Deep Forward Networks

Wednesday 08h15 – 09h00

Géraldine Schaller, Bern Winter School on Machine Learning 2025, Muerren

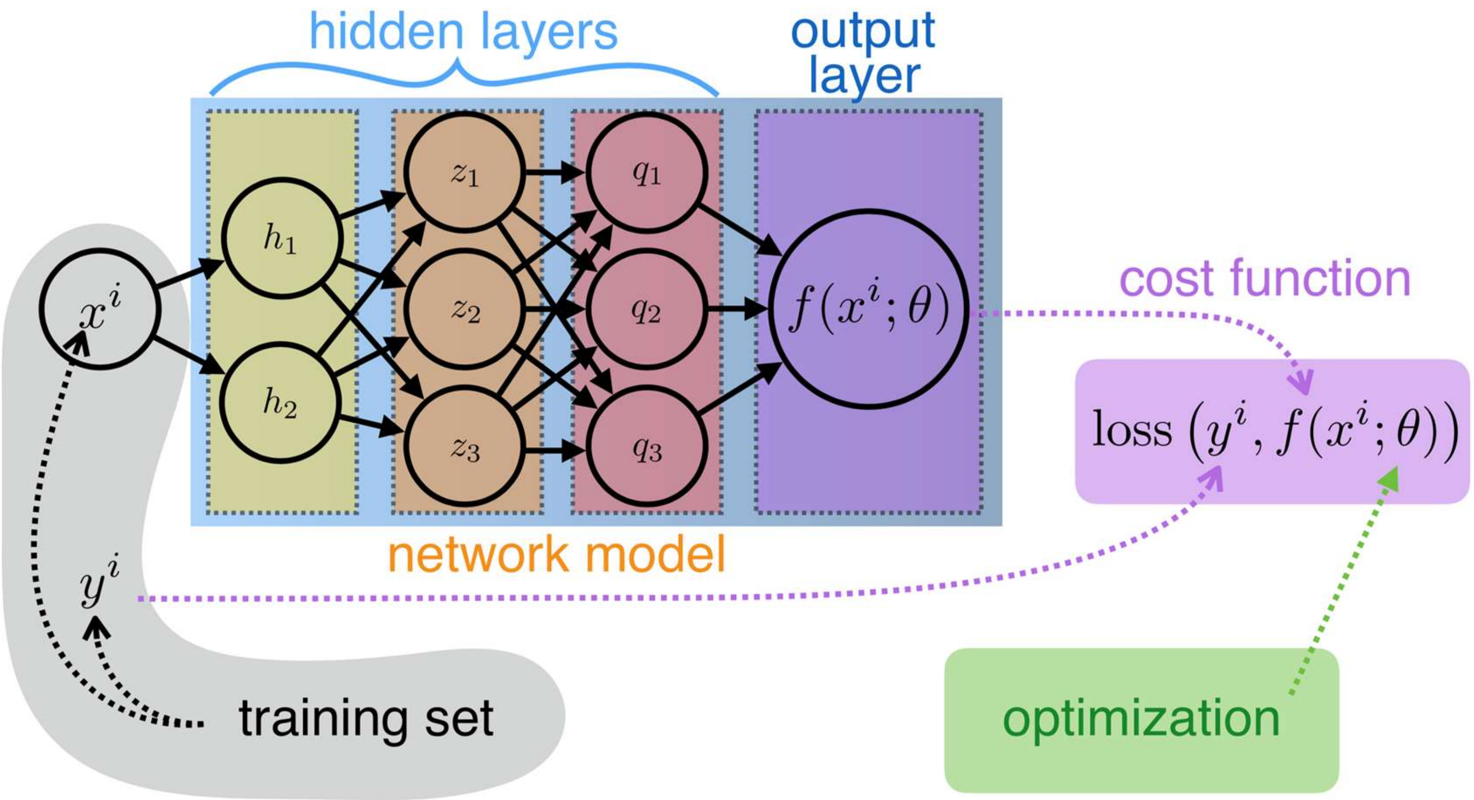
Deploying a Neural Network

Given a task (in terms of **I/O mappings**), we need :

