u} \right|_{u=u_0}$$

1.Order derivative w.r.t  $u$  at  $u = u_0$

### Application #4:

- $f(u) = u^2 \rightarrow \nabla f(u)_{u_0=1} = \left. \frac{\partial f(u)}{\partial u} \right|_{u=1} = \left. \frac{\partial u^2}{\partial u} \right|_{u=1} = 2u|_{u=1} = 2 \cdot 1 = 2$
- $f(u) = \frac{1}{u-1} \rightarrow \nabla f(u)_{u_0=0} = \left. \frac{\partial f(u)}{\partial u} \right|_{u=0} = \left. \frac{0-1}{(u-1)^2} \right|_{u=0} = -1$

## Application #5

### Challenge:

$$x = f(u_1, u_2) = 2u_1^3 + \ln(u_2)$$

Calculate the gradient of  $f(u_1, u_2)$  at  $u = (u_1, u_2)$

### Solution:


$$x = f(u_1, \dots, u_n) \rightarrow \nabla f = \begin{bmatrix} \frac{\partial f}{\partial u_1} \\ \vdots \\ \frac{\partial f}{\partial u_n} \end{bmatrix} \quad \nabla f = \begin{bmatrix} 6u_1^2 \\ \frac{1}{u_2} \end{bmatrix}$$

## Application #6

### Challenge:

$$x = f(u_1, u_2) = -u_2^2 + u_2 + 17$$

Calculate the gradient of  $f(u_1, u_2)$  at  $u = (u_1, u_2)$

### Solution:

$$x = f(u_1, \dots, u_n) \rightarrow \nabla f = \begin{bmatrix} \frac{\partial f}{\partial u_1} \\ \vdots \\ \frac{\partial f}{\partial u_n} \end{bmatrix} \longrightarrow \nabla f = \begin{bmatrix} 0 \\ -2u_2 + 1 \end{bmatrix}$$

## Application #7

### Challenge:

$$x = f(u_1, u_2) = -u_1 u_2^2 + u_1 u_2 + 17u_2$$

Calculate the gradient of  $f(u_1, u_2)$  at  $u = (u_1, u_2)$

### Solution:

$$x = f(u_1, \dots, u_n) \rightarrow \nabla f = \begin{bmatrix} \frac{\partial f}{\partial u_1} \\ \vdots \\ \frac{\partial f}{\partial u_n} \end{bmatrix}$$



$$\nabla f = \begin{bmatrix} -u_2^2 + u_2 \\ -2u_1 u_2 + u_1 + 17 \end{bmatrix}$$




## Application #8

### Challenge:

$$x = f(u_1, u_2, u_3) = -u_1 u_2^2 u_3 + u_1 u_2 + 17u_2 + u_3$$

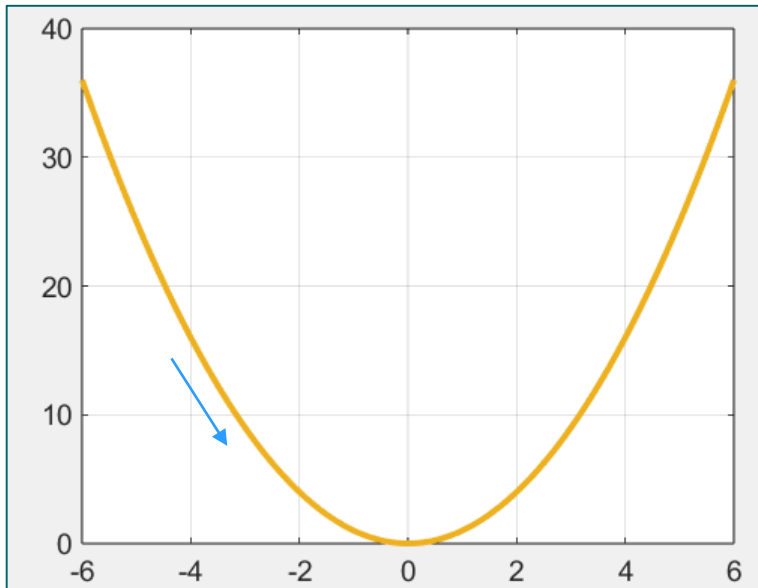
Calculate the gradient of  $f(u_1, u_2, u_3)$  at  $u = (u_1, u_2, u_3)$

### Solution:


$$x = f(u_1, \dots, u_n) \rightarrow \nabla f = \begin{bmatrix} \frac{\partial f}{\partial u_1} \\ \vdots \\ \frac{\partial f}{\partial u_n} \end{bmatrix} \quad \longrightarrow \quad \nabla f = \begin{bmatrix} -u_2^2 u_3 + u_2 \\ -2u_1 u_3 u_2 + u_1 + 17 \\ -u_1 u_2^2 + 1 \end{bmatrix}$$

## Why is the gradient useful?

- Suppose that we have a function  $x = f(u) = u^2$



How to find  $u^*$  that minimize  $f(u)$ ?

## Approach:

$$u_{k+1} = u_k - r \overset{=d}{\nabla f(u)}_{u_k} = u_k - r \frac{\partial f(u)}{\partial u} \Big|_{u=u_k}$$

- $r$  is a **hyperparameter** that reflects the **learning rate**
- The **fastest decay** of  $f(u)$  is the **opposite direction** of the **gradient**  $\nabla f(u)$  of  $f(u)$
- Hence,  $-r \nabla f(u)$  steers the series until the convergence  $u_{k+1} \rightarrow u^*$



**Caution: Many local optima might exist**

## Optimization **routine** based upon the gradient

Goal: find minimum of  $x = f(u) = u^2$

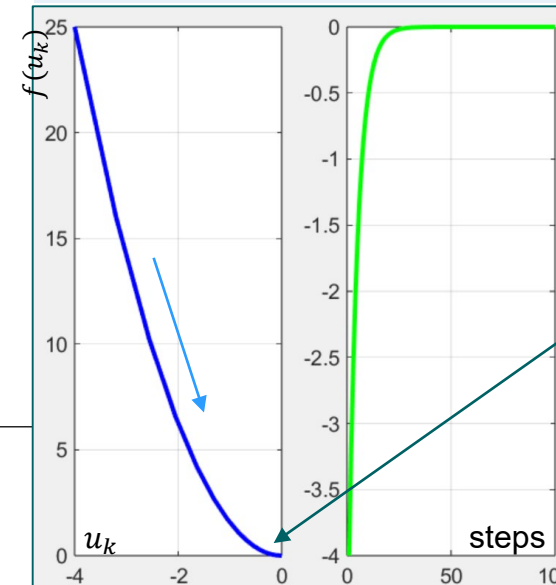
```
1 clear;
2 syms u %symbolic variable
3 f = u^2; %function to be optimized
4 c = gradient(f,u); %symbolic gradient
5 uk = -5; % initial uk value
6 r = 0.1; % learning rate
7 interval=1:100; % 100 steps
8 U=[]; functionValue=[];%container
9 for i=interval
10     u = uk;
11     uk = uk - r*subs(c); %main iteration loop
12     U=[U uk]; % for plotting
13     functionValue = [functionValue (subs(f))];
14 end
15 subplot(1,2,1); plot(U,functionValue,'b');
16 subplot(1,2,2); plot(interval,U,'g');
```

You are welcome to optimize and share the code in our lecture forum!

### Approach:

$$u_{k+1} = u_k - r \nabla f(u)_{u_k} = u_k - r \left. \frac{\partial f(u)}{\partial u} \right|_{u=u_k}$$

- $r$  is a **hyperparameter** that reflects the learning rate
- The **fastest decay** of  $f(u)$  is the **opposite direction** of the **gradient**  $\nabla f(u)$  of  $f(u)$
- Hence,  $-r \nabla f(u)$  steers the series until the convergence  $u_{k+1} \rightarrow u^*$

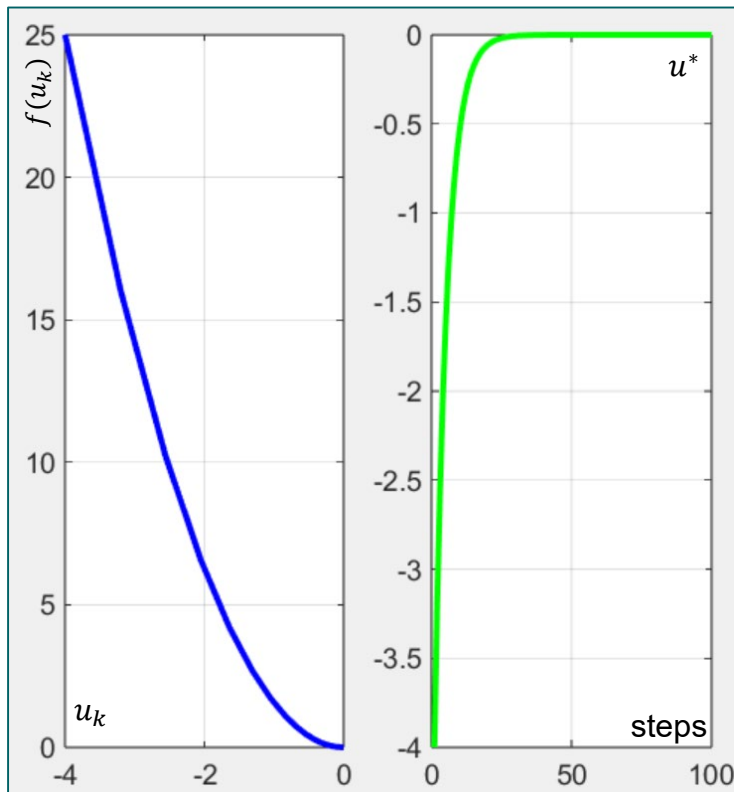


### Observations:

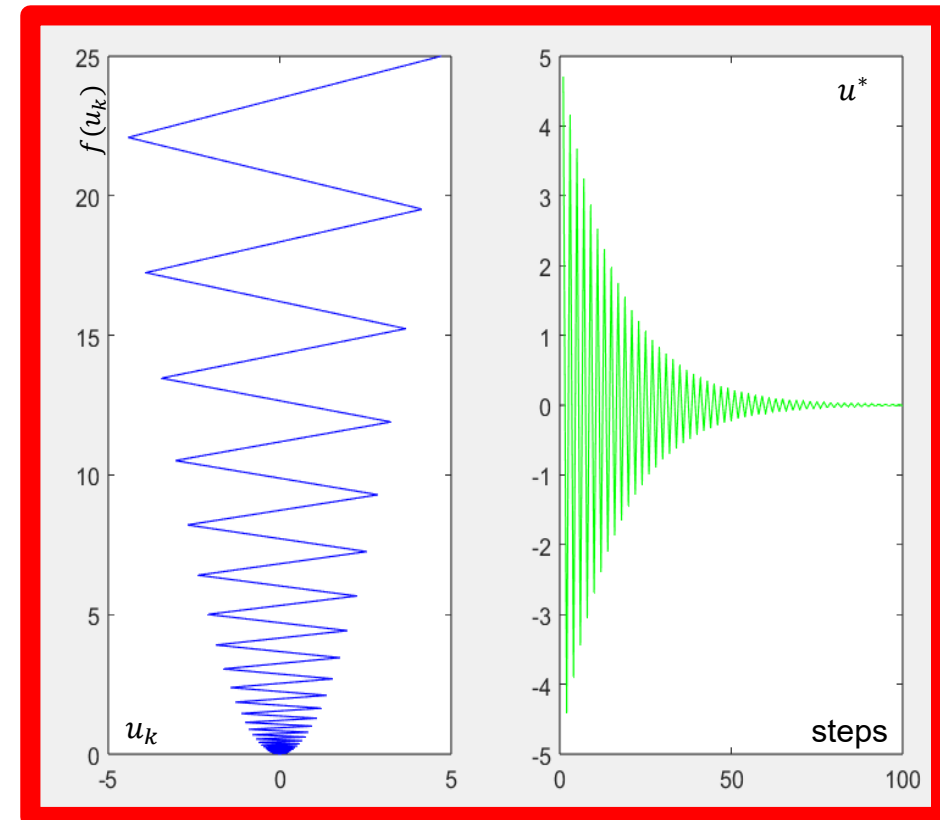
- Goal-oriented decay toward minimum value
- Minimum position  $u^*$  is attained
- **However ...**

We are aware of the gradient usefulness. The path toward usefulness can be **struggling**! Why?

- Minimizing  $x = f(u) = u^2$  to find minimum  $u = u^*$



Learning rate  $r = 0.1$ . Optimization remains smooth and fast.

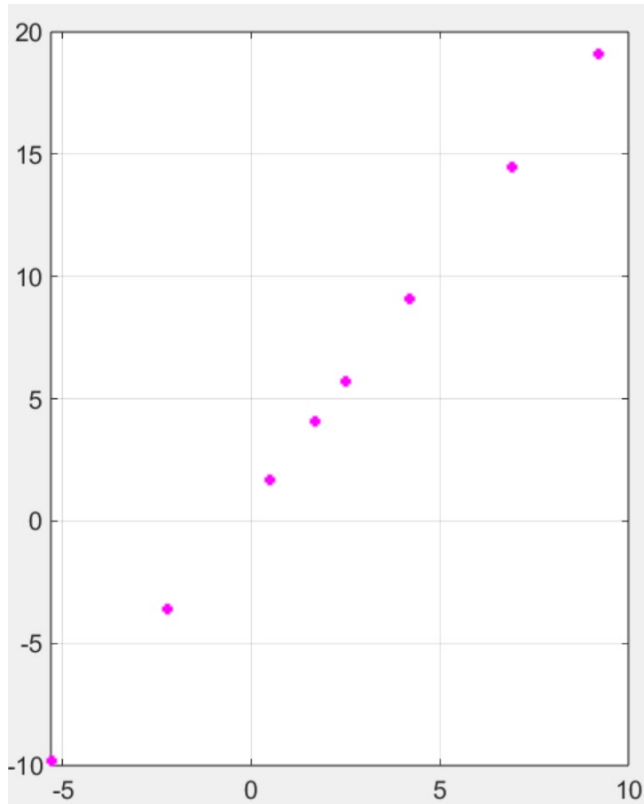


Learning rate  $r = 0.97$ . Optimization takes longer to converge while oscillating!

