FH KREMS
UNIVERSITY OF APPLIED SCIENCES / AUSTRIA

Machine Learning, Artificial Intelligence, and Big Data Analytics (IL, 4th Semester)

Lecture 10

Agenda

- Introduction to Neural Networks
- The building blocks of a neural network
  - The perceptron: Neurons, weights, and activation function
- Deep Neural Network
- Training a neural network
  - Loss function, Gradient descent, backpropagation

- CODING.

Some history in pills

The Rosenblatt perceptron, 1960

- 1949: Donald Hebb proposes the Hebbian Learning principle
- 1951: Marvin Minsky creates the first ANN (Hebbian learning, 40 neurons).
- 1958: Frank Rosenblatt creates a perceptron to classify 20×20 images.

<1974-1980: 1st AI winter>

- 1980: Kunihiko Fukushima presents the Neocognitron, basis for convolutional NN
- 1982: Paul Werbos proposes back-propagation for ANN.

<1987-1993: 2nd AI winter>

- 21st century: Resurgence
- 2010-ongoing: AI spring, deep learning explosion

Why the new AI spring?

- Big data and cloud
  - Large datasets
  - Easier and cheaper collection & storage

- Hardware
  - GPUs/APUs
  - Parallelization

- Software
  - Frameworks and toolboxes

Popular Deep Learning frameworks

TensorFlow + Keras

- Developed by **Alphabet**
- Written in C++
- Now integrates **Keras**

- Popular in production
- Trickier debugging

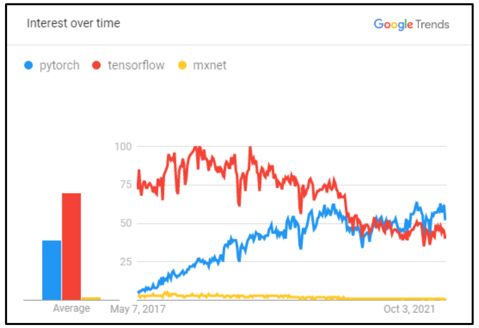
PyTorch

- Developer by **Meta**
- Written in Python/C++
- Based on **Torch**

- Popular in academia
- Easier debugging

mxnet

- Academic and **Apache**
- Written in C++
- Multi-language support but less popular



The perceptron

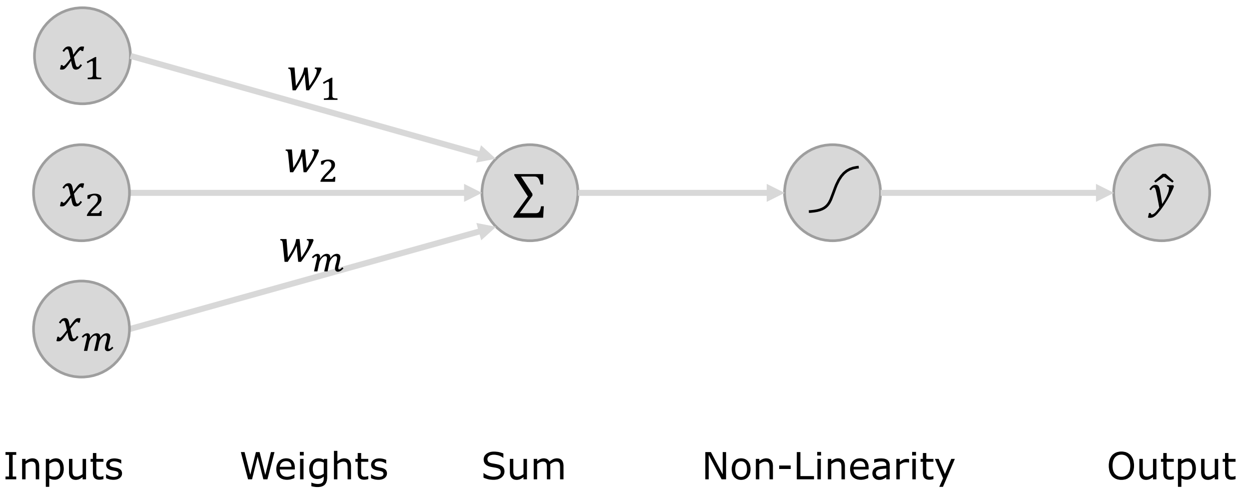
The basic building block of a neural network

Output

Linear combination of inputs

$$\hat{y} = g\left(\sum_{i=1}^{m} x_i w_i\right)$$

Non-linear activation function



The perceptron

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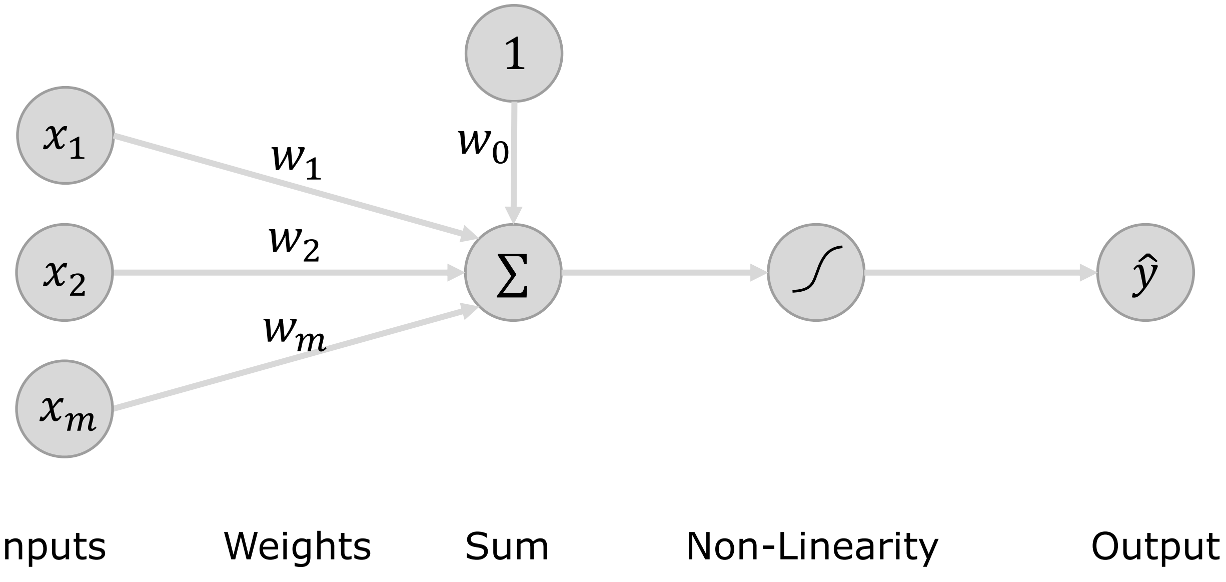


Output

Linear combination of inputs

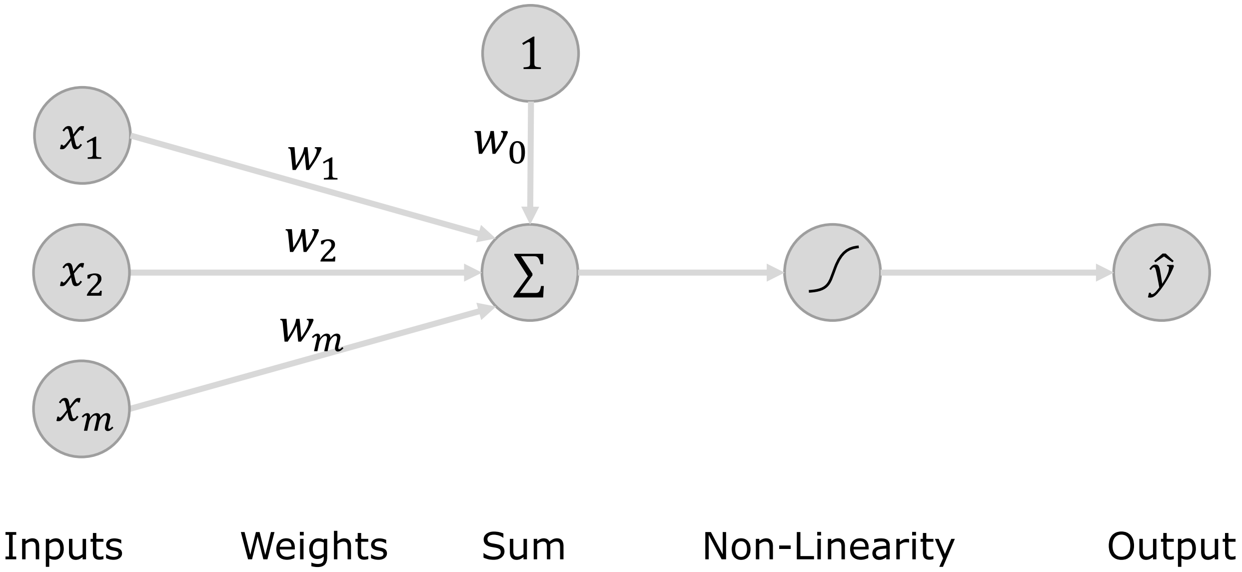
$$\hat{y} = g\left(w_0 + \sum_{i=1}^{m} x_i w_i\right)$$