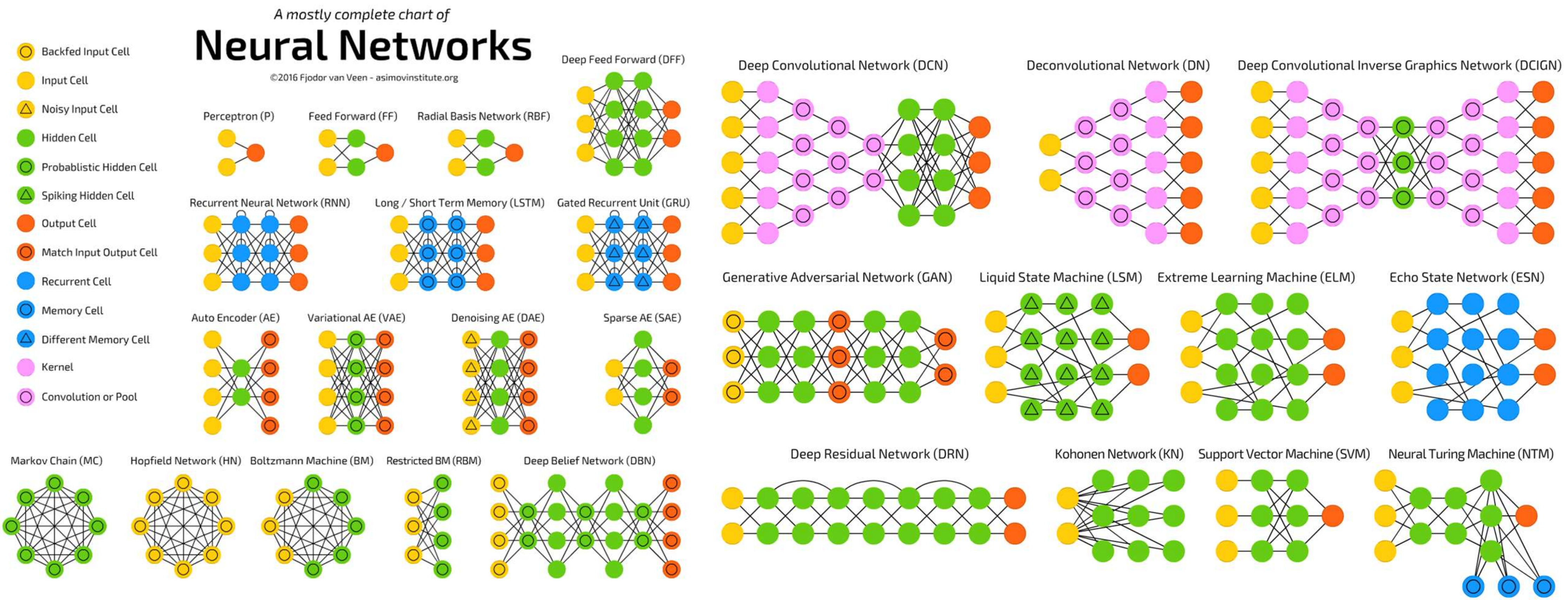
1) **Network model**

2) **Cost function**

3) **Optimization**

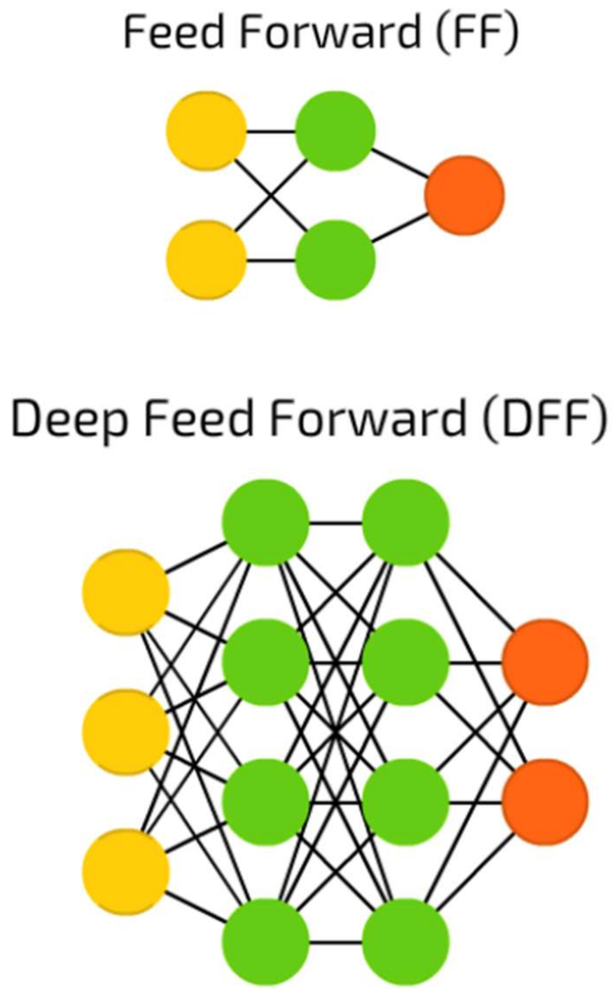


1) Network Model



(Deep) Feedforward NN (DFF)

- the simplest type of neural network
- All units are fully connected (between layers)
- information flows from input to output layer without back loops
- The first single-neuron network was proposed already in 1958 by AI pioneer Frank Rosenblatt
- Deep for "more than 1 hidden layer"

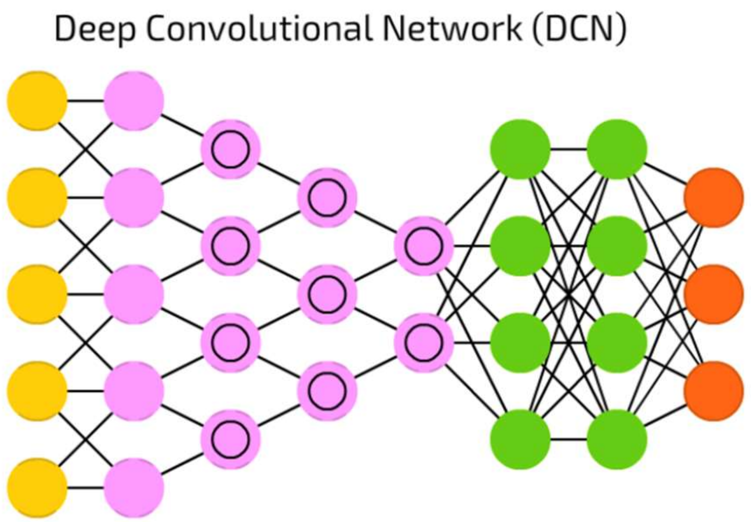


Convolutional Neural Networks (CNN)

- inspired by the organization of the animal visual cortex

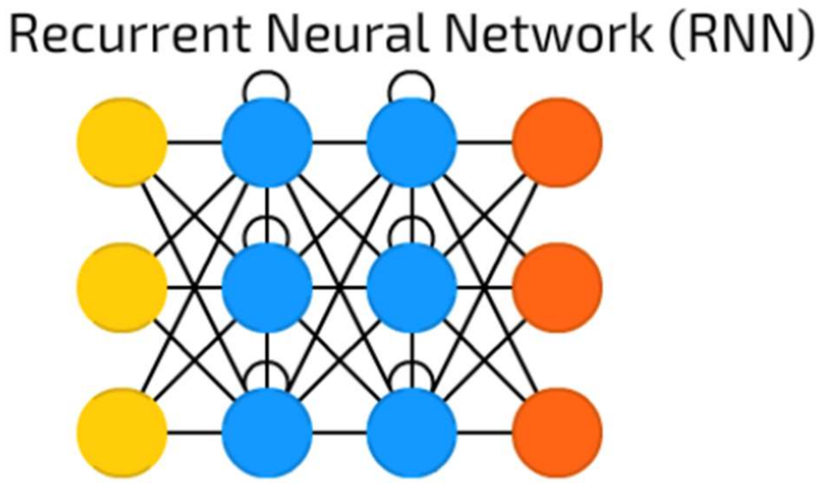
- **Kernel and convolution or pool cells** used to process and simplify input data
  - Weight sharing between *local regions*

- well suited for computer vision tasks
  - Image classification
  - Object detection