**Observation #1:** Values of hyperparameters  $r$  impact optimization processes!

# Linear regression

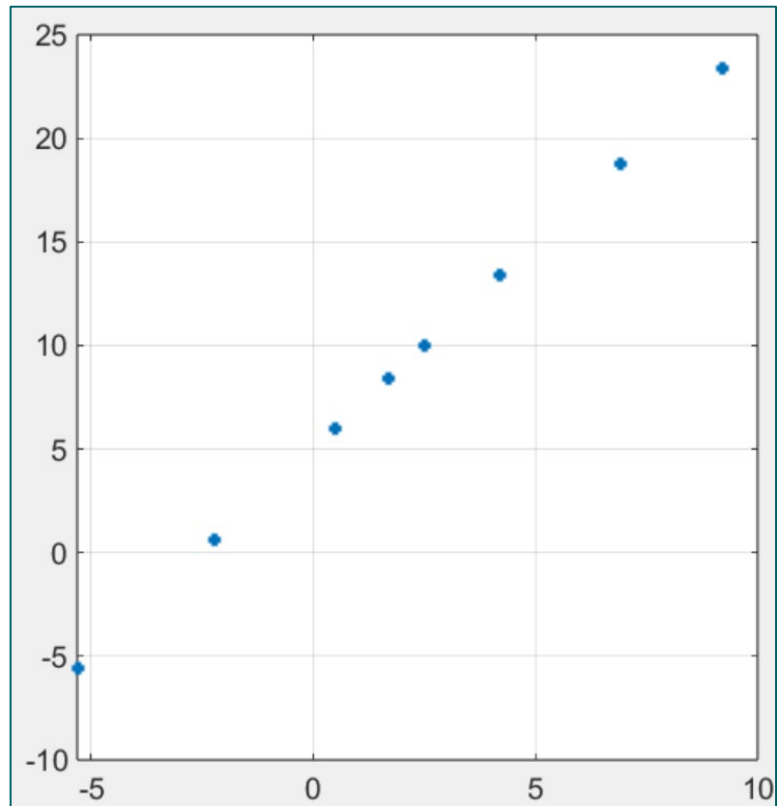
## Objective of regression – Find a function that captures the set of points



- Input:  $u = [-5.3 \ -2.2 \ 0.5 \ 1.7 \ 2.5 \ 4.2 \ 6.9 \ 9.2]^T$ ;
- Output:  $x = [-9.8 \ -3.6 \ 1.70 \ 4.1 \ 5.7 \ 9.1 \ 14.5 \ 19.1]^T$ ;

- Points A (u,x) potentially line up with a line L
- If so, then approxim. of L should read:  $\hat{x} = wu + b$
- $w$  (a scalar) is the slope, given by the **gradient**
- $b$  (also a scalar) is the „bias“

## Objective of regression – Find a function that captures the set of points



- $u = [-5.3 \ -2.2 \ 0.5 \ 1.7 \ 2.5 \ 4.2 \ 6.9 \ 9.2]^T$ ;

- $x = [-5.6 \ 0.6 \ 6.0 \ 8.4 \ 10.0 \ 13.4 \ 18.8 \ 23.4]^T$ ;

$\frac{\partial f}{\partial u_1}$  is growth rate of  $f([u_1 \dots u_n])$  in the  $u_1$  direction

Hint:

$x = f(u_1, \dots, u_n) \rightarrow \nabla f = \begin{bmatrix} \frac{\partial f}{\partial u_1} \\ \vdots \\ \frac{\partial f}{\partial u_n} \end{bmatrix}$  is a vector of  $\mathbb{R}^n$ !

$\nabla f$  is the direction of the steepest **ascent** (hence,  $-\nabla f$  is the direction of steepest **descent**) at  $u$ .

Goal: learning  $w$  and  $b$  that min.  $L(w, b)$

- Gradient  $\nabla L(w, b) = \begin{bmatrix} \frac{\partial L(w, b)}{\partial w} \\ \frac{\partial L(w, b)}{\partial b} \end{bmatrix} = \sum_{i=1}^n \begin{bmatrix} 2u(\hat{x}_i - x_i) \\ 2(\hat{x}_i - x_i) \end{bmatrix}$

- $u_{k+1} = u_k - r \nabla L(u)_{u_k}, u_k = [w_k \ b_k]^T$

Hint:

$$\begin{aligned} \frac{\partial L}{\partial w} &= \frac{\partial L}{\partial \hat{x}} \frac{\partial \hat{x}}{\partial w} \\ \frac{\partial L}{\partial b} &= \frac{\partial L}{\partial \hat{x}} \frac{\partial \hat{x}}{\partial b} \end{aligned}$$

## Optimization pitfall





## When to update the **parameters**?

**Hint:**

$$\frac{\partial L}{\partial w} = \frac{\partial L}{\partial \hat{x}} \frac{\partial \hat{x}}{\partial w}$$
$$\frac{\partial L}{\partial b} = \frac{\partial L}{\partial \hat{x}} \frac{\partial \hat{x}}{\partial b}$$

- Line  $\hat{x} = wu + b$
- Loss  $L(w, b) = \sum_{i=1}^n (\hat{x}_i - x_i)^2$
- Gradient  $\nabla L(w, b) = \begin{bmatrix} \frac{\partial L(w, b)}{\partial w} \\ \frac{\partial L(w, b)}{\partial b} \end{bmatrix} = \sum_{i=1}^n \begin{bmatrix} 2u(\hat{x}_i - x_i) \\ 2(\hat{x}_i - x_i) \end{bmatrix}$
- $u_{k+1} = u_k - r \nabla L(u)_{u_k}, u_k = [w_k \ b_k]^T$

### Gradient descent:

Update after a loss evaluation related to **all training data samples** (after each **epoch**)

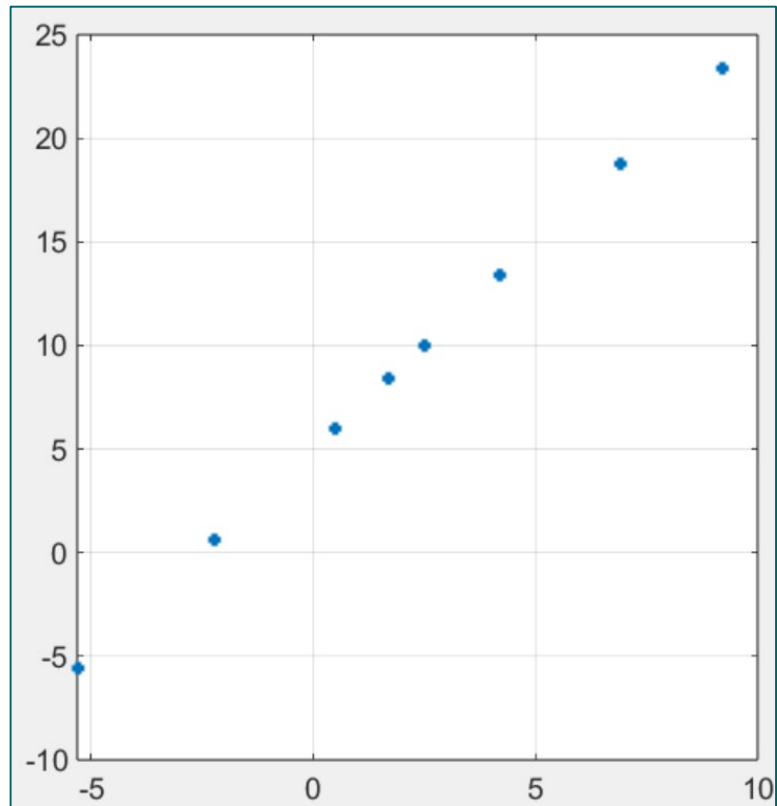
### Stochastic gradient descent:

Update after the loss related to **a training data sample** has been computed

### Mini-**batch** stochastic gradient descent:

Update after the loss related to **a number of training data samples** has been computed

## Application #9: Write and execute a Matlab code that learns $w$ and $b$ !



- $u = [-5.3 \ -2.2 \ 0.5 \ 1.7 \ 2.5 \ 4.2 \ 6.9 \ 9.2]^T$ ;

- $x = [-5.6 \ 0.6 \ 6.0 \ 8.4 \ 10.0 \ 13.4 \ 18.8 \ 23.4]^T$ ;

$\frac{\partial f}{\partial u_1}$  is growth rate of  $f([u_1 \dots u_n])$  in the  $u_1$  direction

- Line  $\hat{x} = wu + b$

- Loss  $L(w, b) = \sum_{i=1}^n (\hat{x}_i - x_i)^2$

Hint:

$x = f(u_1, \dots, u_n) \rightarrow \nabla f = \begin{bmatrix} \frac{\partial f}{\partial u_1} \\ \vdots \\ \frac{\partial f}{\partial u_n} \end{bmatrix}$  is a vector of  $\mathbb{R}^n$ !

Goal: learning  $w$  and  $b$  that min.  $L(w, b)$

- Gradient  $\nabla L(w, b) = \begin{bmatrix} \frac{\partial L(w, b)}{\partial w} \\ \frac{\partial L(w, b)}{\partial b} \end{bmatrix} = \sum_{i=1}^n \begin{bmatrix} 2u(\hat{x}_i - x_i) \\ 2(\hat{x}_i - x_i) \end{bmatrix}$

$\nabla f$  is the direction of the steepest **ascent** (hence,  $-\nabla f$  is the direction of steepest **descent**) at  $u$ .

- $u_{k+1} = u_k - r \nabla L(u)_{u_k}, u_k = [w_k \ b_k]^T$

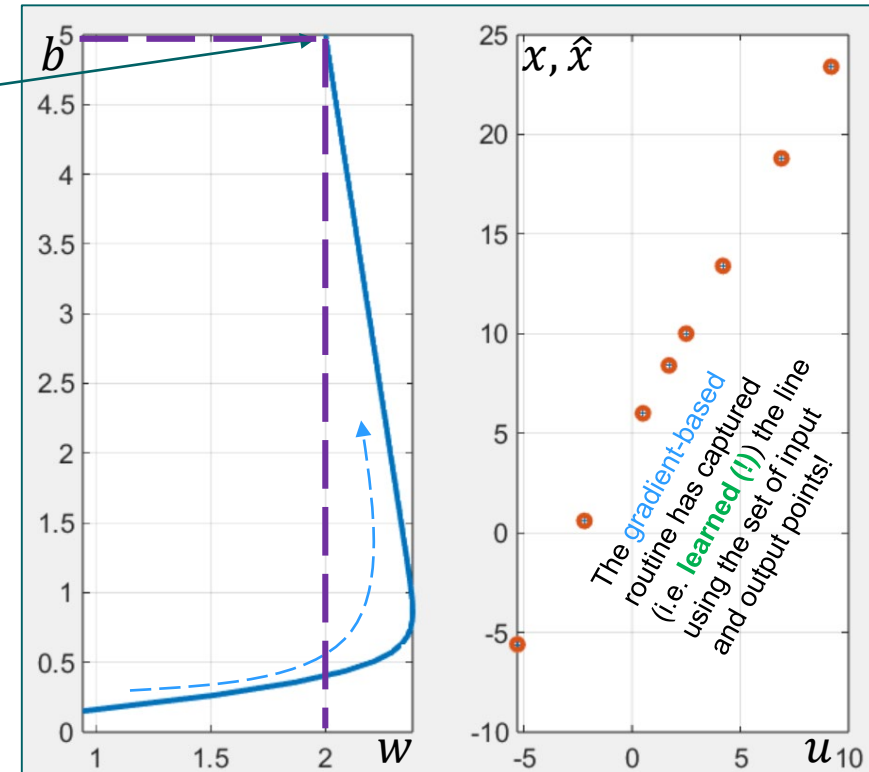
Hint:

$$\begin{aligned} \frac{\partial L}{\partial w} &= \frac{\partial L}{\partial \hat{x}} \frac{\partial \hat{x}}{\partial w} \\ \frac{\partial L}{\partial b} &= \frac{\partial L}{\partial \hat{x}} \frac{\partial \hat{x}}{\partial b} \end{aligned}$$

## Objective of regression – Find a function that captures the set of points

```
1 clear; clc;
2 input = [-5.3 -2.2 0.5 1.7 2.5 4.2 6.9 9.2];
3 output = [-5.6 0.6 6.0 8.4 10.0 13.4 18.8 23.4]; %ou = 2*in+5
4 uk=[0;0];
5 r = 0.001; U = []; w = 0; b = 0;
6 for i = 1:10000
7     uk = uk - r*gradientloss(uk,input,output);
8     U = [U uk]; w = uk(1); b = uk(2);
9 end
10
11 subplot(1,2,1); plot(U(1,:),U(2,:));
12 subplot(1,2,2); plot(input,output,'+'); hold on; plot(input,w*input+b,'o');
13
14 function [r] =gradientloss (uk, in, out)
15     r1 = sum(2*(uk(1)*in+uk(2)-out).*in);
16     r2 = sum(2*(uk(1)*in+uk(2)-out) );
17     r=[r1;r2];
18 end
```

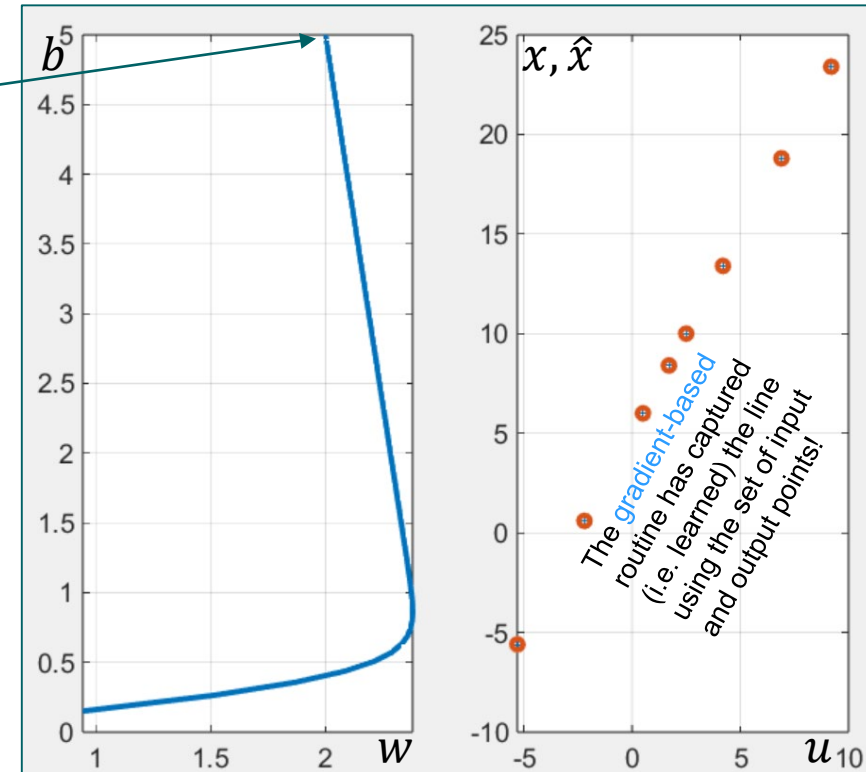
Ground truth



Once we have the weights  $w$  and  $b$ , we have **captured** the mapping between input and output data!