Non-linear activation function

Bias

The perceptron

The basic building block of a neural network



Output

Linear combination of inputs

$$\hat{y} = g\left(w_0 + \sum_{i=1}^{m} x_i w_i\right)$$

Non-linear activation function

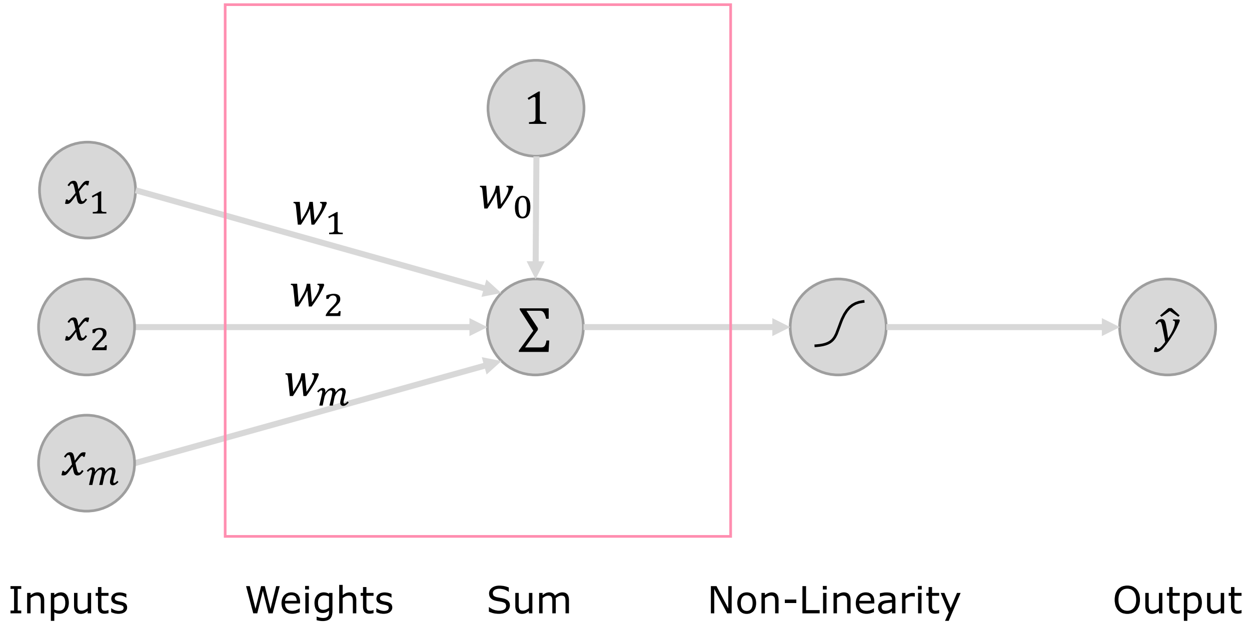
Bias

$$\hat{y} = g(w_0 + \boldsymbol{X}^T \boldsymbol{W})$$

$$where\ \boldsymbol{X} = \begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix}\ and\ \boldsymbol{W} = \begin{bmatrix} w_1 \\ \vdots \\ w_m \end{bmatrix}$$

The perceptron

The basic building block of a neural network



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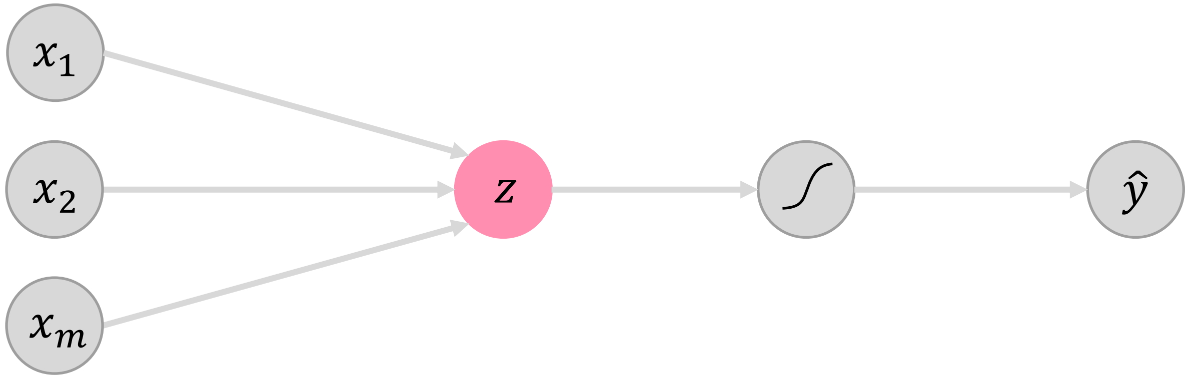
The perceptron