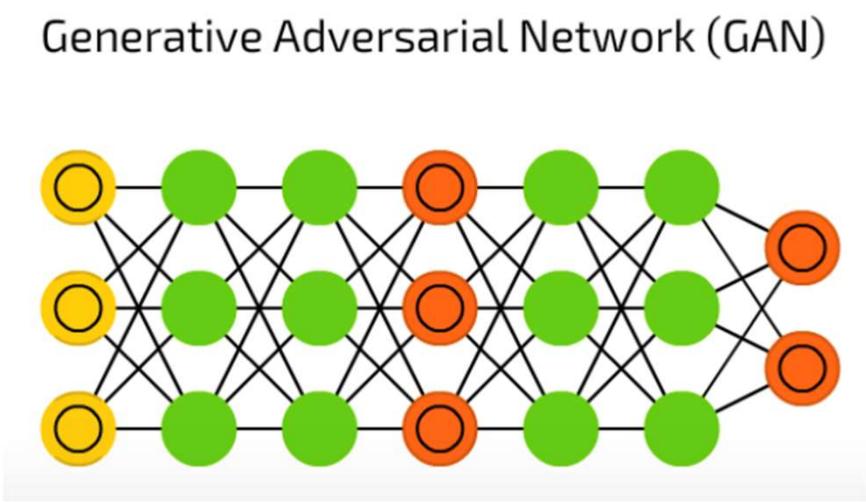
Recurrent Neural Networks (RNN)

- connections between neurons include loops
- **Recurrent cells** (or memory cells) used
  - Weight sharing between *time-steps*
- well-suited for processing sequences of inputs, when context is important
  - Text analysis

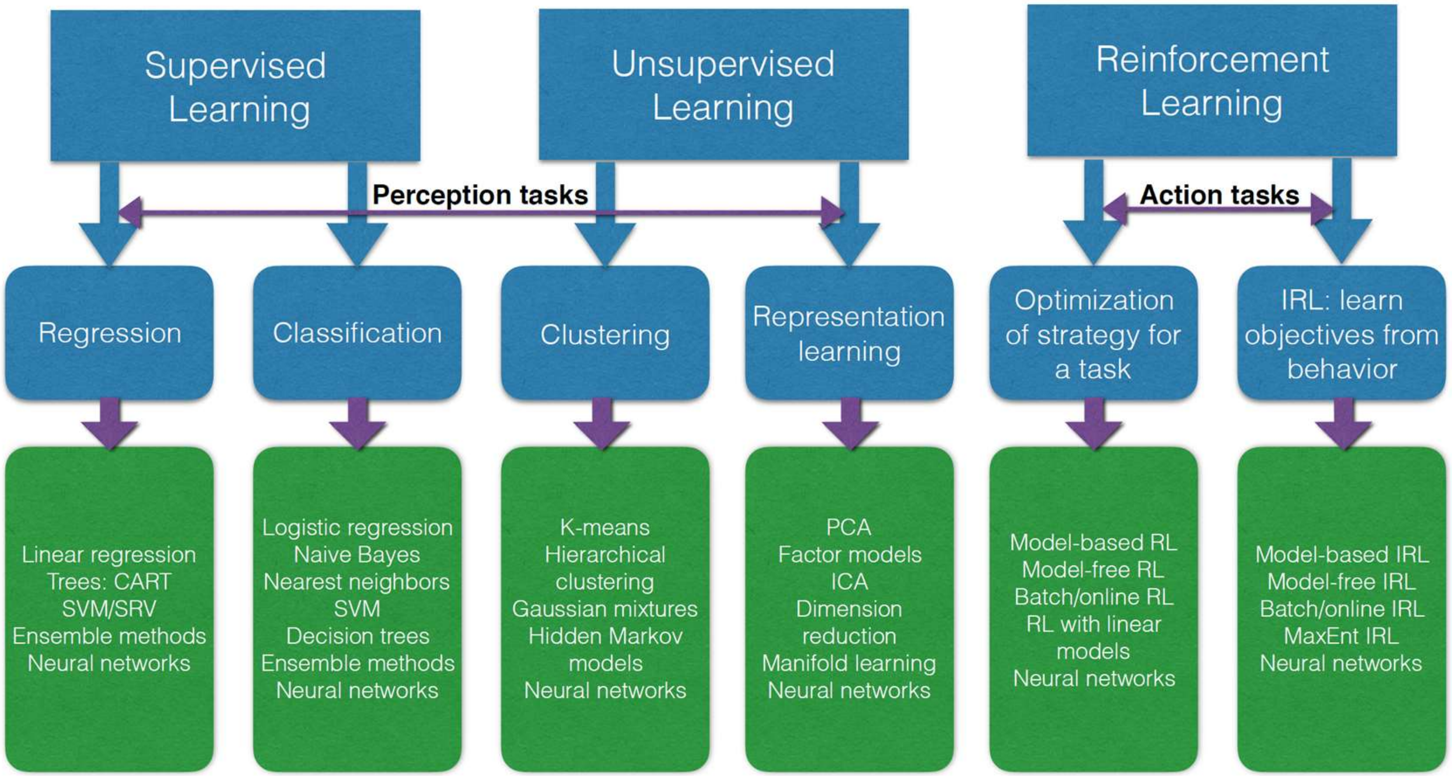


Generative Adversarial Networks (GAN)

- More of a **Training Paradigm** rather than an architecture
- Double networks composed from generator and discriminator.
- They constantly try to fool each other, hence contain **backfed input cells** and **match input output cells**.
- well-suited for generating real-life images, text or speech



Use cases



Supervised Learning
Unsupervised Learning
Reinforcement Learning
Perception tasks
Action tasks
Regression
Classification
Clustering
Representation learning
Optimization of strategy for a task
IRL: learn objectives from behavior
Linear regression
Trees: CART
SVM/SRV
Ensemble methods
Neural networks
Logistic regression
Naive Bayes
Nearest neighbors
SVM
Decision trees
Ensemble methods
Neural networks
K-means
Hierarchical clustering
Gaussian mixtures
Hidden Markov models
Neural networks
PCA
Factor models
ICA
Dimension reduction
Manifold learning
Neural networks
Model-based RL
Model-free RL
Batch/online RL
RL with linear models
Neural networks
Model-based IRL
Model-free IRL
Batch/online IRL
MaxEnt IRL
Neural networks