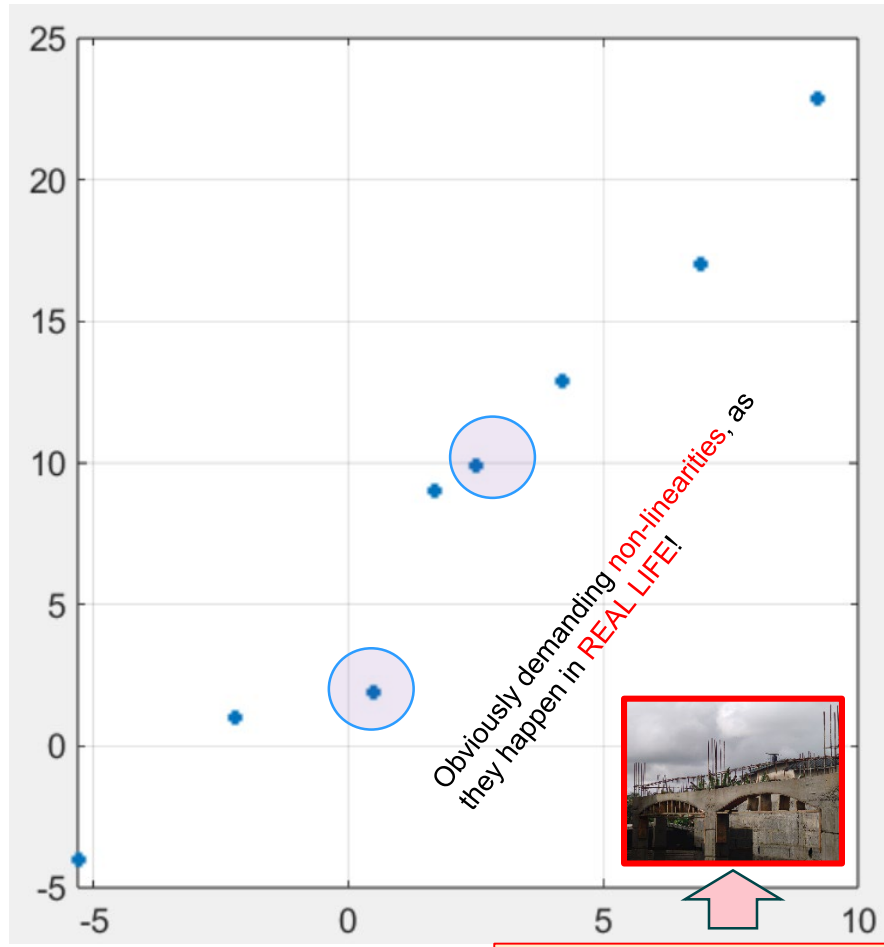
## Objective of regression – Find a function that captures the set of points

```
1 clear; clc;
2 input = [-5.3 -2.2 0.5 1.7 2.5 4.2 6.9 9.2];
3 output = [-5.6 0.6 6.0 8.4 10.0 13.4 18.8 23.4]; %ou = 2*in+5
4 uk = [0;0];
5 r = 0.001; U = []; w = 0; b = 0;
6 for i = 1:10000
7     uk = uk - r*gradientloss(uk,input,output);
8     U = [U uk]; w = uk(1); b = uk(2);
9 end
10
11 subplot(1,2,1); plot(U(1,:),U(2,:));
12 subplot(1,2,2); plot(input,output,'+'); hold on; plot(input,w*input+b,'o');
13
14 function [r] = gradientloss (uk, in, out)
15     r1 = sum(2*(uk(1)*in+uk(2)-out).*in);
16     r2 = sum(2*(uk(1)*in+uk(2)-out));
17     r = [r1;r2];
18 end
```



**Observation #2:** Gradient helps LEARN the mapping (Here:  $\hat{x} = wu + b$ ) using input & output data! However...

## Objective – Find a function that captures the set of points



- $u = [-5.3 \ -2.2 \ 0.5 \ 1.7 \ 2.5 \ 4.2 \ 6.9 \ 9.2];$
- $x = [-4.0 \ 1.0 \ 1.9 \ 9.0 \ 9.90 \ 12.9 \ 17.0 \ 22.9];$

- Still a line  $\hat{x} = wu + b$  ?!

- Loss  $L(w, b) = \sum_{i=1}^n (\hat{x}_i - x_i)^2$

- Gradient  $\nabla L(w, b) = \begin{bmatrix} \frac{\partial L(w, b)}{\partial w} \\ \frac{\partial L(w, b)}{\partial b} \end{bmatrix} = \sum_{i=1}^n \begin{bmatrix} 2u(\hat{x}_i - x_i) \\ 2(\hat{x}_i - x_i) \end{bmatrix}$

- $u_{k+1} = u_k - r \nabla L(u)_{u_k}, u_k = [w_k \ b_k]^T$

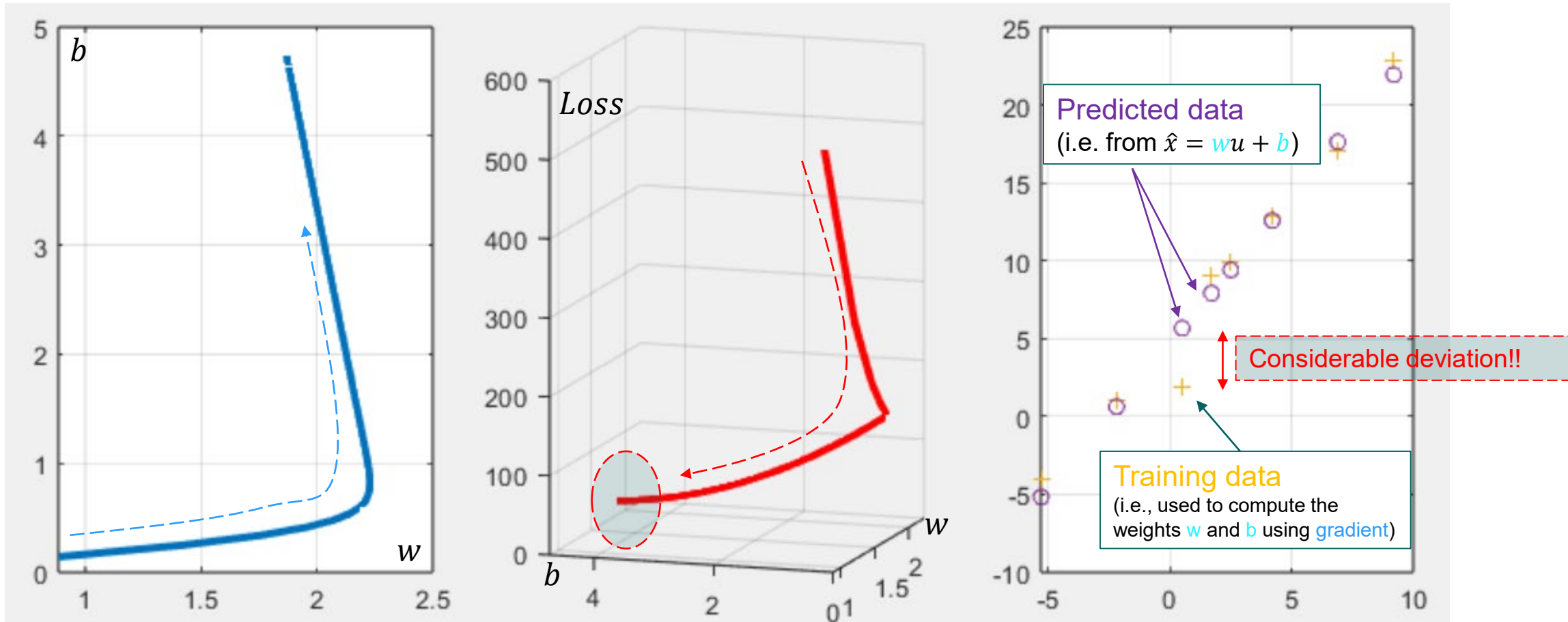
Hint:

$$x = f(u_1, \dots, u_n) \rightarrow \nabla f = \begin{bmatrix} \frac{\partial f}{\partial u_1} \\ \vdots \\ \frac{\partial f}{\partial u_n} \end{bmatrix}$$

...how good does this approach with **linearity assumption** perform?!

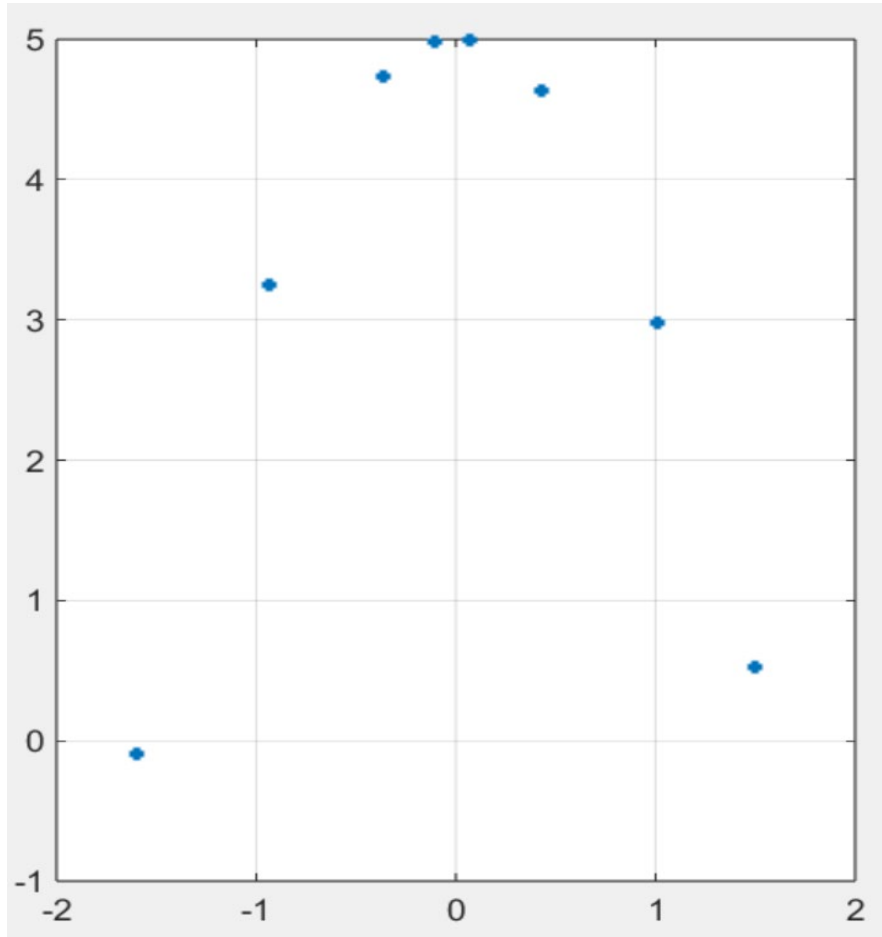
**Recall:** the real world (and thus application data...) is (mostly) **non-linear**.

## Objective – Find a function that captures the set of points



Dynamics of optimization of weights

## Objective – Find a function that captures the set of points



- $u = [-1.5967 \quad -0.9356 \quad -0.3599 \quad -0.1040 \quad 0.0666 \quad 0.4292 \quad 1.0049 \quad 1.4954];$
- $x = [-0.0990 \quad 3.2492 \quad 4.7410 \quad 4.9784 \quad 4.9911 \quad 4.6316 \quad 2.9802 \quad 0.5275];$

- Obviously **not** a line  $\hat{x} = wu + b!$

- Loss  $L(w, b) = \sum_{i=1}^n (\hat{x}_i - x_i)^2$

- Gradient  $\nabla L(w, b) = \begin{bmatrix} \frac{\partial L(w, b)}{\partial w} \\ \frac{\partial L(w, b)}{\partial b} \end{bmatrix} = \sum_{i=1}^n \begin{bmatrix} 2u(\hat{x}_i - x_i) \\ 2(\hat{x}_i - x_i) \end{bmatrix}$

- $u_{k+1} = u_k - r \nabla L(u)_{u_k}, u_k = [w_k \ b_k]^T$

Hint:

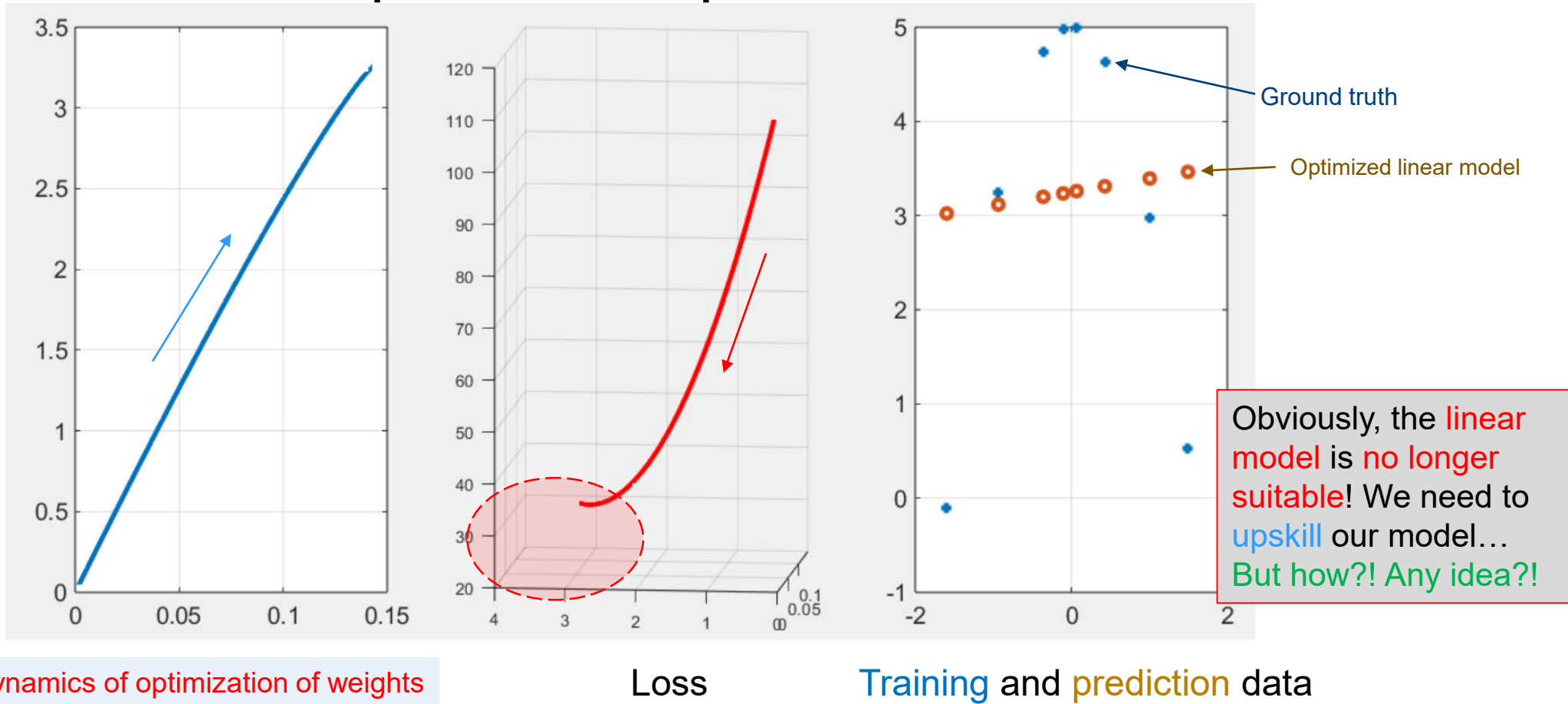
$$x = f(u_1, \dots, u_n) \rightarrow \nabla f = \begin{bmatrix} \frac{\partial f}{\partial u_1} \\ \vdots \\ \frac{\partial f}{\partial u_n} \end{bmatrix}$$

...**how good** does this approach with **linearity assumption** perform?!



