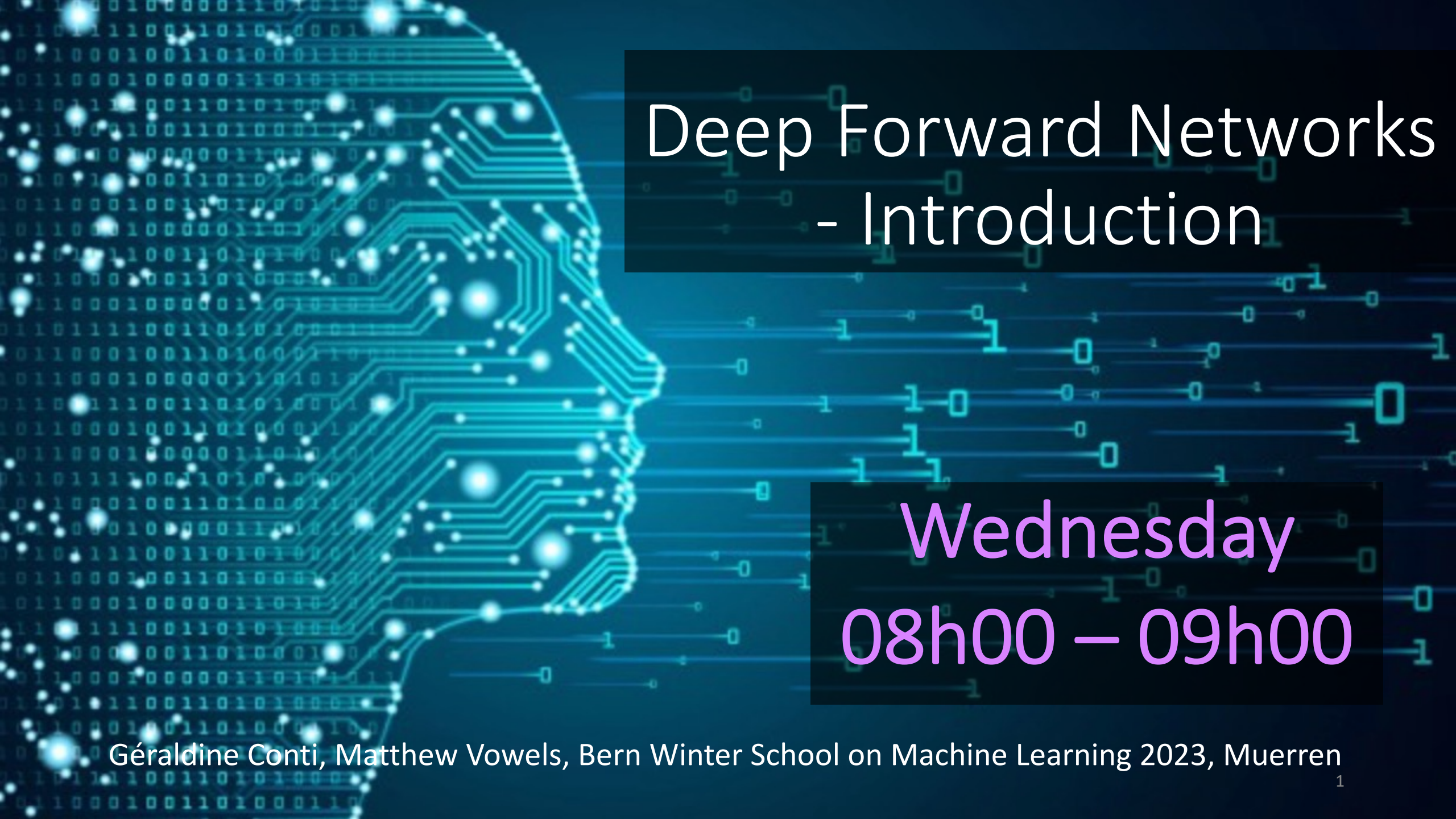


Deep Forward Networks - Introduction

Wednesday 08h00 – 09h00

Géraldine Conti, Matthew Vowels, Bern Winter School on Machine Learning 2023, Muerren