2) Loss and Cost functions

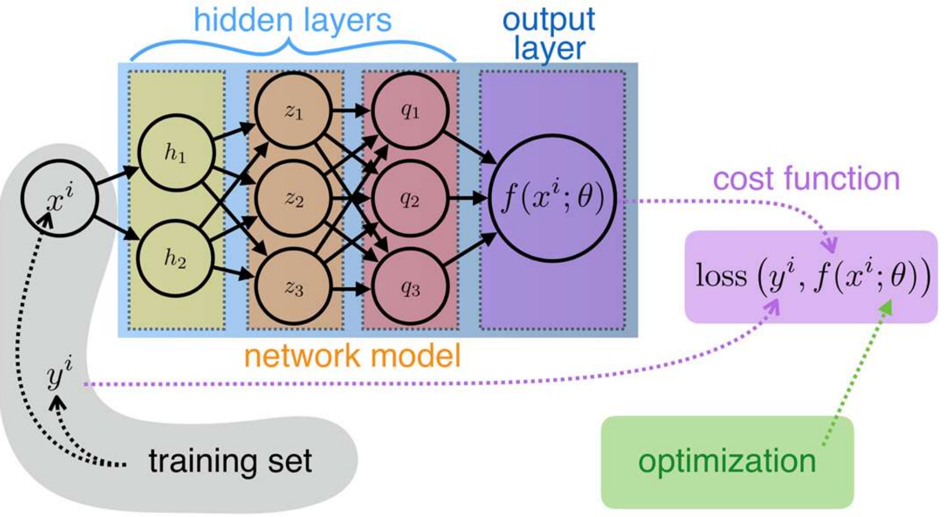
- Loss function $L\left(\hat{y}^{(i)}, y^{(i)}\right)$, also called error function, measures how different the prediction $\hat{y} = f(x)$ and the desired output y are

- Cost function $J(w, b)$ is the average of the loss function on the *entire training set*

$$J(w, b) = \frac{1}{m} \sum_{i=1}^{m} L(\hat{y}^{(i)}, y^{(i)})$$

- Goal of the optimization is to find the *parameters* $\theta = (w, b)$ that minimize the cost function

3) Optimization



- Given a task we define
  - Training data $\{x^i, y^i\}_{i=1,\ldots,m}$
  - Network $f(x;\theta)$
  - Cost function $J(\theta) = \sum_{i=1}^{m} \text{loss}\left(y^i, f(x^i;\theta)\right)$
  - Parameter initialization (weights, biases)
    - *random weights*, *biases initialized to small values (0.1)*
- Next, we *optimize the network parameters θ* (training)
- In addition, we have to set values for hyperparameters

Maximum Likelihood

- Given IID input/output samples : $(x^i, y^i) \sim p_{\text{data}}(x, y)$

- Conditional Maximum Likelihood estimate (between model pdf and data pdf):

$$\theta_{\text{ML}} = \arg\max_{\theta} \prod_{i=1}^{m} p_{\text{data}}(y^i | x^i; \theta)$$

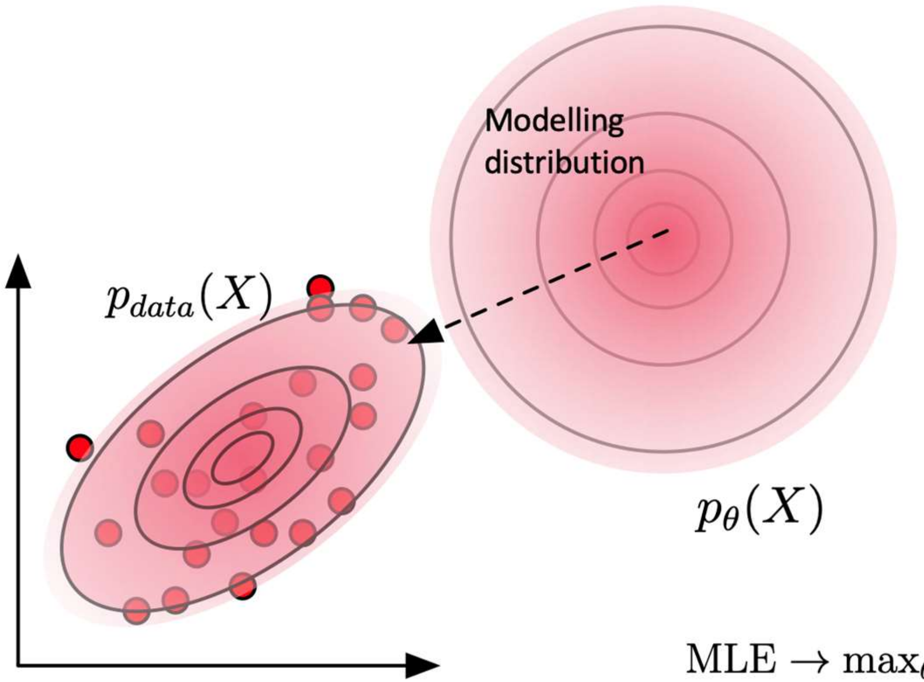
- Mathematical tricks :

$$= \arg\max_{\theta} \sum_{i=1}^{m} \log p_{\text{data}}(y^i | x^i; \theta)$$

$$\min_{\theta} -E_{x,y\sim\hat{p}_{\text{data}}}[\log p_{\text{model}}(y|x;\theta)]$$

*Maximize the likelihood == **Minimize the negative log-likelihood***

Maximum Likelihood



$$\text{MLE} \rightarrow \max_{\theta\in\Theta} \frac{1}{N}\sum_{i=1}^{N} \log p_\theta(x_i)$$

Fisher 1922

$$\min_{\theta\in\mathcal{M}} KL\left(P_{\text{data}}, P_\theta\right) = \mathbb{E}_{\mathbf{x}\sim P_{\text{data}}}\left[\log \frac{p_{\text{data}}(\mathbf{x})}{p_\theta(\mathbf{x})}\right]$$

Loss function choice

- Choice determined by the output representation
  - Probability vector (**classification**) : Cross-entropy

$$\hat{y} = \sigma(w^\top h + b) \qquad\qquad p(y|\hat{y}) = \hat{y}^{y}(1-\hat{y})^{(1-y)}$$

$$\boxed{L(\hat{y}, y) = -\log p(y|\hat{y}) = -\big(y\ \log(\hat{y}) + (1-y)\log(1-\hat{y})\big)}$$

(binary classification)