# Robotics and Machine Learning – Model Capture

**Objective – Find a function that captures the set of points**

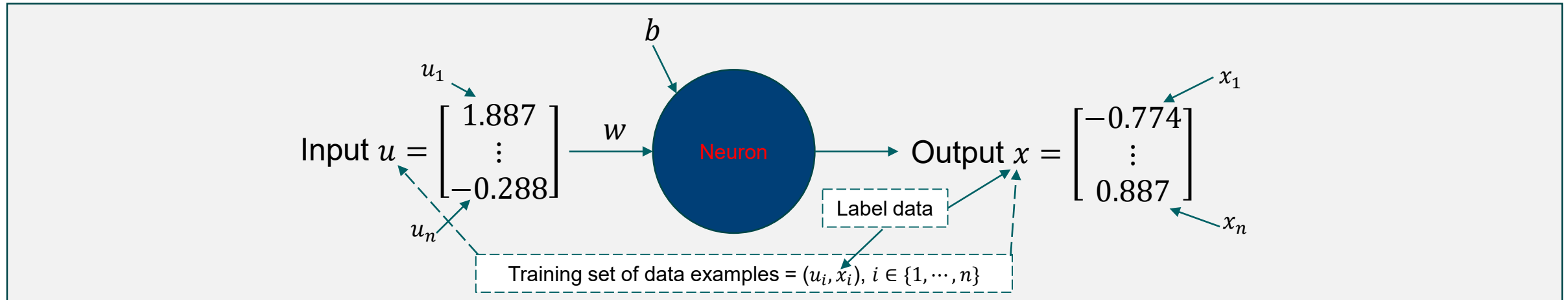


**Observation #3:** The performance of  $\hat{x} = wu + b$  drops as non-linearities and outliers are involved in training data!



# Learning using a neuron

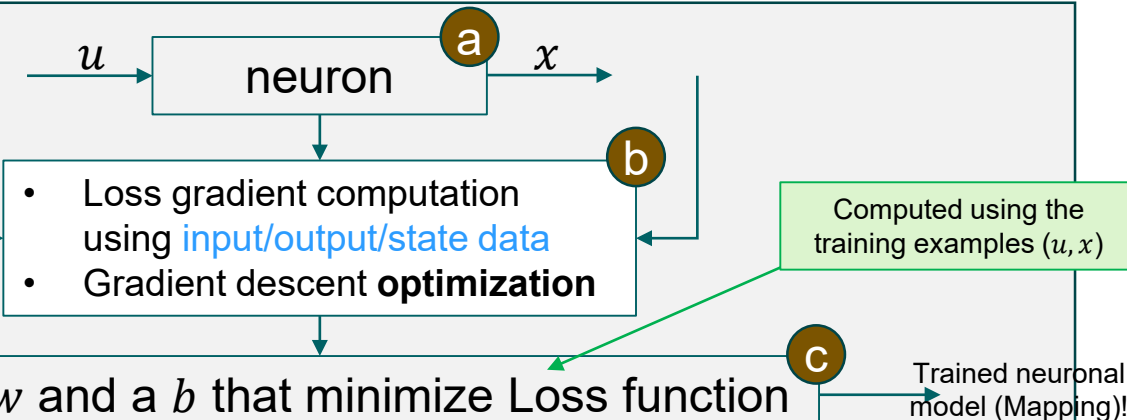
## 1 neuron case : Optimization of the weights using (Input data, Output data) and gradient



**Objectives:** How to find suitable  $w$  and  $b$ , two scalars, that (**learn to**) **associate (or map)** multiple input examples in  $u$  with corresponding output examples (i.e., labels) in  $x$  ?

.. and with good **generalization**!

### Approach:



new  $u$  not seen before

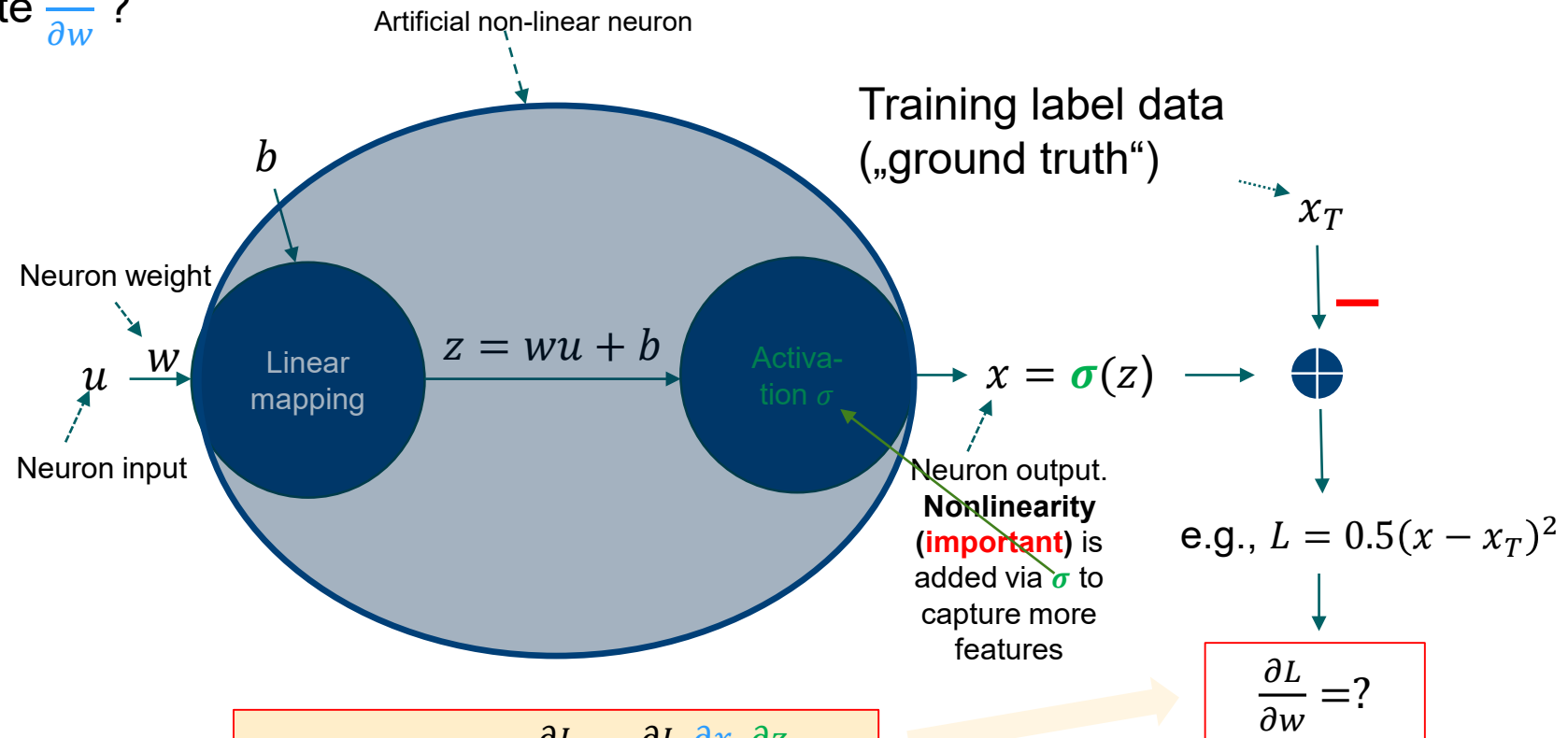
Learned mapping  
as the AI model

Accurately predicted  $x$

(Use in tests/applications testdata **normalized** with same normalization parameters as training)

## Neuron-related gradient computation

**Objective:** How to compute  $\frac{\partial L}{\partial w}$  ?



**Observe that:**  $\frac{\partial L}{\partial w} = \frac{\partial L}{\partial x} \frac{\partial x}{\partial z} \frac{\partial z}{\partial w}$

## Neuron-related gradient computation

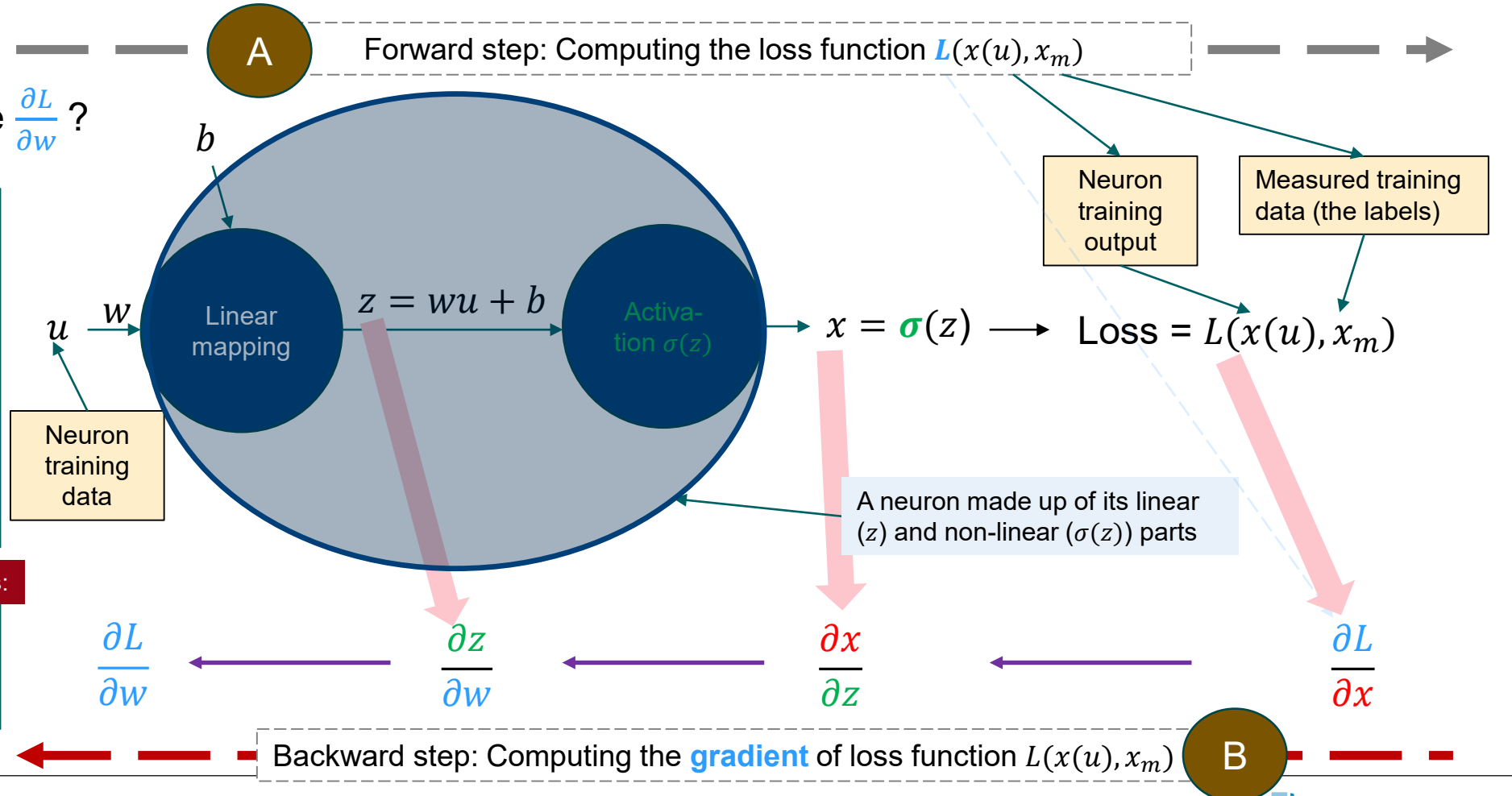
**Objective:** How to compute  $\frac{\partial L}{\partial w}$  ?

**Rationale:** We need the **derivative** (i.e.,  $\frac{\partial L}{\partial w}$ ) to be aware of the **direction of fastest decrease** (given by  $-\frac{\partial L}{\partial w}$ ) of  $L$  as a function of  $w$  to update  $w_{k+1}$ . Recall that we strive to find  $w_{k+1} = w_k - r \frac{\partial L}{\partial w} \rightarrow w^*$  that minimizes  $L$ !