The basic building block of a neural network



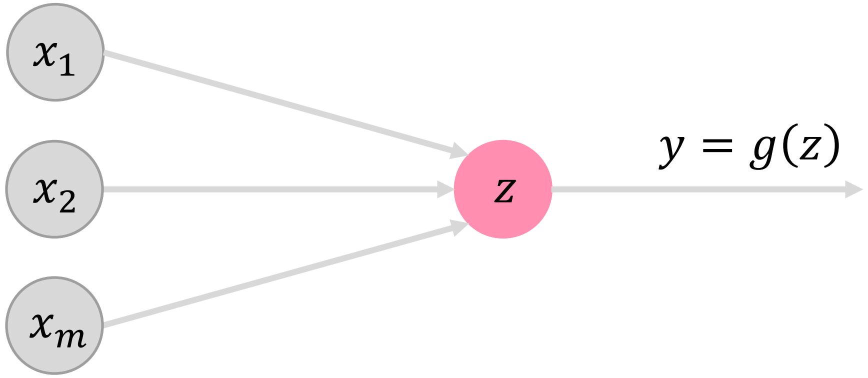
Inputs

$z = w_0 + \sum_{j=1}^{m} x_j w_j$

Output

The perceptron

The basic building block of a neural network

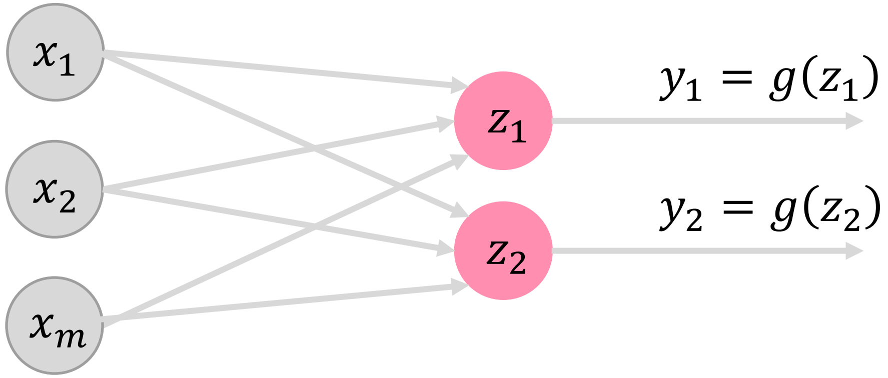


Inputs

$$z = w_0 + \sum_{j=1}^{m} x_j w_j$$

The perceptron

The basic building block of a neural network



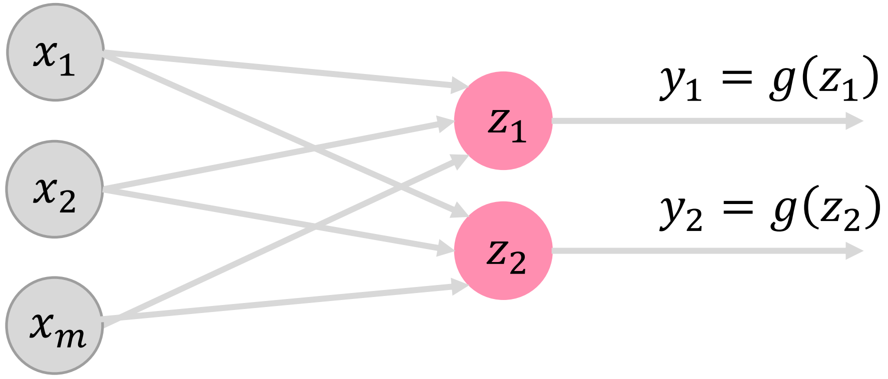
Inputs

$$z_i = w_{0,i} + \sum_{j=1}^{m} x_j w_{j,i}$$

Multi-output perceptron

The perceptron

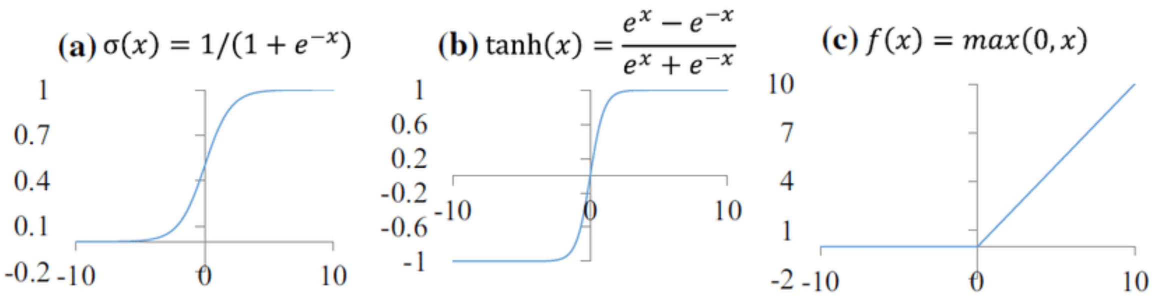
The basic building block of a neural network



Inputs

$z_i = w_{0,i} + \sum_{j=1}^{m} x_j w_{j,i}$

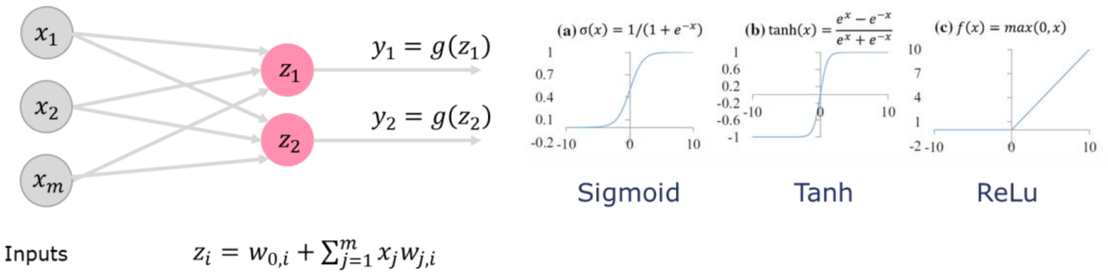
Common activation functions g



Sigmoid

Tanh

ReLu



The perceptron

Example of output from the multi-output perceptron

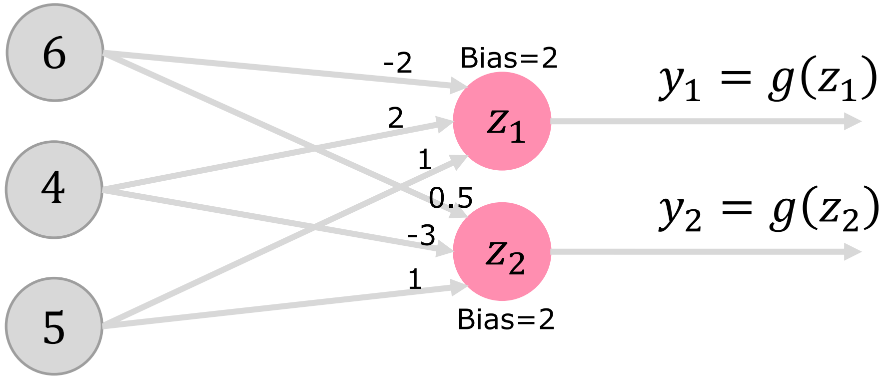
$x_1 = 6$
$x_2 = 4$
$x_3 = 5$

$w_{0,1} = 2$ $\quad$ $w_{0,2} = 2$

$w_{1,1} = -2$ $\quad$ $w_{1,2} = 0.5$

$w_{2,1} = 2$ $\quad$ $w_{2,2} = -3$

$w_{3,1} = 1$ $\quad$ $w_{3,2} = 1$

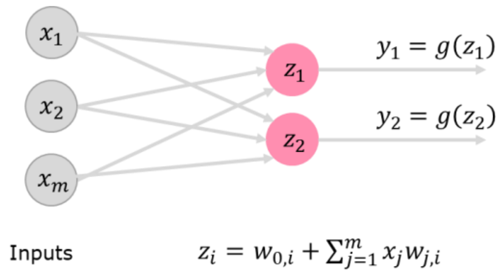


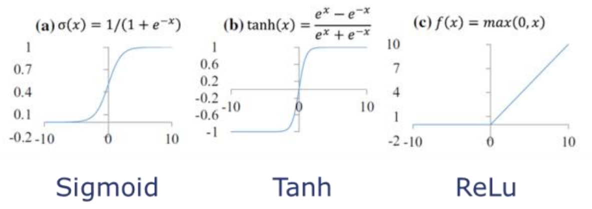
$$z_1 = 2 + (-2 * 6) + (2 * 4) + (1 * 5) = 3$$

$$z_2 = 2 + (0.5 * 6) + (-3 * 4) + (1 * 5) = -2$$

$$y_1 = g(z_1) = \begin{cases} \sigma(3) = \sim 0.952 \\ \tanh(3) = \sim 0{,}995 \\ \mathrm{ReLU}(3) = 3 \end{cases}$$

$$y_2 = g(z_2) = \begin{cases} \sigma(-2) = \sim 0.119 \\ \tanh(-2) = \sim -0{,}964 \\ \mathrm{ReLU}(-2) = 0 \end{cases}$$