  - Mean estimate (**regression**) : Mean Squared Error, L2 loss

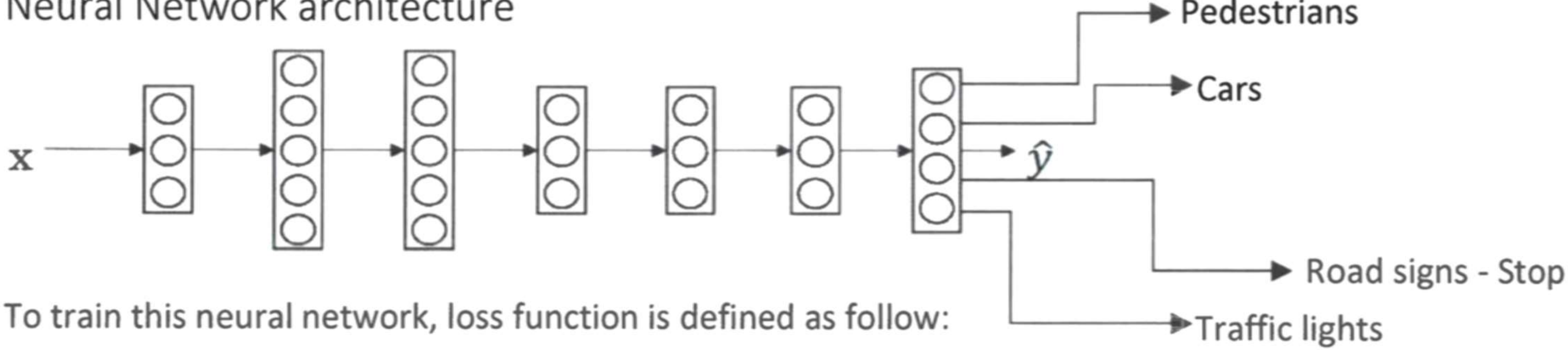
$$\hat{y} = W^\top h + b \qquad\qquad p(y|\hat{y}) = \mathrm{N}(y; \hat{y})$$

$$\boxed{L_2(\hat{y}, y) = -\log p(y|\hat{y}) = \sum_{i=0}^{m} \left(y^i - \hat{y}^i\right)^2}$$

Loss function example

- NN does simultaneously several tasks (multi-task)

Neural Network architecture

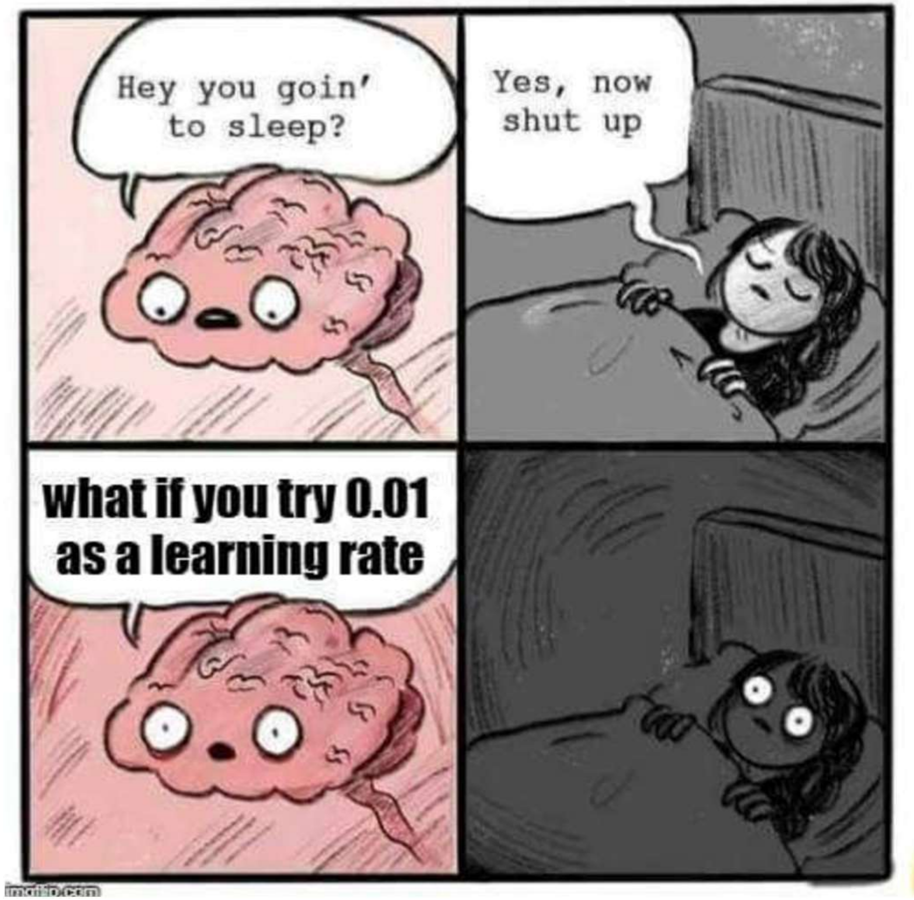


To train this neural network, loss function is defined as follow:

$$-\frac{1}{m}\sum_{i=1}^{m}\boxed{\sum_{j=1}^{4}}\left(y_j^{(i)}\log\left(\hat{y}_j^{(i)}\right)+\left(1-\ y_j^{(i)}\right)\log\left(1-\hat{y}_j^{(i)}\right)\right)$$

Hyperparameters

- Parameters that cannot be learnt directly from training data
- A long list…
  - Learning rate α
  - Number of iterations (epochs)
  - Number of hidden layers
  - Number of hidden units
  - Choice of activation function
  - *More to come !*



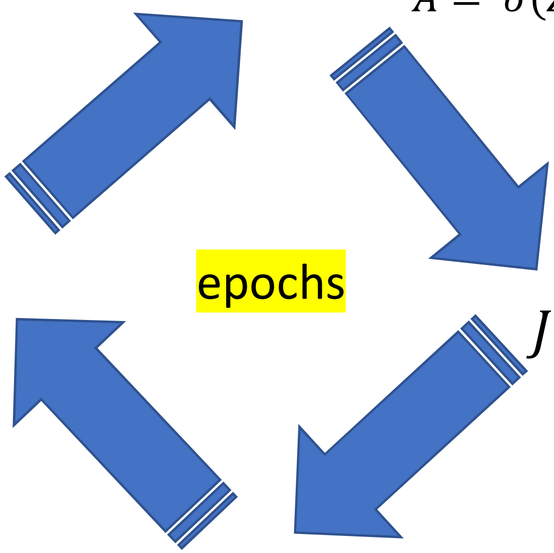
Training

- *Iterative* process

Forward propagation

$$Z = w^T x + b$$

$$A = \sigma(Z)$$



epochs

Cost function

$$J(w, b) = J(\theta)$$

Backward propagation

(dJ/dw, dJ/db)