This has implications:

**How? Observe that:**

$$\frac{\partial L}{\partial w} = \frac{\partial L}{\partial x} \frac{\partial x}{\partial z} \frac{\partial z}{\partial w}$$

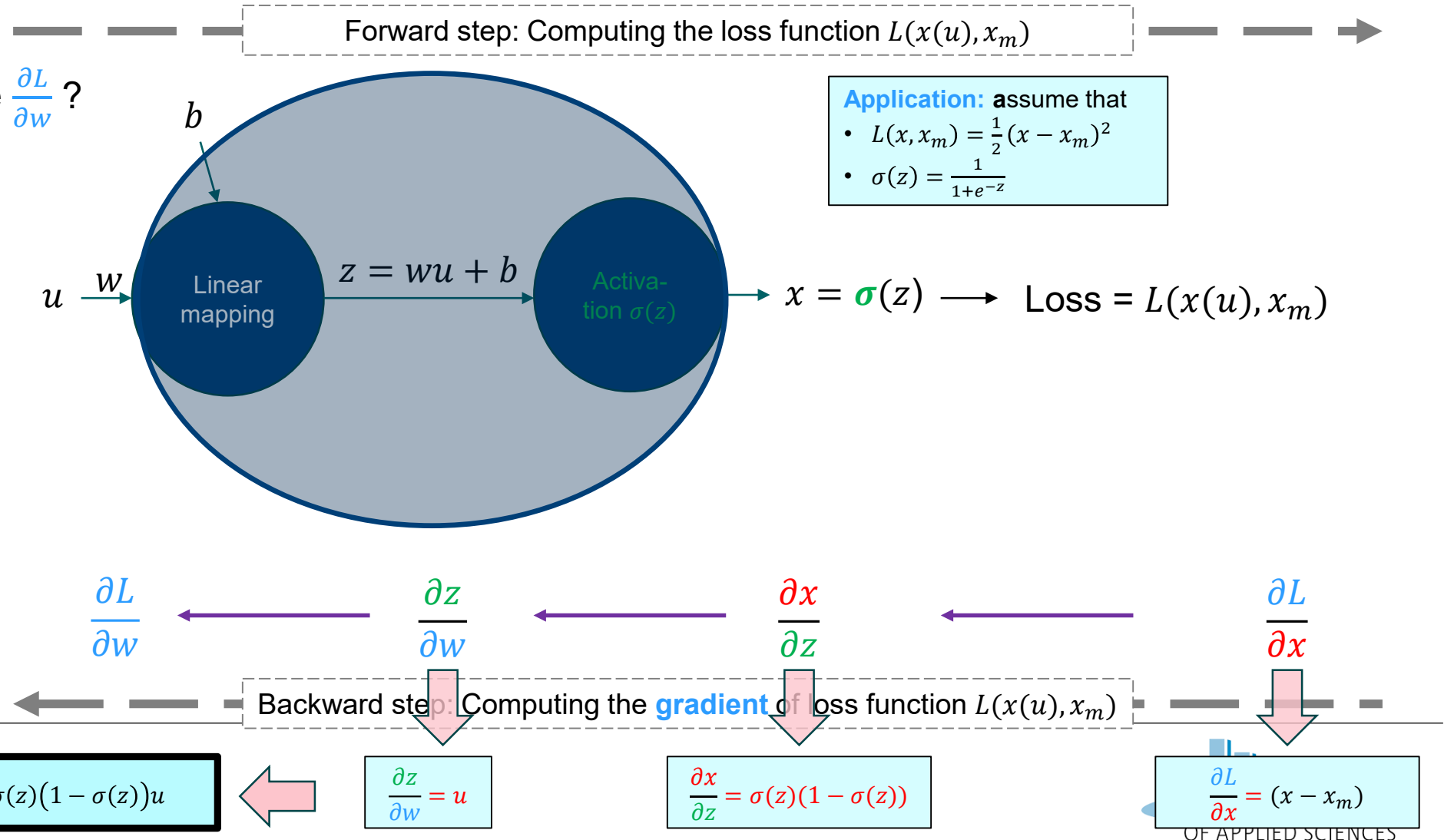


**Observation:** Gradient  $\frac{\partial L}{\partial w}$  computed (to optimize  $w$ ) through a **backward propagation**!

## Neuron-related gradient computation

**Objective:** How to compute  $\frac{\partial L}{\partial w}$  ?

**Rationale:** We need the **derivative** (i.e.,  $\frac{\partial L}{\partial w}$ ) to be aware of the **direction of fastest decrease** (given by  $-\frac{\partial L}{\partial w}$ ) of  $L$  as a function of  $w$  to update  $w_{k+1}$ . Recall that we strive to find  $w_{k+1} = w_k - r \frac{\partial L}{\partial w} \rightarrow w^*$  that minimizes  $L$ !



## Neuron-related gradient computation

**Objective:** How to compute  $\frac{\partial L}{\partial w}$  ?

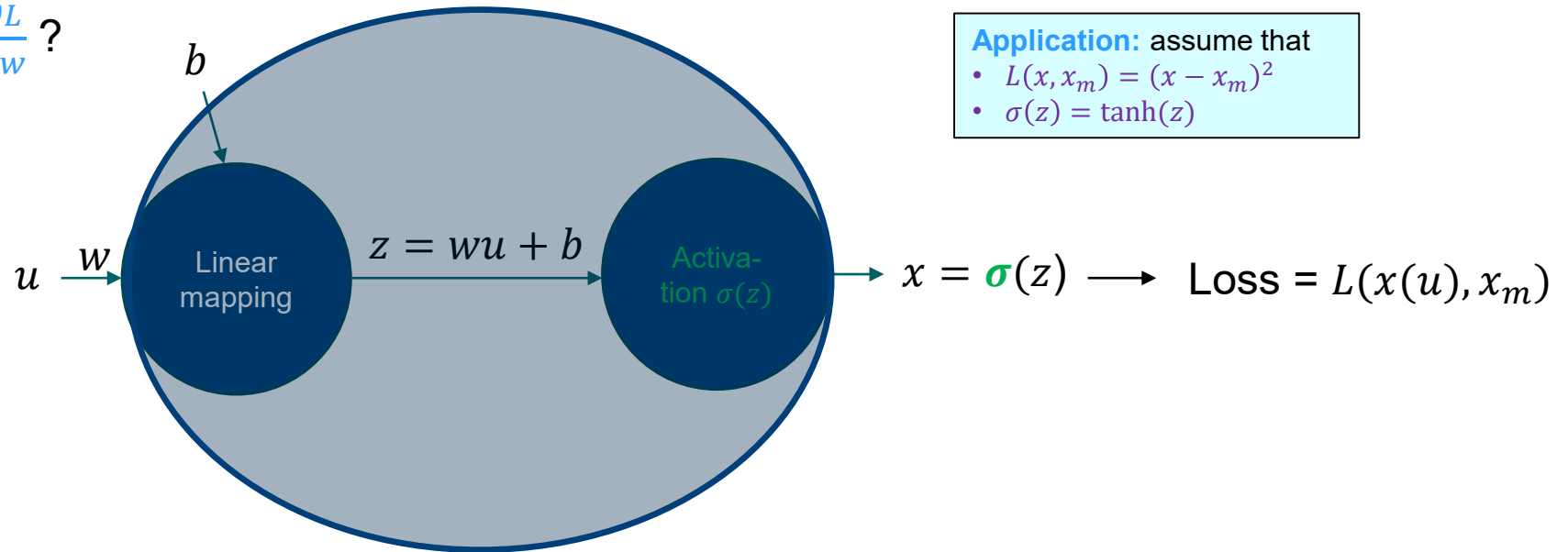
**Rationale:** We need the **derivative** (i.e.,  $\frac{\partial L}{\partial w}$ ) to be aware of the **direction of fastest decrease** (given by  $-\frac{\partial L}{\partial w}$ ) of  $L$  as a function of  $w$  to update  $w_{k+1}$ .

Recall that we strive to find  $w_{k+1} = w_k - r \frac{\partial L}{\partial w} \rightarrow w^*$  that minimizes the loss  $L$ !

**How? Observe that:**

$$\frac{\partial L}{\partial w} = \frac{\partial L}{\partial x} \frac{\partial x}{\partial z} \frac{\partial z}{\partial w}$$

Forward step: Computing the loss function  $L(x(u), x_m)$



**Application:** assume that

- $L(x, x_m) = (x - x_m)^2$
- $\sigma(z) = \tanh(z)$

$$\frac{\partial L}{\partial w}$$

$$\frac{\partial z}{\partial w}$$

$$\frac{\partial x}{\partial z}$$

$$\frac{\partial L}{\partial x}$$

Backward step: Computing the **gradient** of loss function  $L(x(u), x_m)$

$$\frac{\partial L}{\partial w} = 2(x - x_m)(1 - \sigma^2(z))u$$

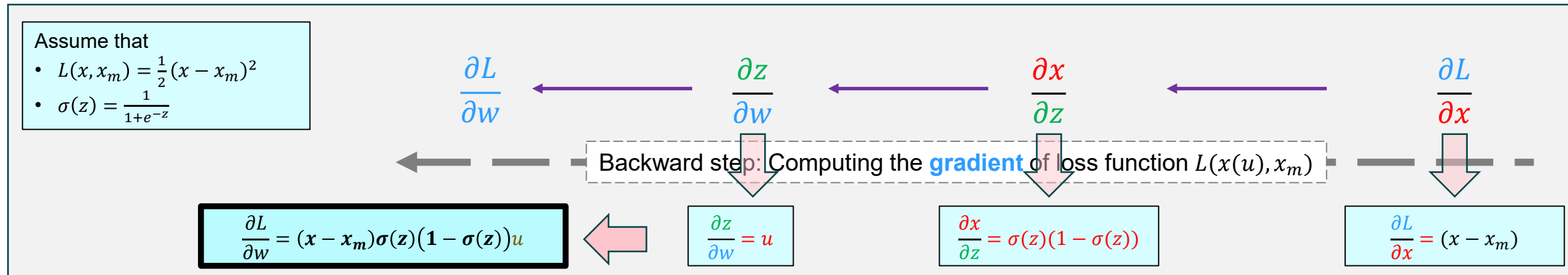
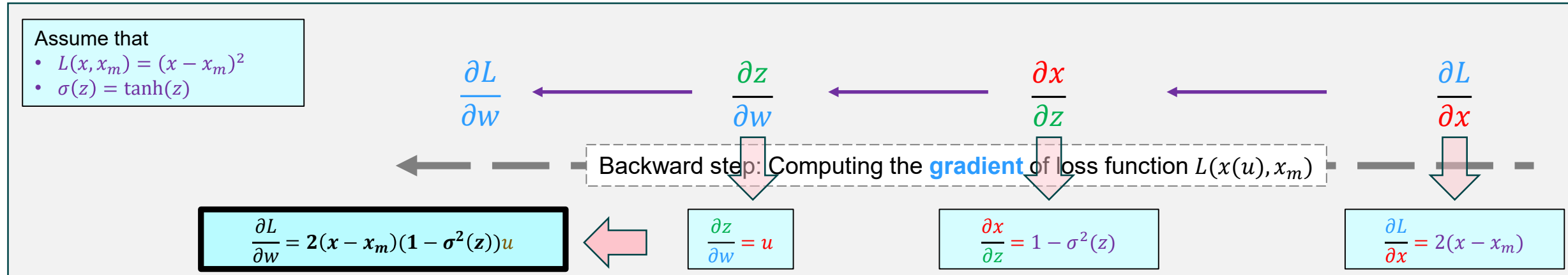
$$\frac{\partial z}{\partial w} = u$$

$$\frac{\partial x}{\partial z} = 1 - \sigma^2(z)$$

$$\frac{\partial L}{\partial x} = 2(x - x_m)$$

## Neuron-related gradient computation

Known activation function  $\sigma(z)$



Observe that:

$$\frac{\partial L}{\partial w} = \frac{\partial L}{\partial x} \frac{\partial x}{\partial z} \frac{\partial z}{\partial w} = p \frac{\partial z}{\partial w}$$

with  $p = \frac{\partial L}{\partial x} \frac{\partial x}{\partial z} = \frac{\partial L}{\partial z}$

Impact of the **activation function** on  $p$  is kept hidden!

Unknown  
activation  
function  $\sigma(z)$

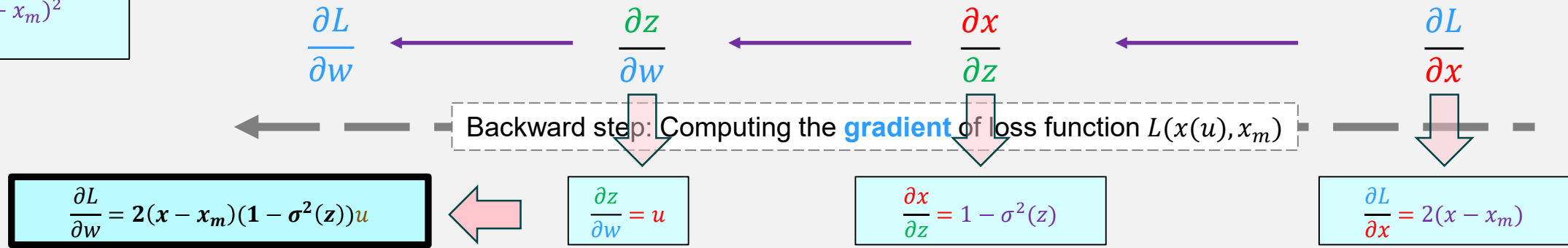
# Robotics and Machine Learning – Model Capture

## Neuron-related gradient computation

Known activation function  $\sigma(z)$

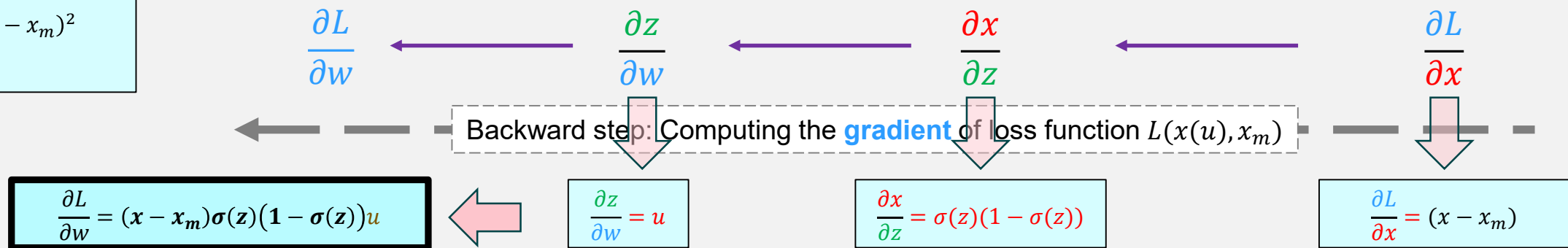
Assume that

- $L(x, x_m) = (x - x_m)^2$
- $\sigma(z) = \tanh(z)$



Assume that

- $L(x, x_m) = \frac{1}{2}(x - x_m)^2$
- $\sigma(z) = \frac{1}{1 + e^{-z}}$



Observe that:

$$\frac{\partial L}{\partial w} = \frac{\partial L}{\partial x} \frac{\partial x}{\partial z} \frac{\partial z}{\partial w} = pu$$

with  $p = \frac{\partial L}{\partial x} \frac{\partial x}{\partial z} = \frac{\partial L}{\partial z}$