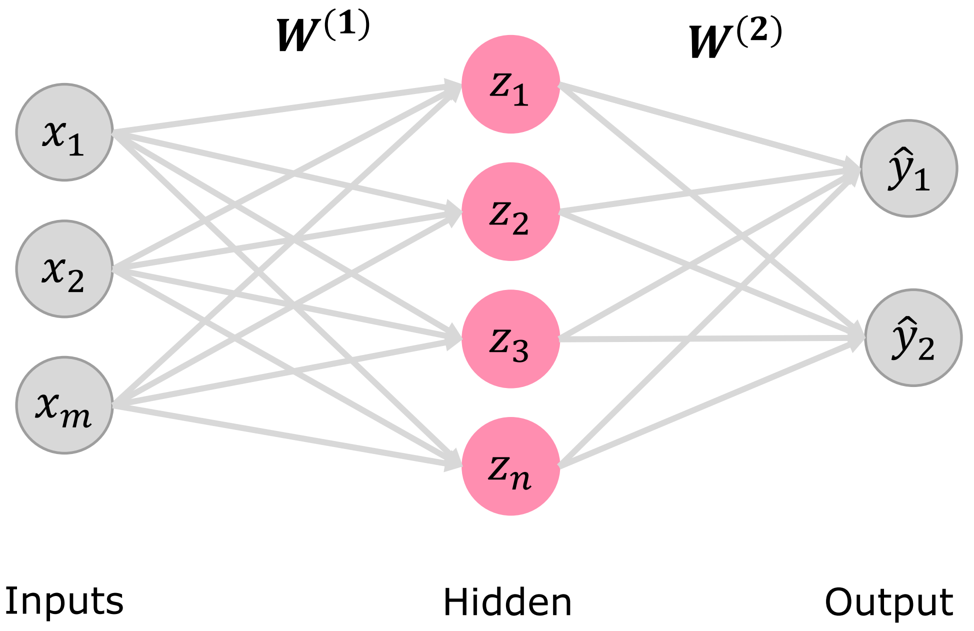
The perceptron

Exercise

$x_1 = 2$
$x_2 = 4$
$x_3 = 1$

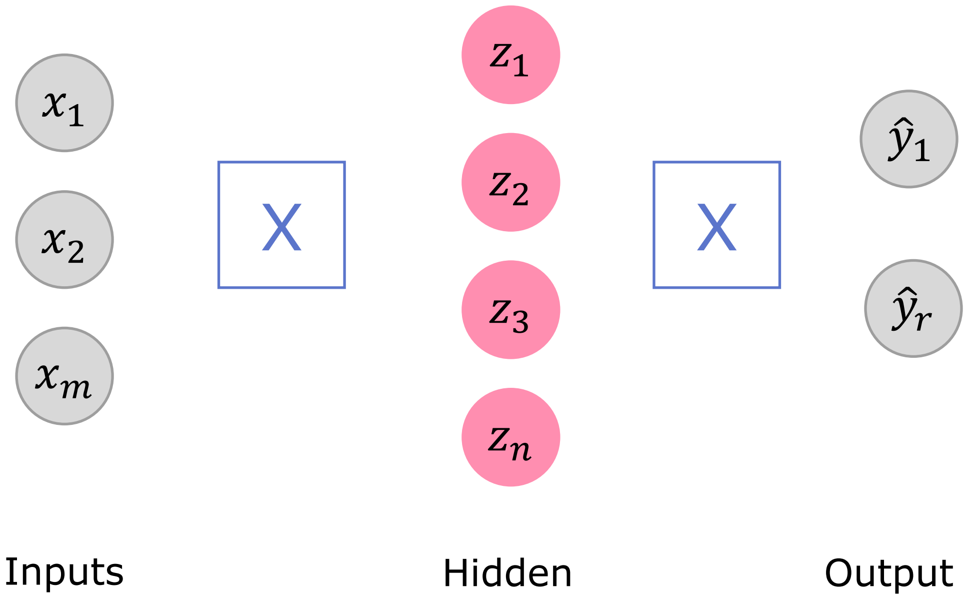
$$W = \begin{pmatrix} 2 & -1 \\ -1 & 1 \\ 1 & -2 \\ 2 & 2 \end{pmatrix}$$

Single layer neural network



Single layer neural network

Dense layers



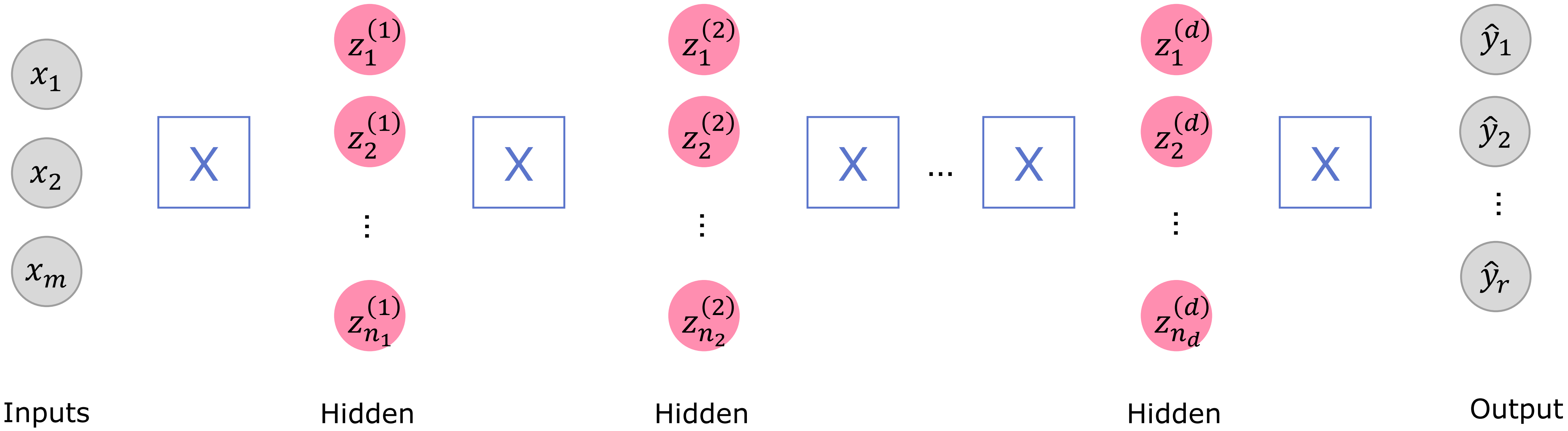
Since they are densely connected, they are called **dense layers**.

Here we have one input layer and two dense layers:

- 1 dense layer with m inputs and n outputs
- 1 dense layer with n inputs and 2 outputs

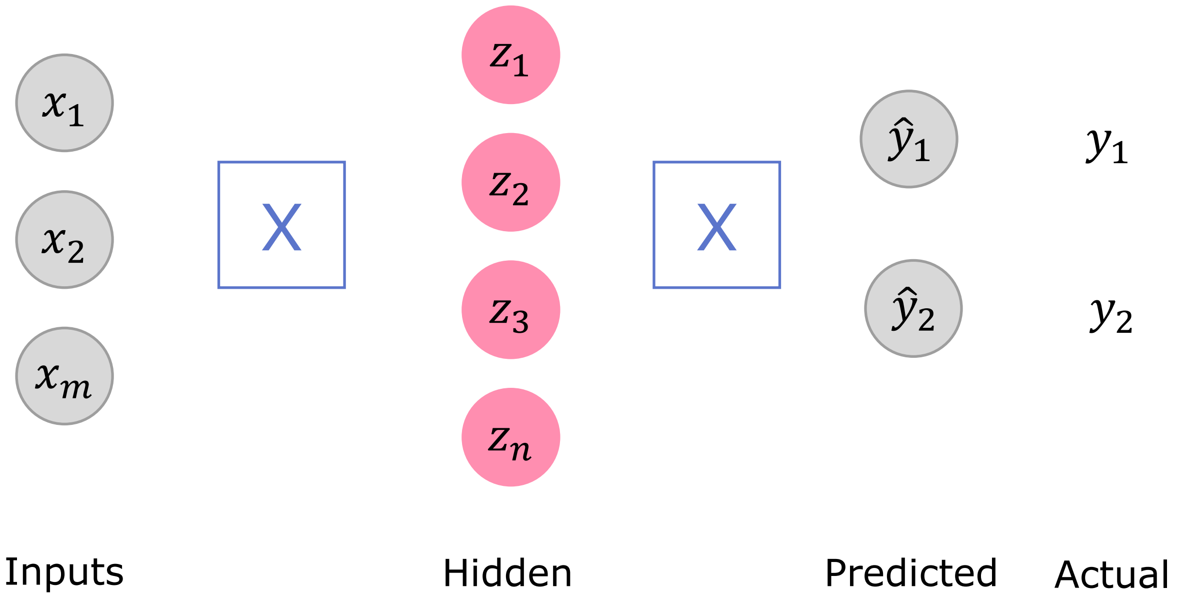
Multiple layer (deep) neural network

Generalization



Training a neural network

Objective



<u>Goal</u>

Identifying parameters (biases and weights) such that the output of the neural network is as close as possible to the ground-truth.