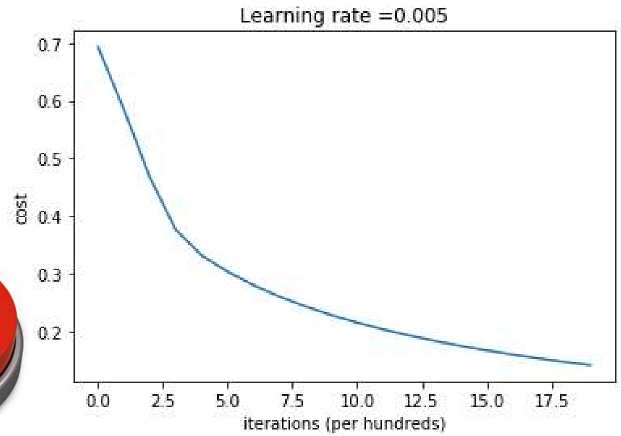
Parameter update

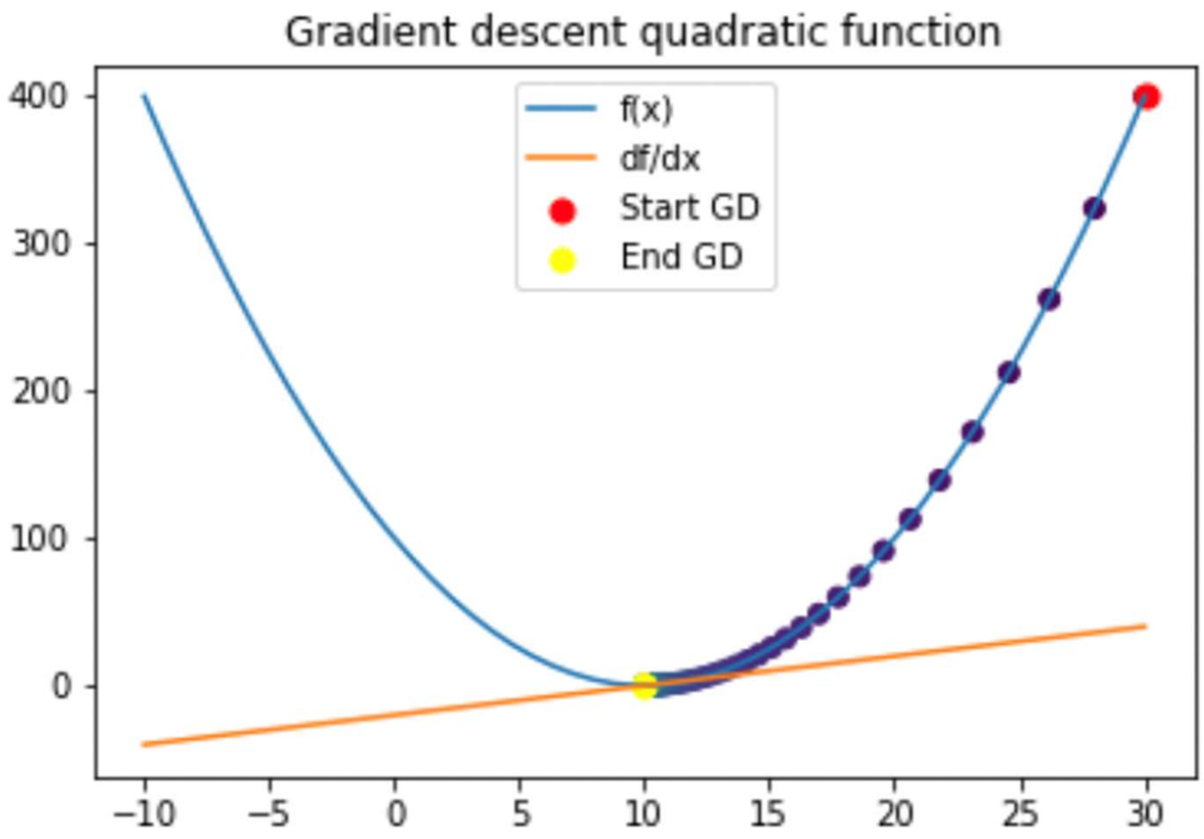
(gradient descent)

learning rate α

$$\boxed{\theta_{t+1} = \theta_t - \alpha \nabla J(\theta_t)}$$

Learning curve

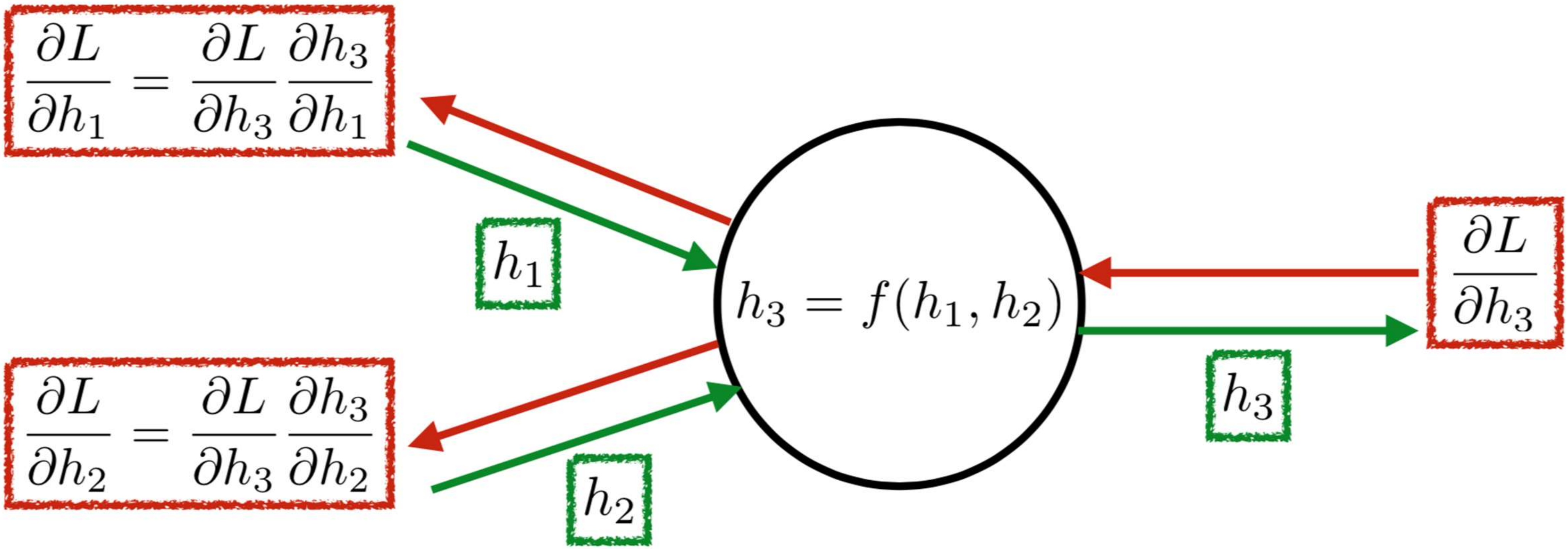




Gradient descent quadratic function
f(x)
df/dx
Start GD
End GD
400
300
200
100
0
−10
−5
0
5
10
15
20
25
30