Weight update:  $w_{k+1} = w_k - r \frac{\partial L}{\partial w} = w_{k+1} + w_k - rpu$

Unknown  
activation  
function  $\sigma(z)$

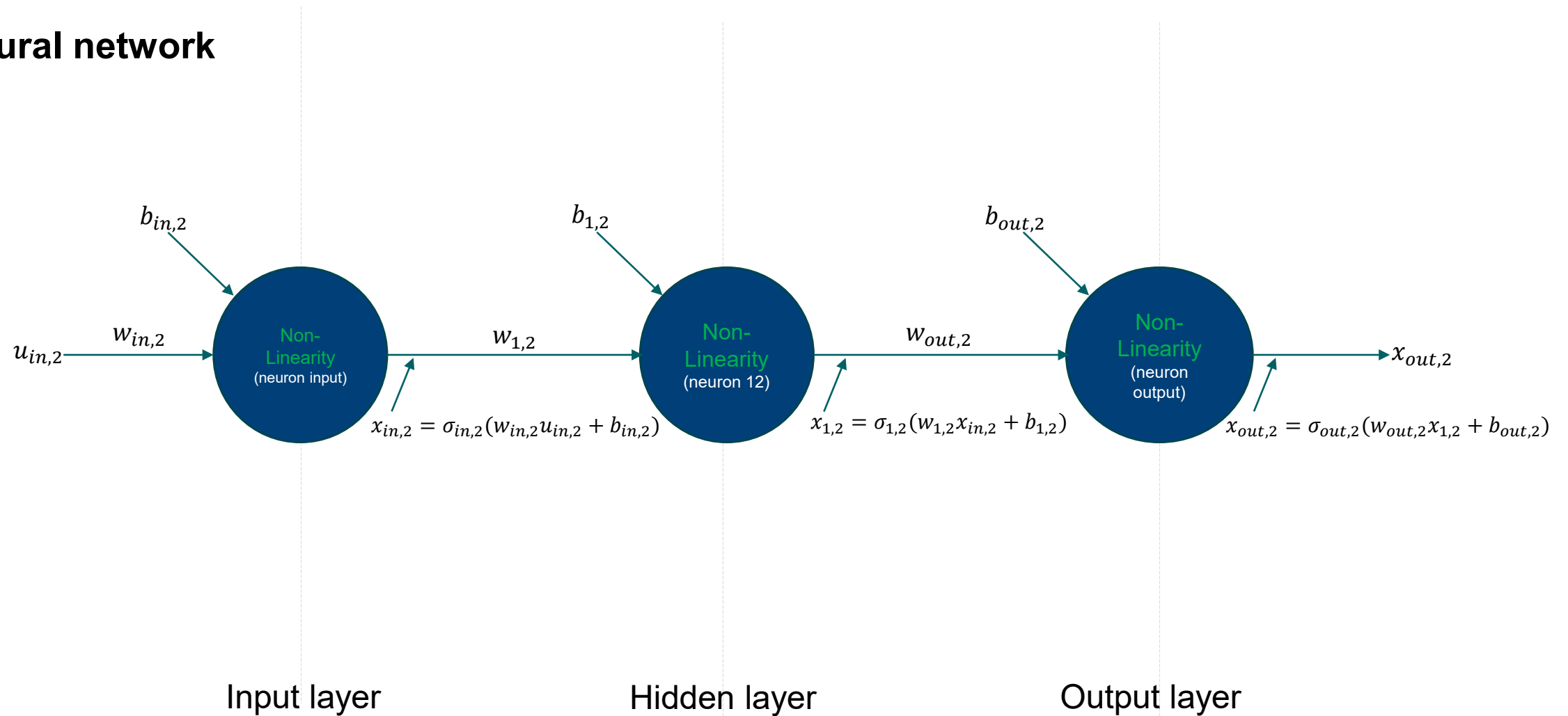


## Application

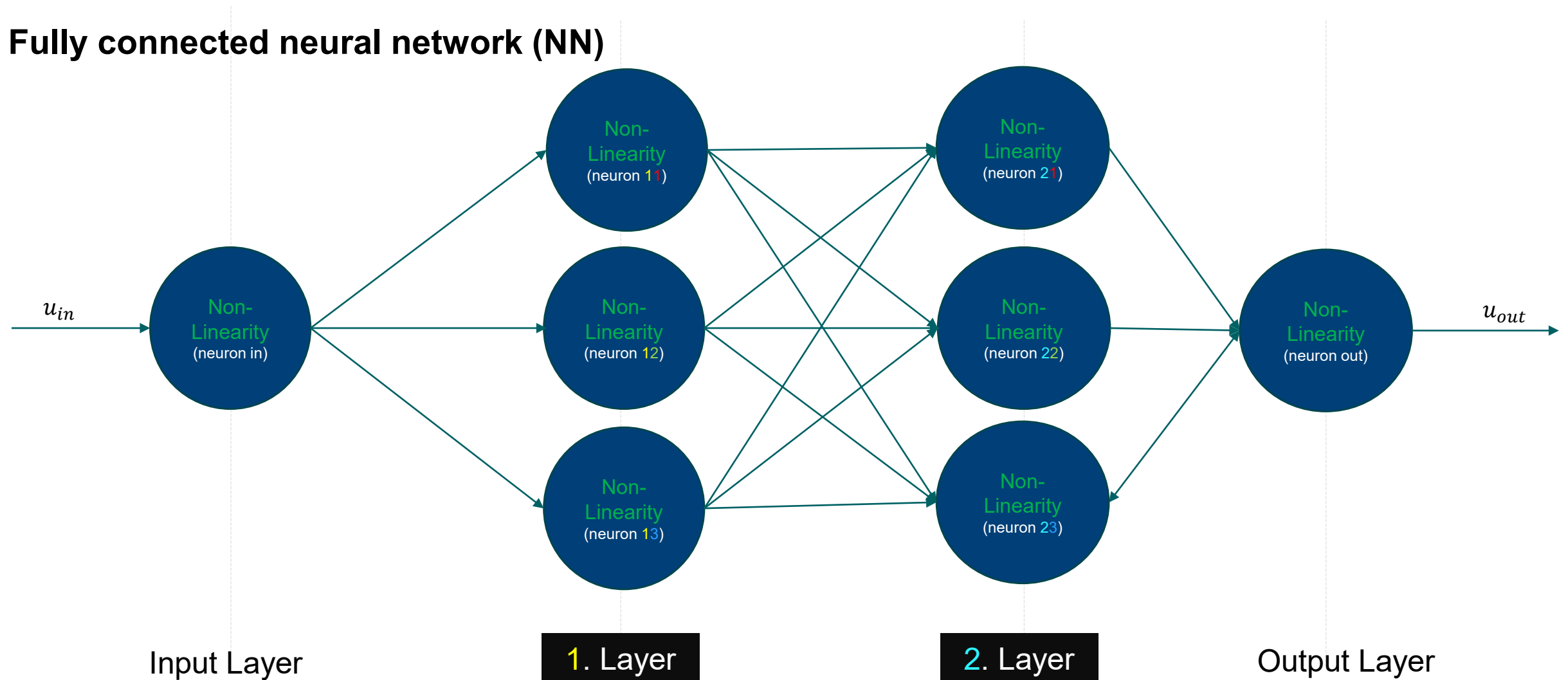
- 1) Generate the **set  $u$  of input training data** made up of **10000 random numbers** between -1 and 1
- 2) Generate the set  $y = x_m$  of label data with  $y = x_m = 243.5 * u - 162$
- 3) Implement a neuron with **input  $u$ , weight  $w$ , bias  $b$ , state  $z$ , identity output  $x$**  as activation (i.e.,  $x(z) = \sigma(z) = z$ ) in Matlab. The neuron maps the input signal  $u$  to an output signal  $x$
- 4) Write a loop (the maximum number of iterations is  $10^4$ ) that uses the neuron to run the
  - a) **Forward propagation** (from  $u$  to the current neural network output  $x$ )
  - b) **Compute the gradient of the loss function  $L$**  (what is a **useful** one?) by **using  $u, x$ , and  $x_m$**
  - c) **Update the weights ( $w, b$ )** of the neuron
- 5) Did you retrieve ( $w = 243.5, b = 162$ )? What do you observe while increasing/decreasing the learning rate  $r$ ?
- 6) Repeat from 2) with  $x_m = 2u^2 + 1$ . What did you observe?

# Learning with several fully connected neurons

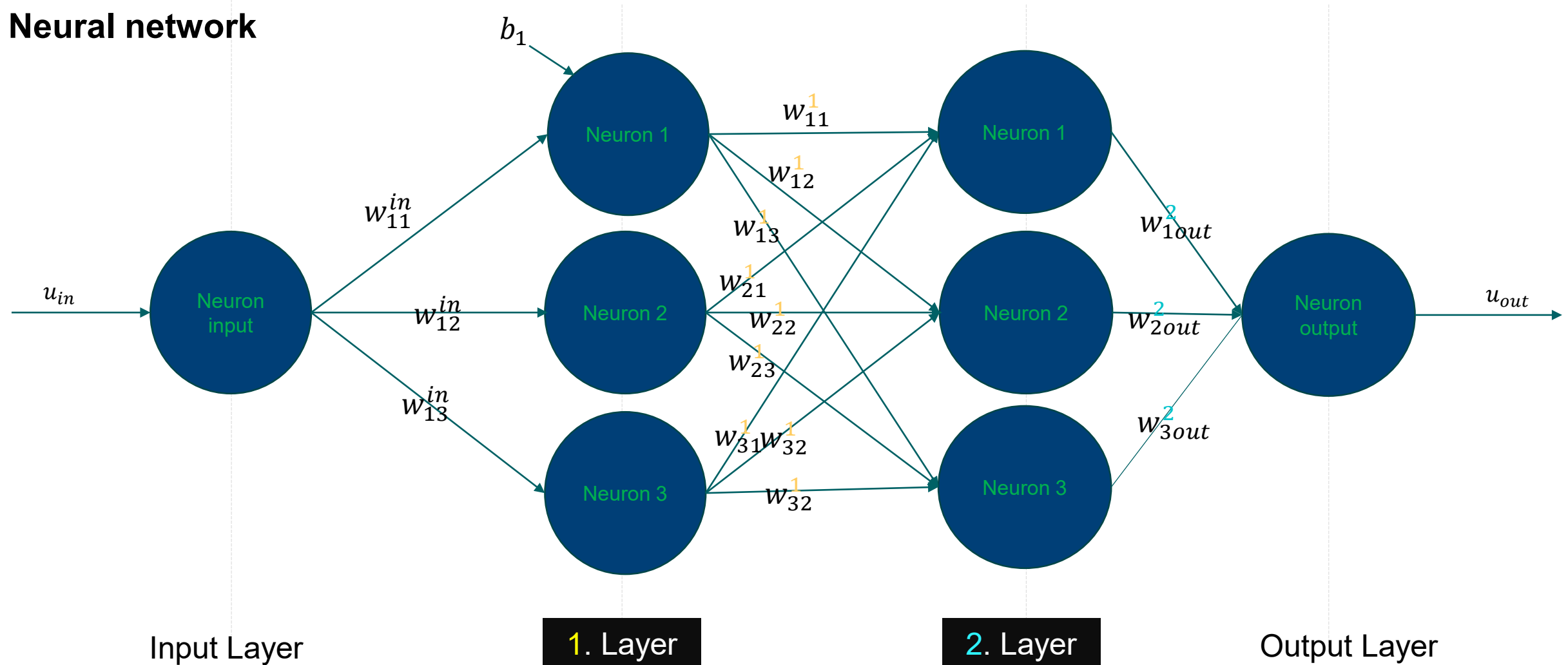
## Neural network



## Fully connected neural network (NN)



## Neural network



## Gradient via **backpropagation**

Recall that:

$$\frac{\partial L}{\partial w} = \frac{\partial L}{\partial x} \frac{\partial x}{\partial z} \frac{\partial z}{\partial w}$$