In other words: **Minimize a loss function.**

Training a neural network

Loss functions

- Examples:

  Regression: Mean Squared Error Loss

$$L(y, \hat{y}) = \frac{1}{N} \sum_{i=0}^{N} (y_i - \hat{y}_i)^2$$

  Classification: Binary Cross Entropy Loss (Log-loss)

$$L(y, \hat{y}) = \frac{1}{N} \sum_{i=0}^{N} -(y_i * \log(\hat{y}_i) + (1 - y_i) * \log(1 - \hat{y}_i))$$

Training a neural network

Loss functions

- Examples:

  Regression: Mean Squared Error Loss

$$L(y,\hat{y}) = \frac{1}{N}\sum_{i=0}^{N}(y_i - \hat{y}_i)^2$$

Example

$$\begin{array}{cc} \hat{y} & y \\ \begin{bmatrix}12\\23\\41\end{bmatrix} & \begin{bmatrix}10\\25\\40\end{bmatrix} \end{array} \qquad L(y,\hat{y}) = \frac{(2)^2+(-2)^2+1^2}{3} = 3$$

  Classification: Binary Cross Entropy Loss (Log-loss)

$$L(y,\hat{y}) = \frac{1}{N}\sum_{i=0}^{N} -(y_i * \log(\hat{y}_i) + (1-y_i) * \log(1-\hat{y}_i))$$

Example

$$\begin{array}{cc} \hat{y} & y \\ \begin{bmatrix}0.1\\0.7\\0.2\end{bmatrix} & \begin{bmatrix}0\\1\\0\end{bmatrix} \end{array}$$

$$L(y,\hat{y}) = $$

$$= \frac{-(\log(1-0.1) + \log(0.7) + \log(1-0.2))}{3}$$

$$= \frac{0.29}{3} = \sim 0.1$$

Loss optimization

The gradient

- The loss is a mathematical function of the various weights in the network
- We want to find the set of weights that achieve the lowest loss

$\boldsymbol{W}^* = \mathrm{argmin}_w \, J(\boldsymbol{W})$, where J is the average Loss

- Gradient of a function: A vector that points in the direction of steepest ascent.
- If we take the opposite direction of the gradient we move towards a local minimum

Loss optimization

The gradient descent algorithm

Example in two dimensions

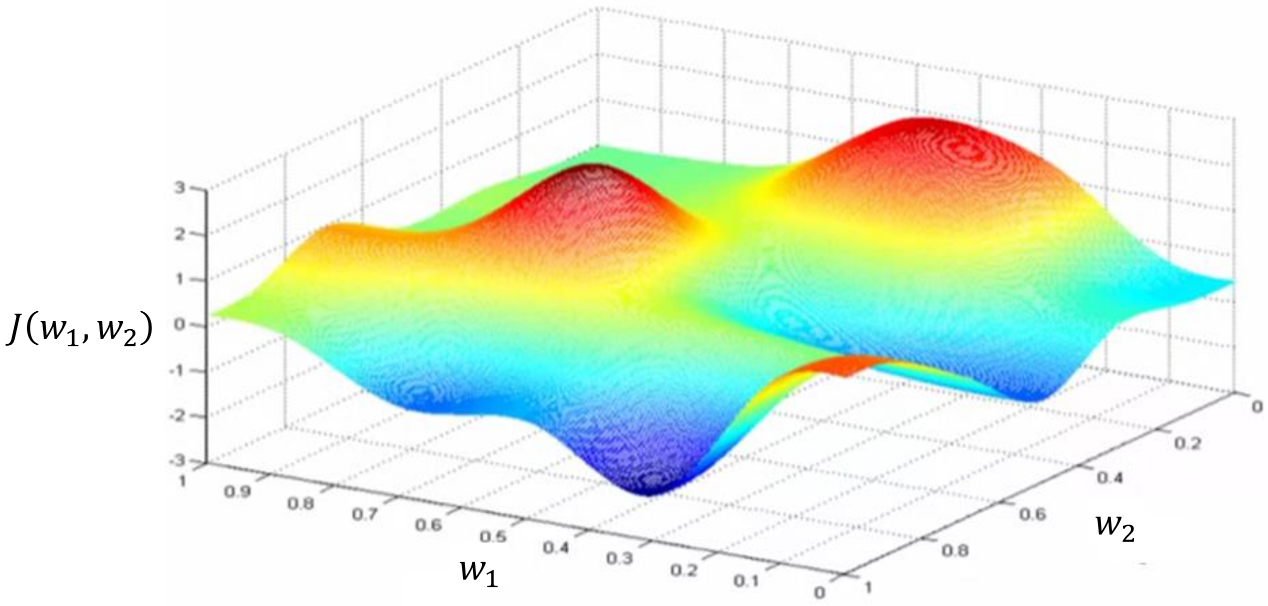


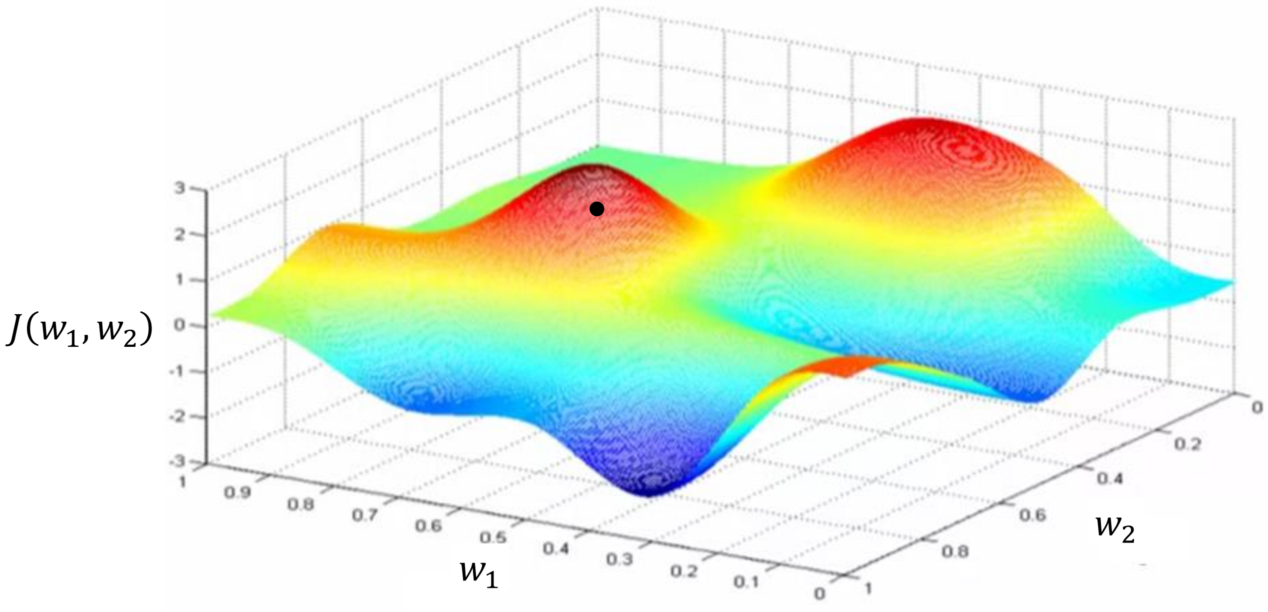
Image from: Andrew Ng (Coursera) https://www.coursera.org/learn/machine-learning/lecture/8SpIM/gradient-descent