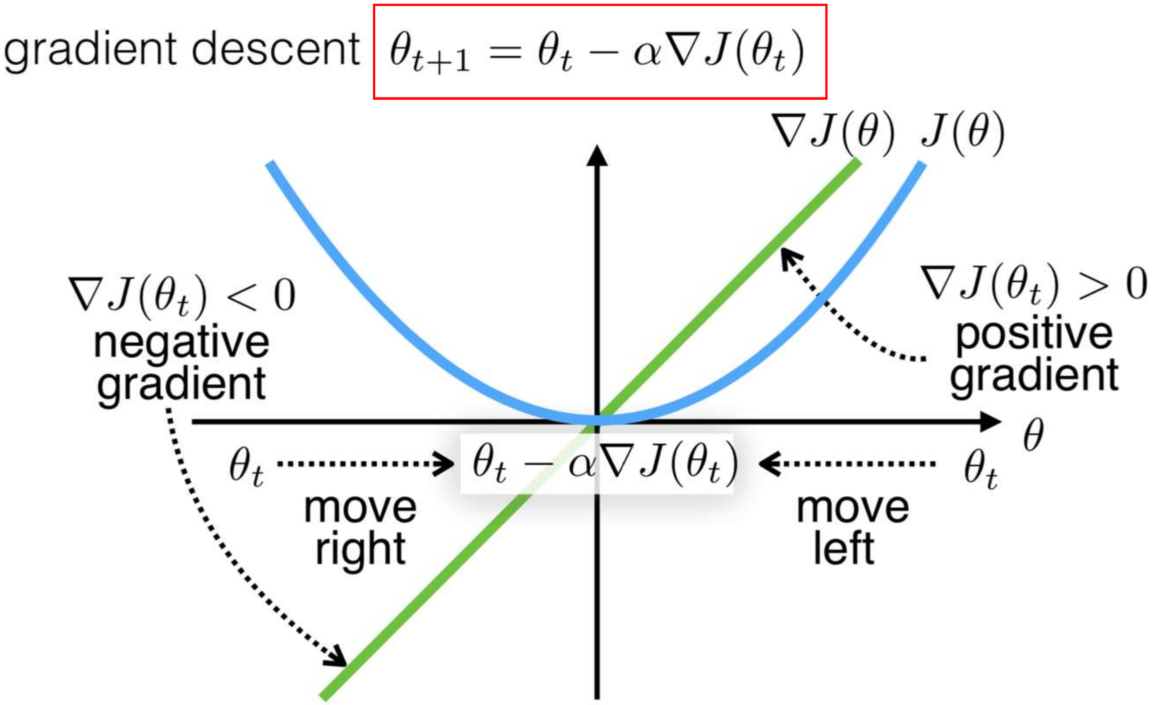
Backpropagation

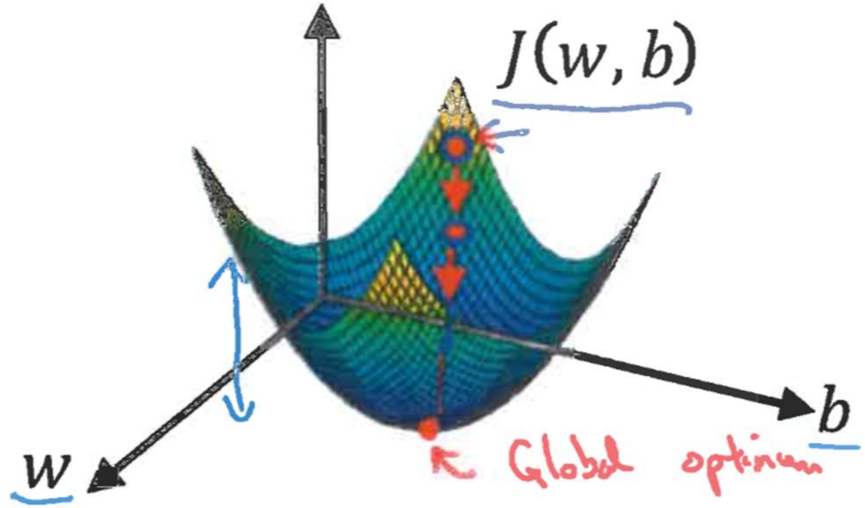
- Efficient implementation of the chain-rule to compute derivatives with respect to network weights



Gradient Descent

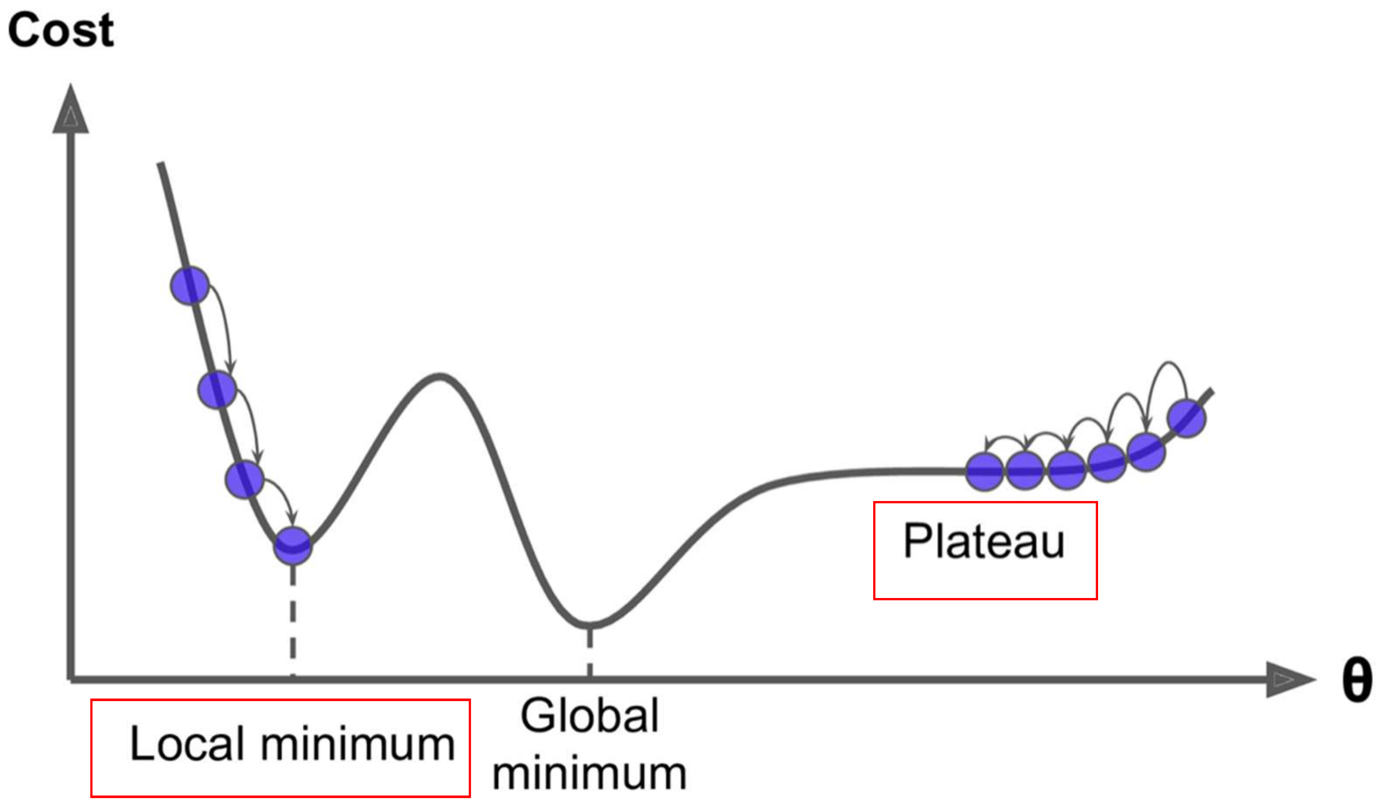
- Iterative method to find the parameters $\theta = (w, b)$ that minimize $J(\theta)$