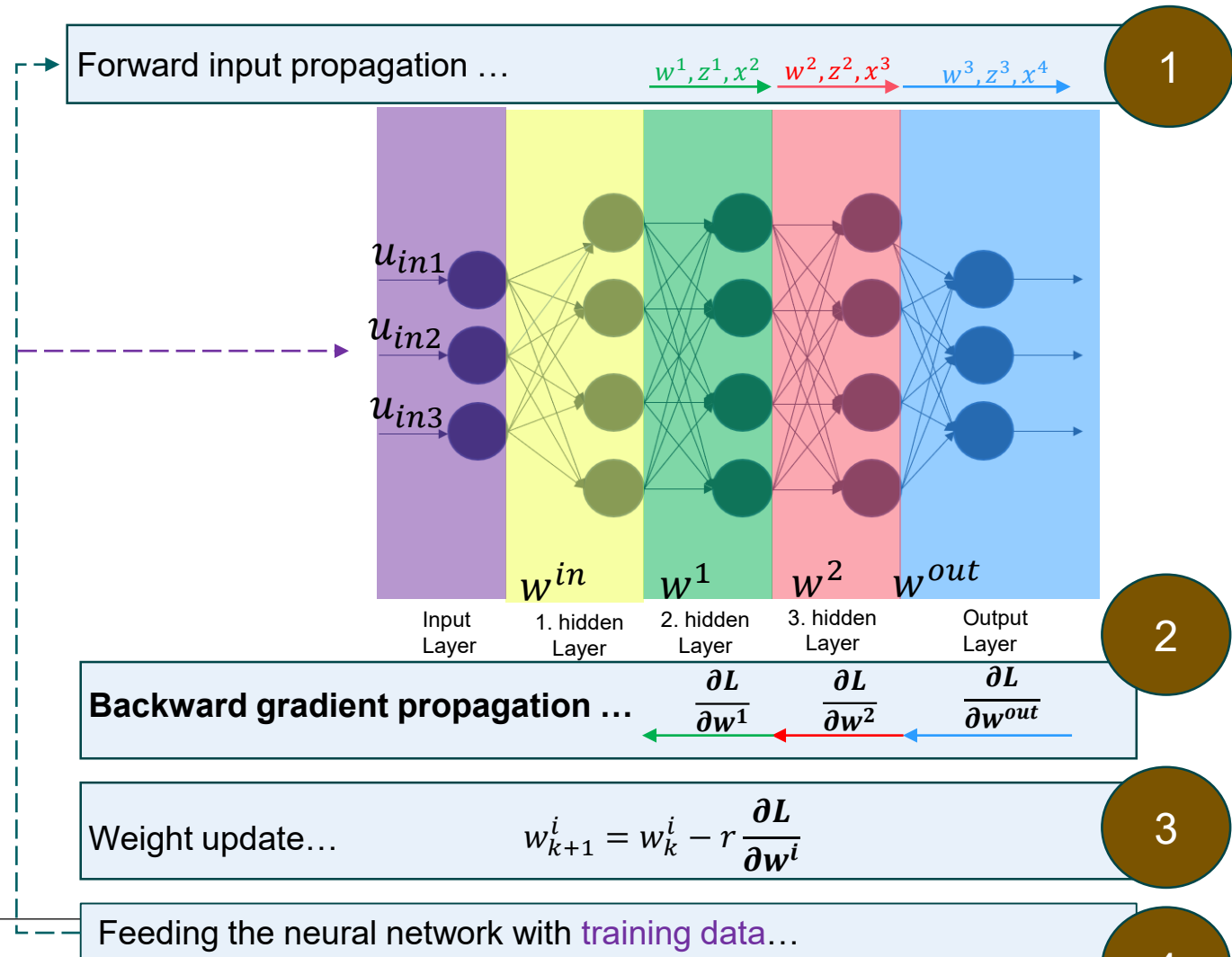


$$\frac{\partial L}{\partial w^4} = \frac{\partial L}{\partial x^3} \frac{\partial x^3}{\partial z^3} \frac{\partial z^3}{\partial w^4}$$

$$\frac{\partial L}{\partial w^3} = \frac{\partial L}{\partial x^3} \frac{\partial x^3}{\partial z^3} \frac{\partial z^3}{\partial x^2} \frac{\partial x^2}{\partial z^2} \frac{\partial z^2}{\partial w^3}$$

$$\frac{\partial L}{\partial w^2} = \frac{\partial L}{\partial x^3} \frac{\partial x^3}{\partial z^3} \frac{\partial z^3}{\partial x^2} \frac{\partial x^2}{\partial z^2} \frac{\partial z^2}{\partial x^1} \frac{\partial x^1}{\partial z^1} \frac{\partial z^1}{\partial w^2}$$

$w^n$  means weights  $w$  w.r.t  $n$ -th layer



## Gradient via backpropagation

Recall that:

$$\frac{\partial L}{\partial w} = \frac{\partial L}{\partial x} \frac{\partial x}{\partial z} \frac{\partial z}{\partial w}$$



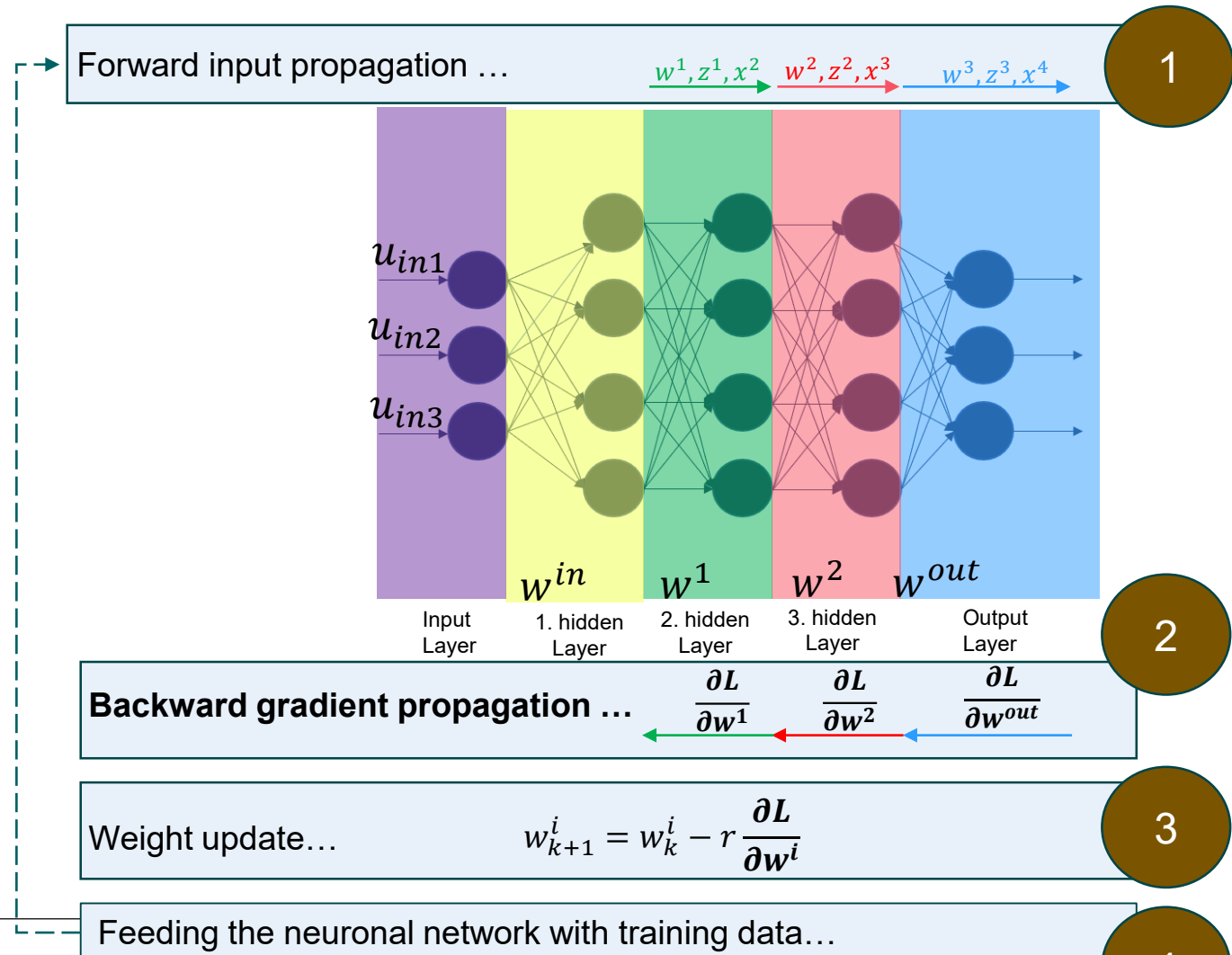
$$\frac{\partial L}{\partial w^4} = \frac{\partial L}{\partial x^3} \frac{\partial x^3}{\partial z^3} \frac{\partial z^3}{\partial w^4}$$

$$\frac{\partial L}{\partial w^3} = \frac{\partial L}{\partial x^3} \frac{\partial x^3}{\partial z^3} \frac{\partial z^3}{\partial x^2} \frac{\partial x^2}{\partial z^2} \frac{\partial z^2}{\partial w^3}$$

$$\frac{\partial L}{\partial w^2} = \frac{\partial L}{\partial x^3} \frac{\partial x^3}{\partial z^3} \frac{\partial z^3}{\partial x^2} \frac{\partial x^2}{\partial z^2} \frac{\partial z^2}{\partial x^1} \frac{\partial x^1}{\partial z^1} \frac{\partial z^1}{\partial w^2}$$

**Observations:**

Some **terms** appear **many times** in the gradient-related chain!



## Gradient via backpropagation

Recall that:

$$\frac{\partial L}{\partial w} = \frac{\partial L}{\partial x} \frac{\partial x}{\partial z} \frac{\partial z}{\partial w}$$



$$\frac{\partial L}{\partial w^4} = \frac{\partial L}{\partial x^3} \frac{\partial x^3}{\partial z^3} \frac{\partial z^3}{\partial w^4}$$

$$\frac{\partial L}{\partial w^3} = \frac{\partial L}{\partial x^3} \frac{\partial x^3}{\partial z^3} \frac{\partial z^3}{\partial x^2} \frac{\partial x^2}{\partial z^2} \frac{\partial z^2}{\partial w^3}$$

$$\frac{\partial L}{\partial w^2} = \frac{\partial L}{\partial x^3} \frac{\partial x^3}{\partial z^3} \frac{\partial z^3}{\partial x^2} \frac{\partial x^2}{\partial z^2} \frac{\partial z^2}{\partial x^1} \frac{\partial x^1}{\partial z^1} \frac{\partial z^1}{\partial w^2}$$

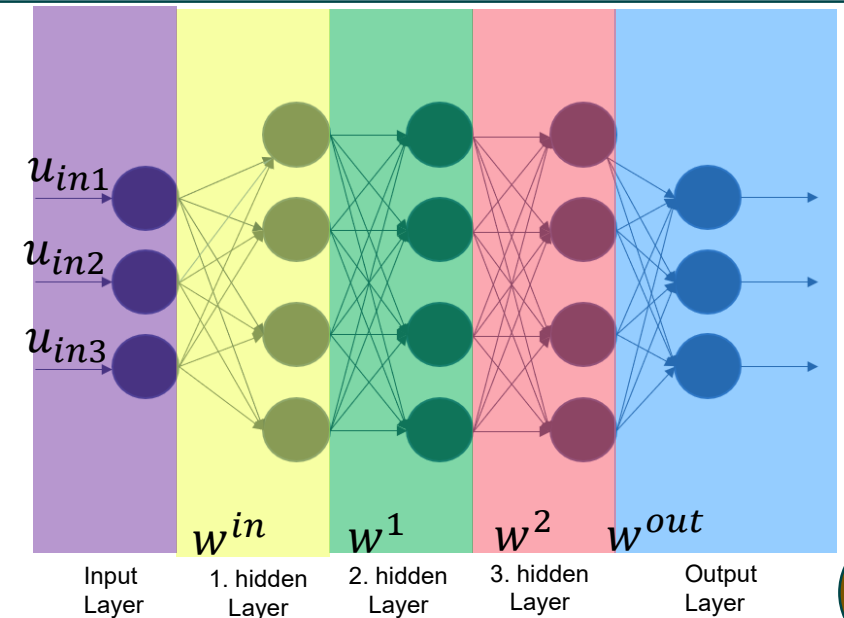
**Observation:**

If some of the  $\frac{\partial 0}{\partial 0}$  (e.g.,  $\frac{\partial x^2}{\partial z^2}$ ) in the chain are too small or simply vanish, the **gradient** is likely to **disappear**!

What does it **implicate**?

Big challenge faced by **deep neural networks**!

Forward input propagation ...



Backward gradient propagation ...

$$\frac{\partial L}{\partial w^1} \quad \frac{\partial L}{\partial w^2} \quad \frac{\partial L}{\partial w^{out}}$$

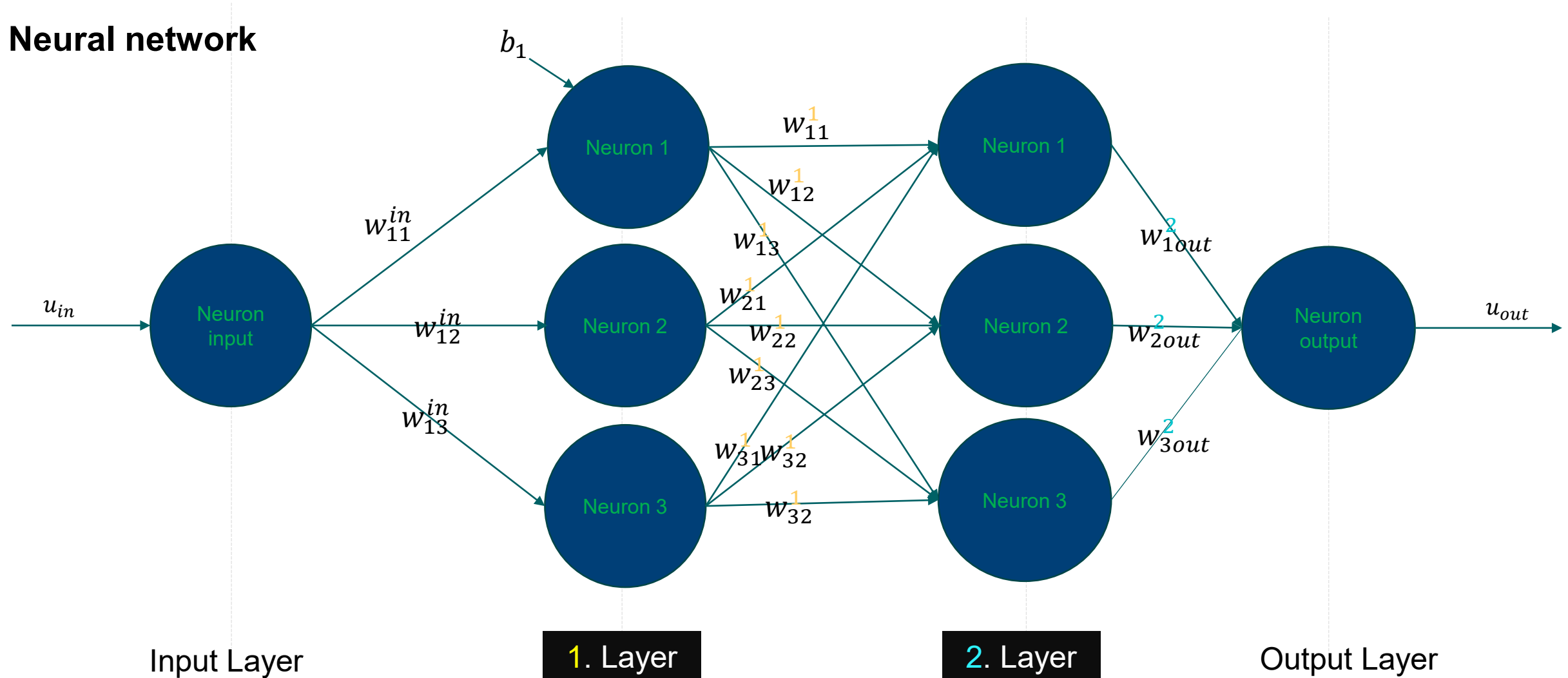
Weight update...

$$w_{k+1}^i = w_k^i - r \frac{\partial L}{\partial w^i}$$

Feeding the neuronal network with training data...