Loss optimization

The gradient descent algorithm

Example in two dimensions

1. Pick a point (initialize weights)



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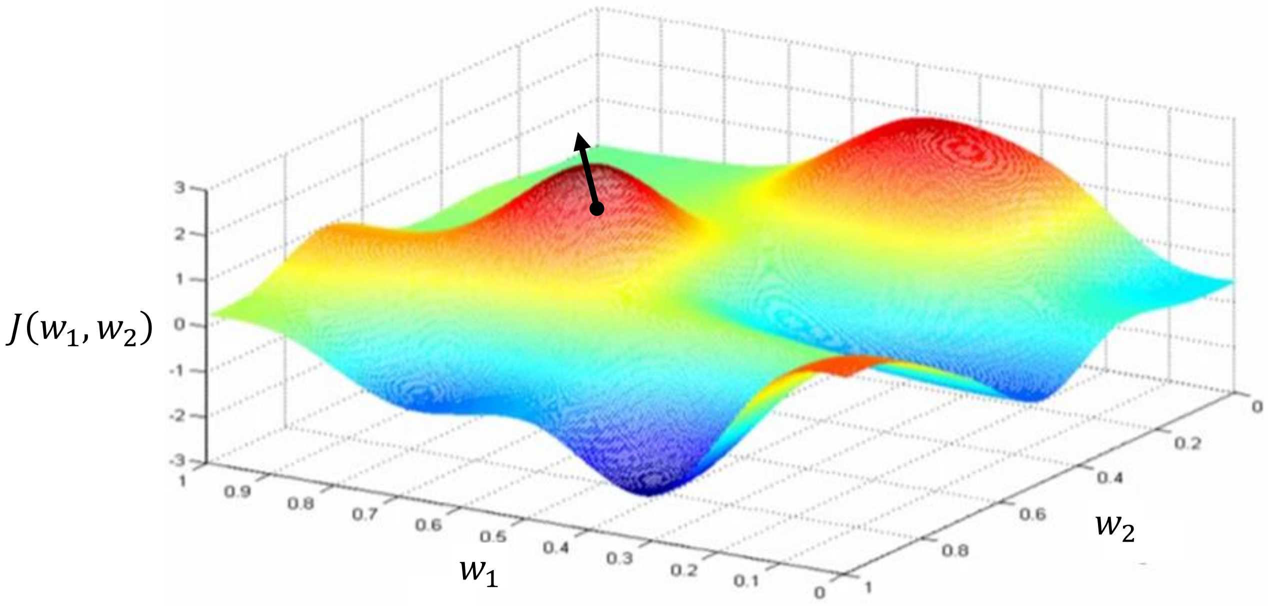
Loss optimization

The gradient descent algorithm

1. Pick a point (initialize weights)
2. Compute the gradient $\frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}$

Example in two dimensions



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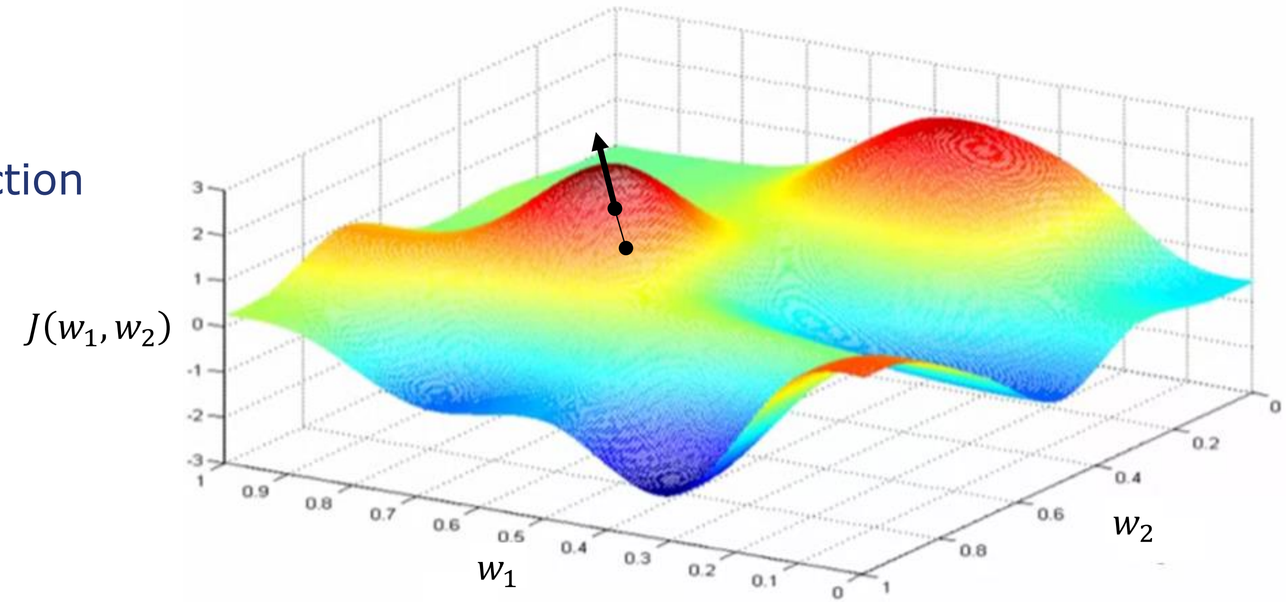
Loss optimization

The gradient descent algorithm

Example in two dimensions

1. Pick a point (initialize weights)
2. Compute the gradient $\frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}$
3. Take a step in the opposite direction

$$\boldsymbol{W} \leftarrow \boldsymbol{W} - \eta \frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}$$



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Loss optimization

The gradient descent algorithm

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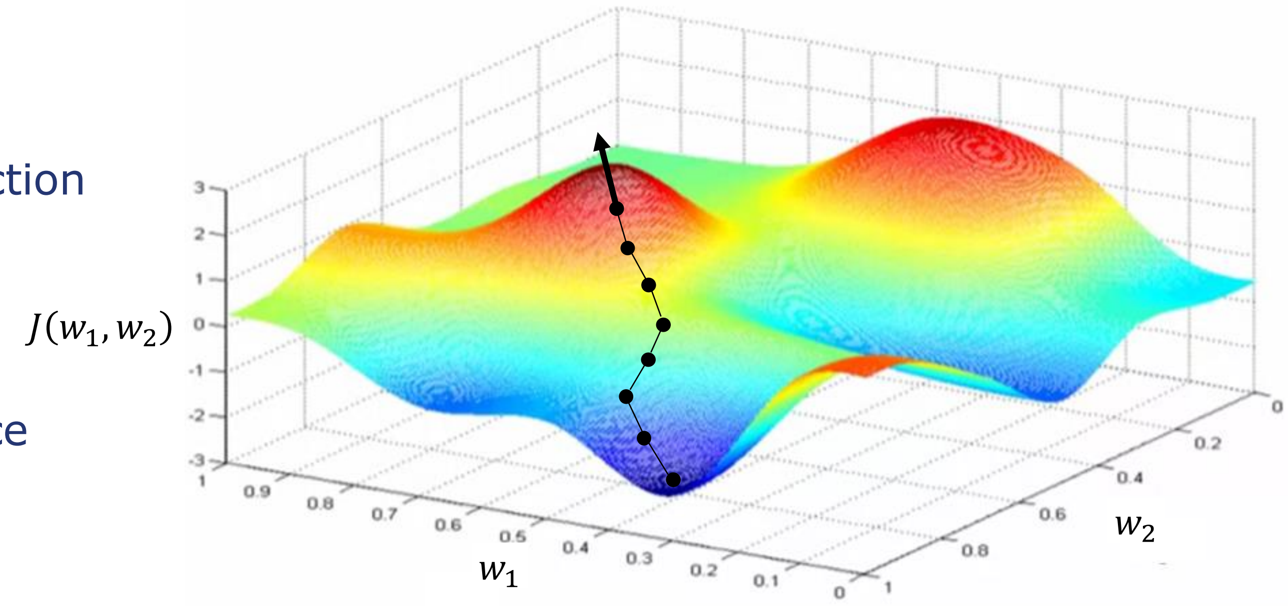
$$\boldsymbol{W} \leftarrow \boldsymbol{W} - \eta \frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}$$