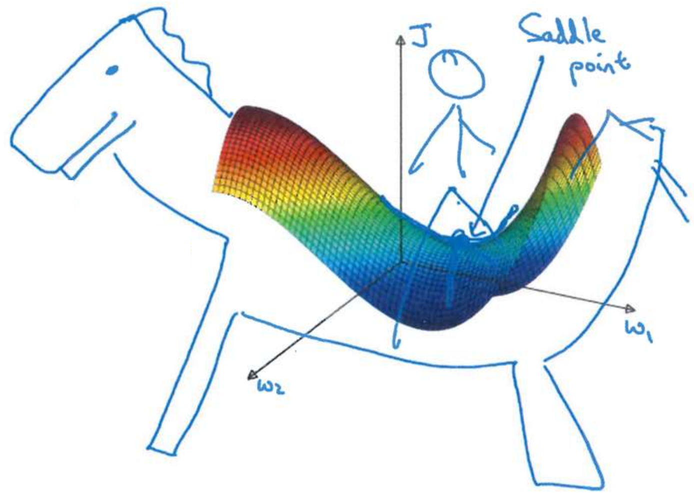


$$\nabla J(w) = \frac{dJ(w,b)}{dw} \qquad \nabla J(b) = \frac{dJ(w,b)}{db}$$

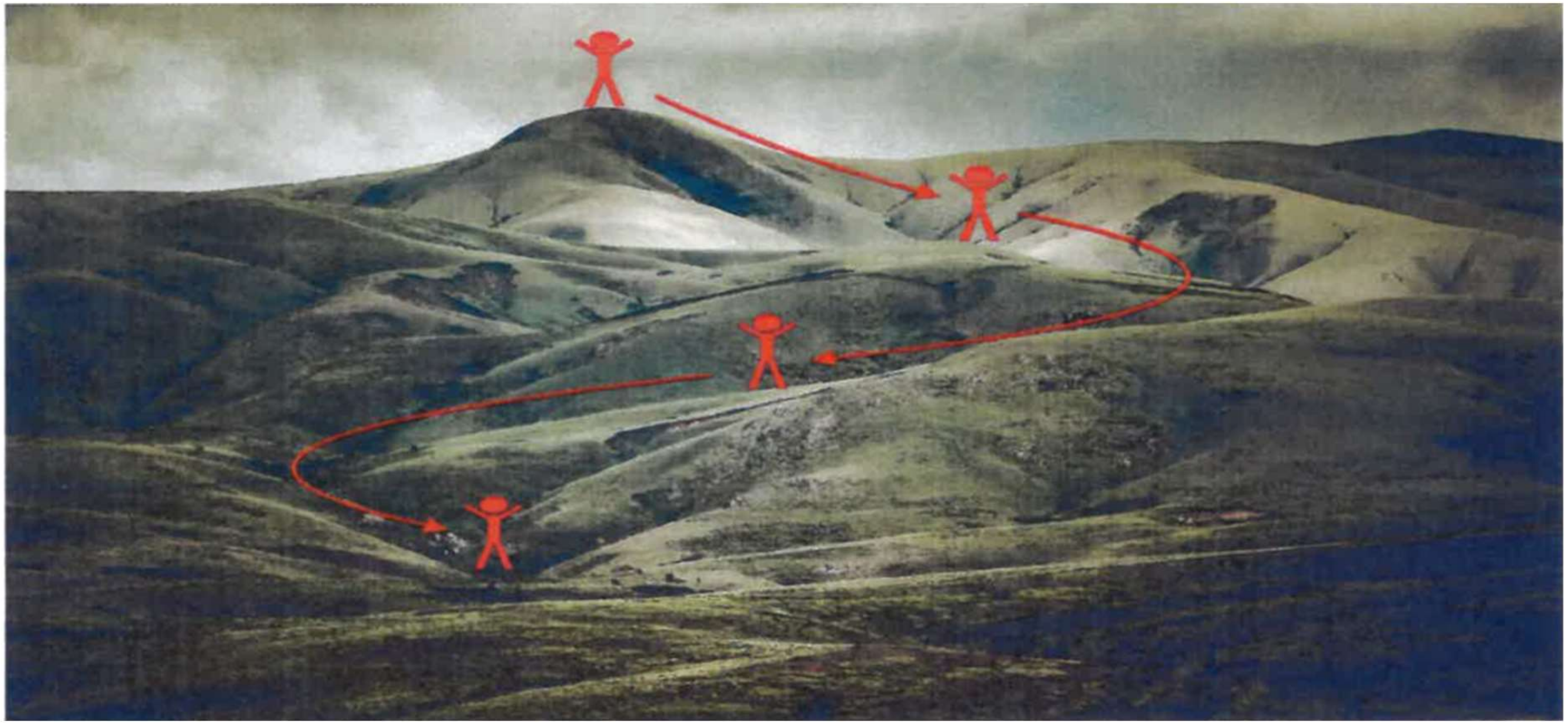
Optimization pitfalls



Saddle point



Gradient Descent Illustration



Tutorial / Practical