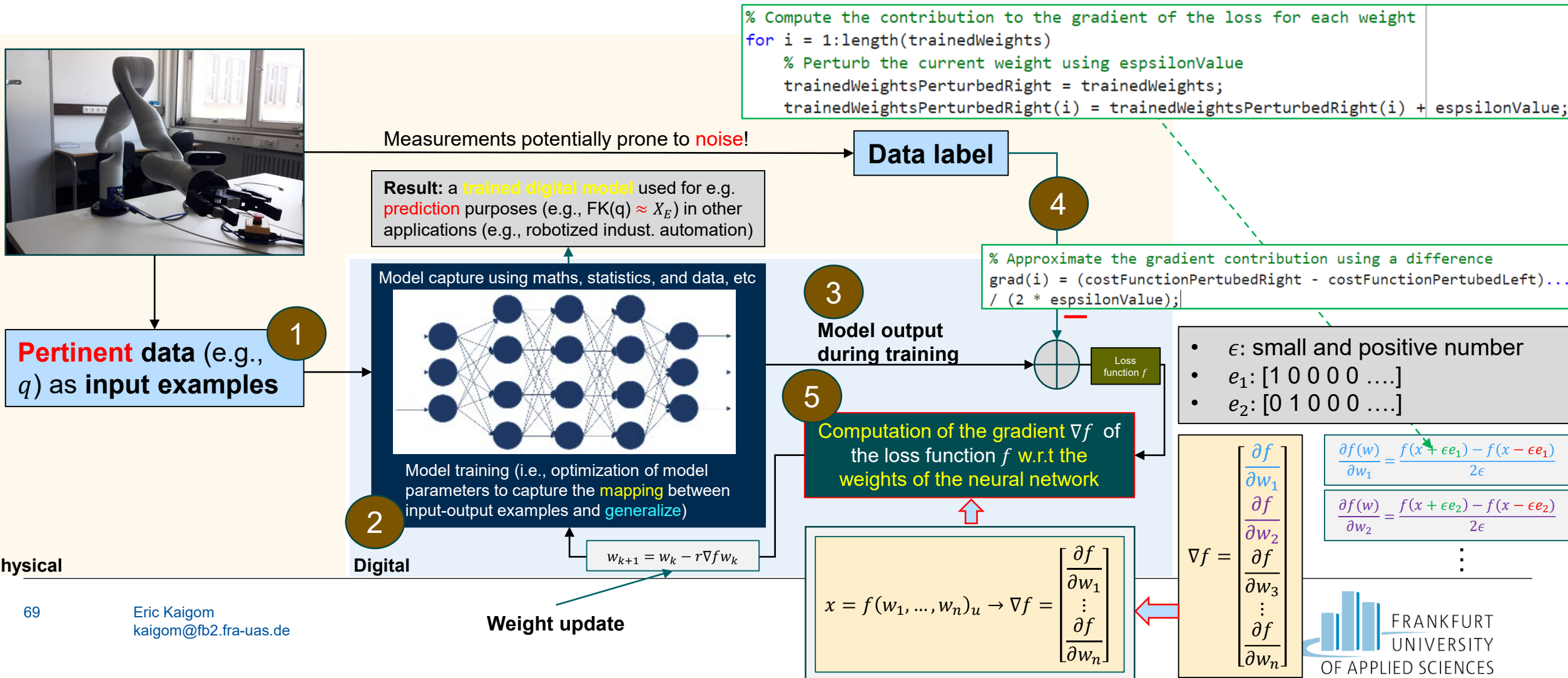
## Neural network



## Application

- 1) Implement a matlab function **[x1, x2] = forward(q1, q2, w)** that reflects a fully connected neural network made up of **two hidden layers** with **two neurons** for each of them. The function receives the following parameters
  - a) Two real inputs **q1** and **q2**
  - b) A vector **w** of weights for all layersand returns two real outputs **x1** and **x2**
- 2) Implement a loop that runs  $10^6$  times, feeds **forward(q1, q2, w)** with randomly generated **q1**, **q2**, and **w**.
- 3) Set **q1** and **q2** as a vector of 1000 random values between -1 and 1. Furthermore, assume (ground truth) that
  - **X1 = q1 + q2**
  - **X2 = q1 - q2**
- 4) Run the loop while feeding the network (i.e., **forward (...)**) with **q1** and **q2** value pairwise and compute a meaningful loss function for each epoch using **X1** and **X2**.

## Machine Learning – Updating the weights of the neural network in practice



## Machine Learning – Adapting the learning rate via moment estimation

- $m_{k+1} = \beta_1 m_k + (1 - \beta_1) \nabla f$

- $v_{k+1} = \beta_2 v_k + (1 - \beta_2) (\nabla f)^2$

- $\hat{m}_{k+1} = \frac{m_{k+1}}{1 - \beta_1^{k+1}}$

- $\hat{v}_{k+1} = \frac{v_{k+1}}{1 - \beta_2^{k+1}}$

adaptation

- $w_{k+1} = w_k - \alpha \frac{1}{\sqrt{\hat{v}_{k+1} + \epsilon}} \hat{m}_k$

$\beta_1$  and  $\beta_2$  induce an exponential decay (from  $\beta_1 = 0.9, \beta_2 = 0.999$ )

- $\alpha = 0.001$
- $\epsilon = 10^{-8}$

```
% Compute the contribution to the gradient of the loss for each weight
for i = 1:length(trainedWeights)
    % Perturb the current weight using espilonValue
    trainedWeightsPerturbedRight = trainedWeights;
    trainedWeightsPerturbedRight(i) = trainedWeightsPerturbedRight(i) + espilonValue;
```

Data label

4

```
% Approximate the gradient contribution using a difference
grad(i) = (costFunctionPertubedRight - costFunctionPertubedLeft)...
/ (2 * espilonValue);
```

3

Model output during training

5

- $\epsilon$ : small and positive number
- $e_1$ : [1 0 0 0 0 ...]
- $e_2$ : [0 1 0 0 0 ...]

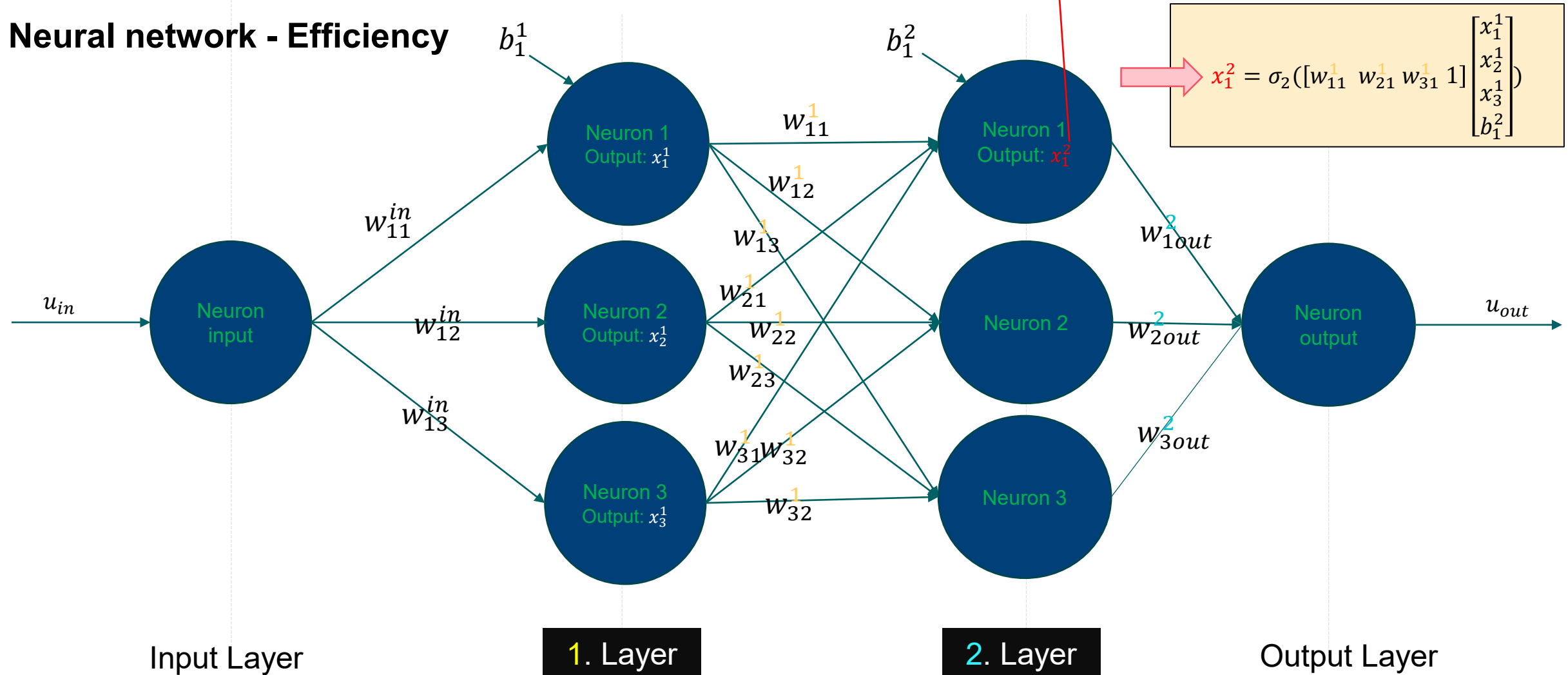
$$w_{k+1} = w_k - r \nabla f(w) w_k$$

Instead of ...

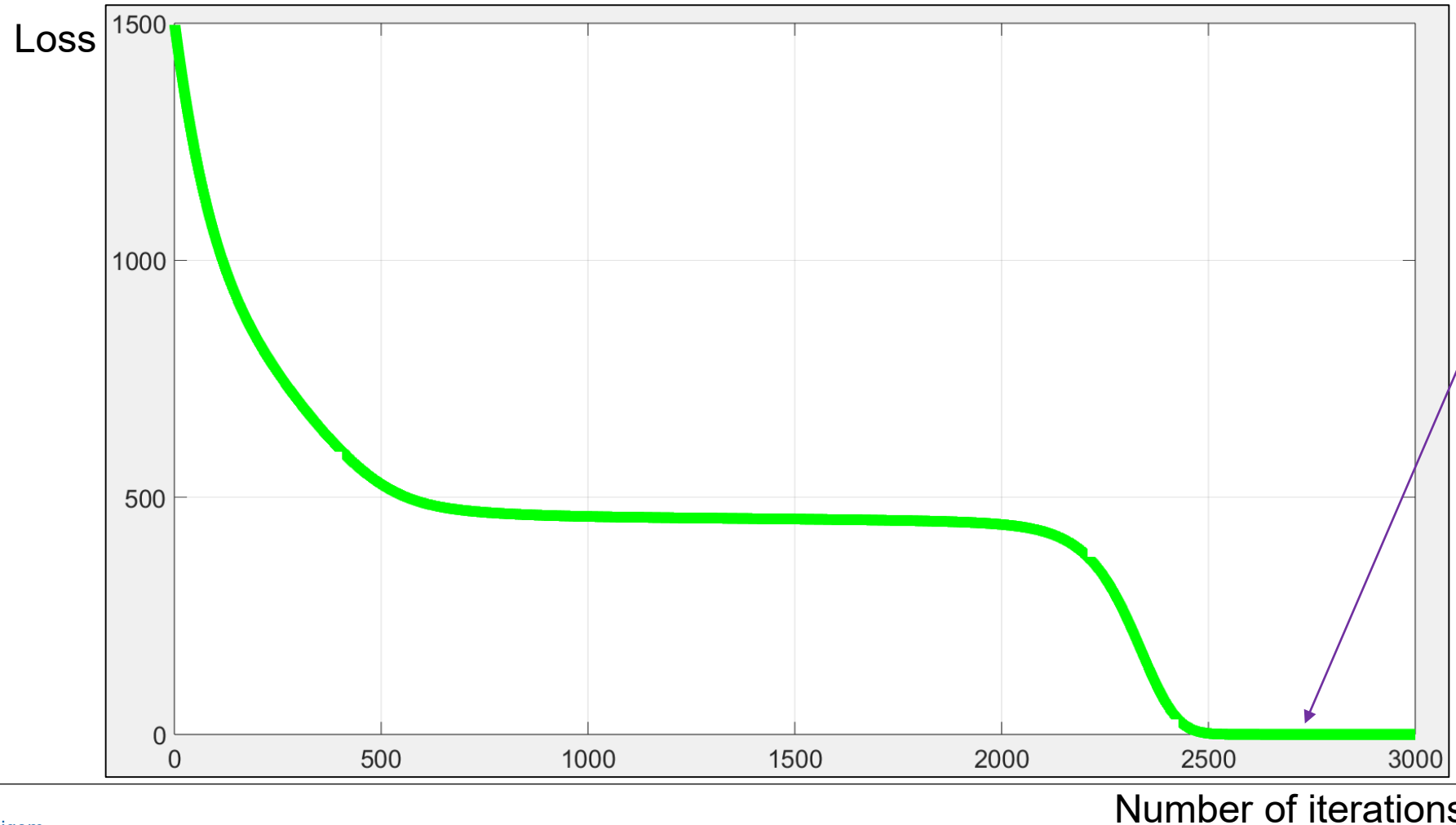
...harness the following insight:

$$x_1^2 = \sigma_2(w_{11}^1 x_1^1 + w_{21}^1 x_2^1 + w_{31}^1 x_3^1 + b_1^2)$$

## Neural network - Efficiency



### Optimization of the prediction accuracy (under adaptive moment-based learning rate) - Result



### Project (presentation: 29.01.25, 8:15 h, groups of min. 2 /max. 3 students, Duration max. 20 Min)

- Improve our model (see the file withStudentsNew.m) to learn

- $X1 = q1 + q2 - 1$
- $X2 = q1 - q2 + 1$

and

- $X1 = q1 + q2.*q2 - 1$
  - $X2 = q1 - q2 + 1$
- When and why is an enhancement necessary?
  - How did you enhance the model?
  - What did you observe? Explain your observation with your own words

**Thank you  
for your attention!**