4. Repeat 2 and 3 until convergence

Example in two dimensions



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Loss optimization

The gradient descent algorithm

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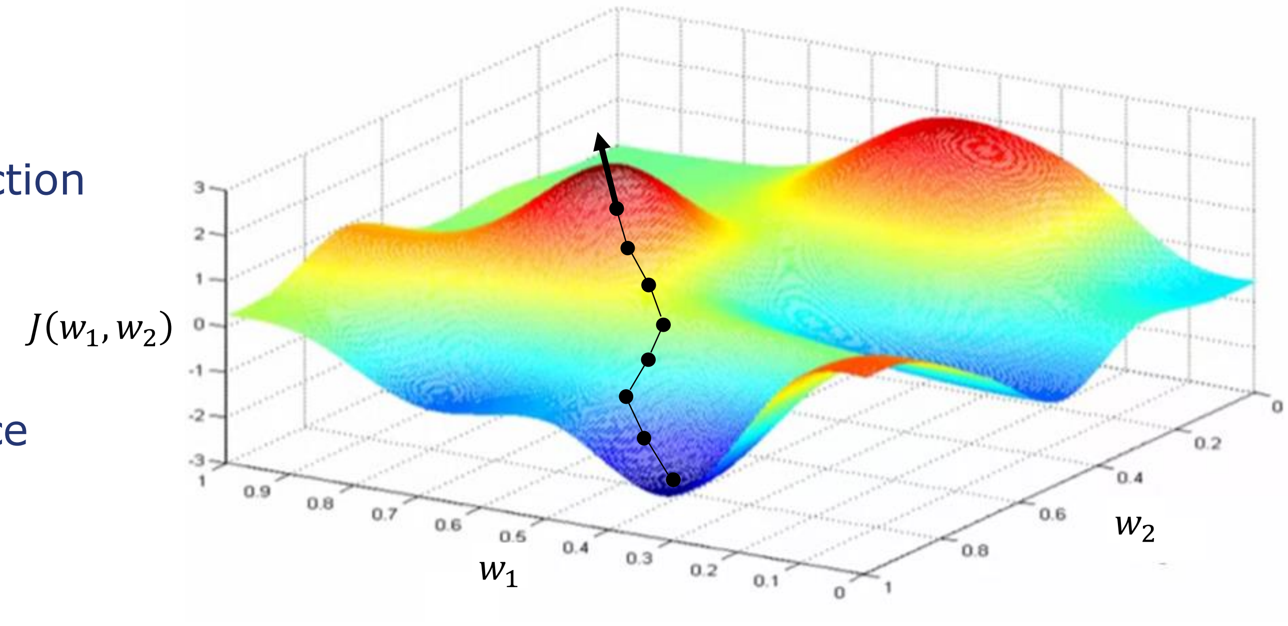
2. Compute the gradient $\frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}$
3. Take a step in the opposite direction

$$\boldsymbol{W} \leftarrow \boldsymbol{W} - \boxed{\eta} \frac{\partial J(\boldsymbol{W})}{\partial \boldsymbol{W}}$$

Learning rate

4. Repeat 2 and 3 until convergence

Example in two dimensions



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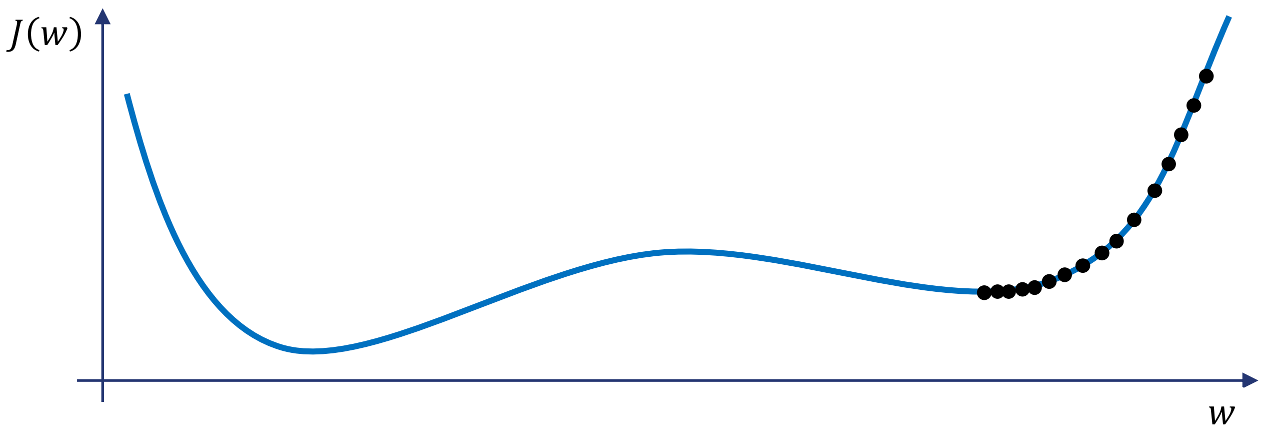
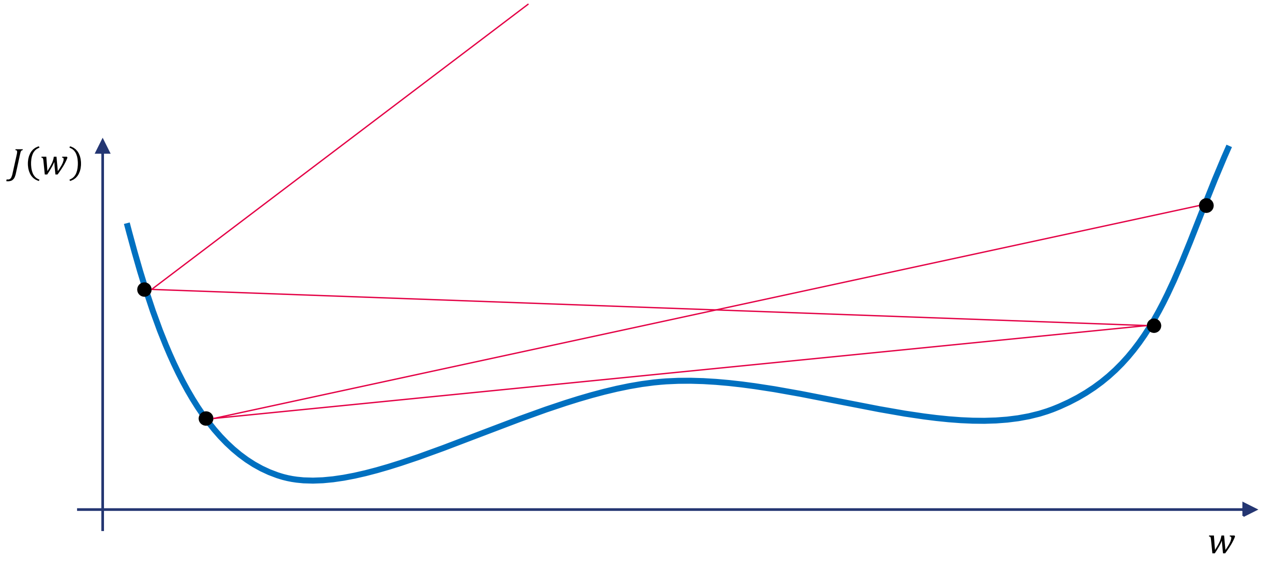
Learning rate η

- **Small** learning rates increase the change of getting stuck into local minima



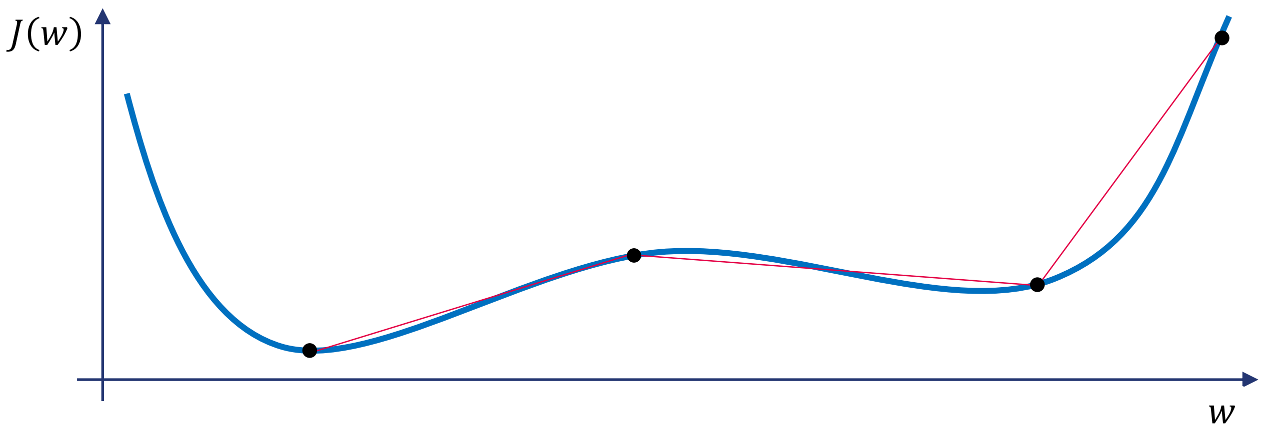
Learning rate η

- **Large** learning rates increase the chance of divergence



Learning rate η

- **Optimal learning rates** are hard to find



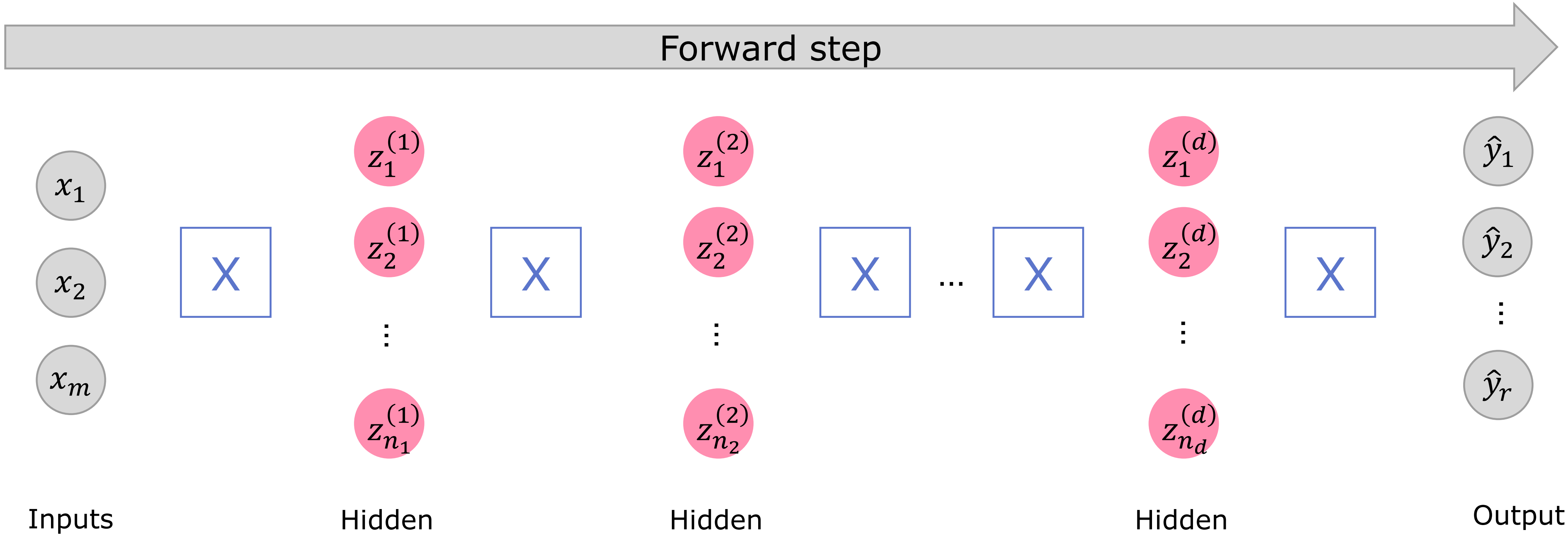
How to identify the right one?

1. Trying multiple learning rates
2. Adaptive learning rates
   - SGD
   - Adam
   - Adadelta
   - Adagrad
   - …

Many available in TF & pyTorch

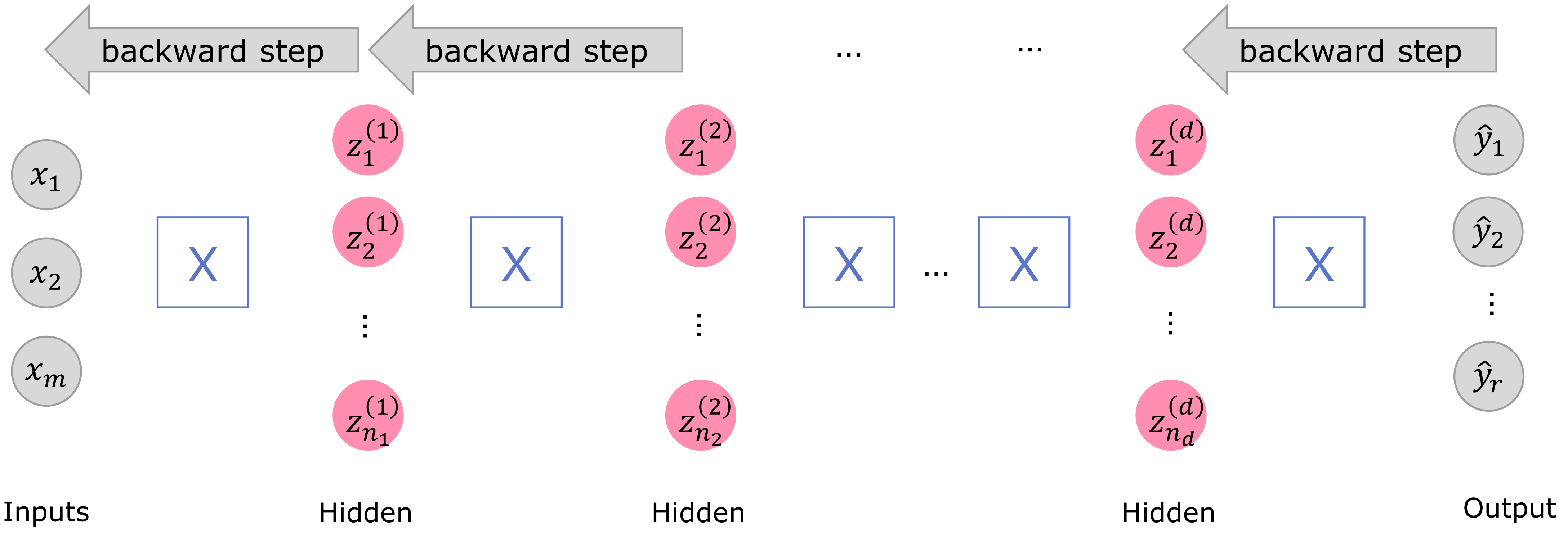
Back-propagation

Why is it called backpropagation?



Back-propagation

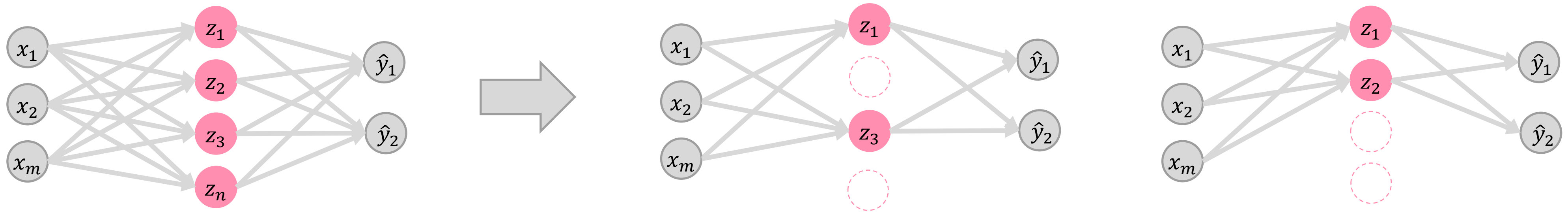
Why is it called backpropagation?



Overfitting in deep learning

Typical approaches

- Drop-out (randomly set some activation functions to 0).



- Early stop (stop training as soon as test error starts increasing)
  - Very similar to the traditional ML approach

Summary

- Fundamental building block: **The Perceptron**
- Stacking multi-output perceptrons sequentially: **Feed-Forward Neural Network**
- Training: finding the weights that **minimize a loss** function
  - Gradient Descent and back-propagation
- Overfitting: **Drop-out** or **early-stop**

- A short video and then… coding session

Exercise 4
Neural Networks

1. **Load the *Dry_Bean dataset***
   (HINT: library *readxl* to read excel files)
2. **Explore the dataset** (e.g. how many observations? How many classes? How many observations per class? How is each numeric variable distributed among classes? Are the classes distinguishable? etc.)
3. Create a **feed forward neural network** to predict the class of the beans by using the other variables as predictors
   1. Split the data (with ratio 80-20)
   2. Convert to tensors
   3. Experiments with different num of layer and nodes.
   4. Show results on training and test set

- **Due date: ??, 23.59 CET (Late submission +1week, 7 pts)**
- R Students: Use Rmarkdown/Rnotebook/Jupyter.
- Py Students: Use Jupyter
- Reports must contain code and results (no need to rerun)