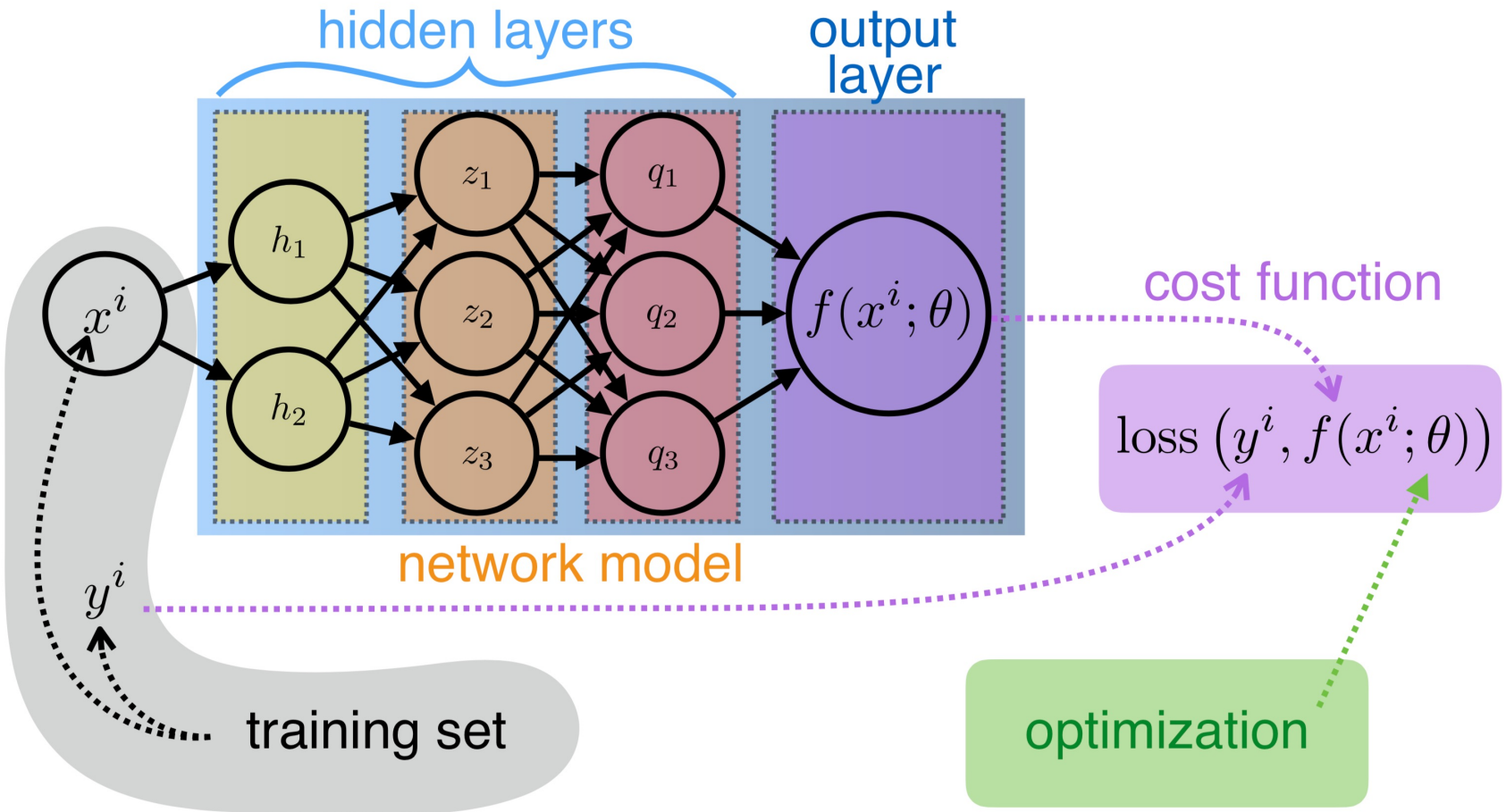
Deploying a Neural Network

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

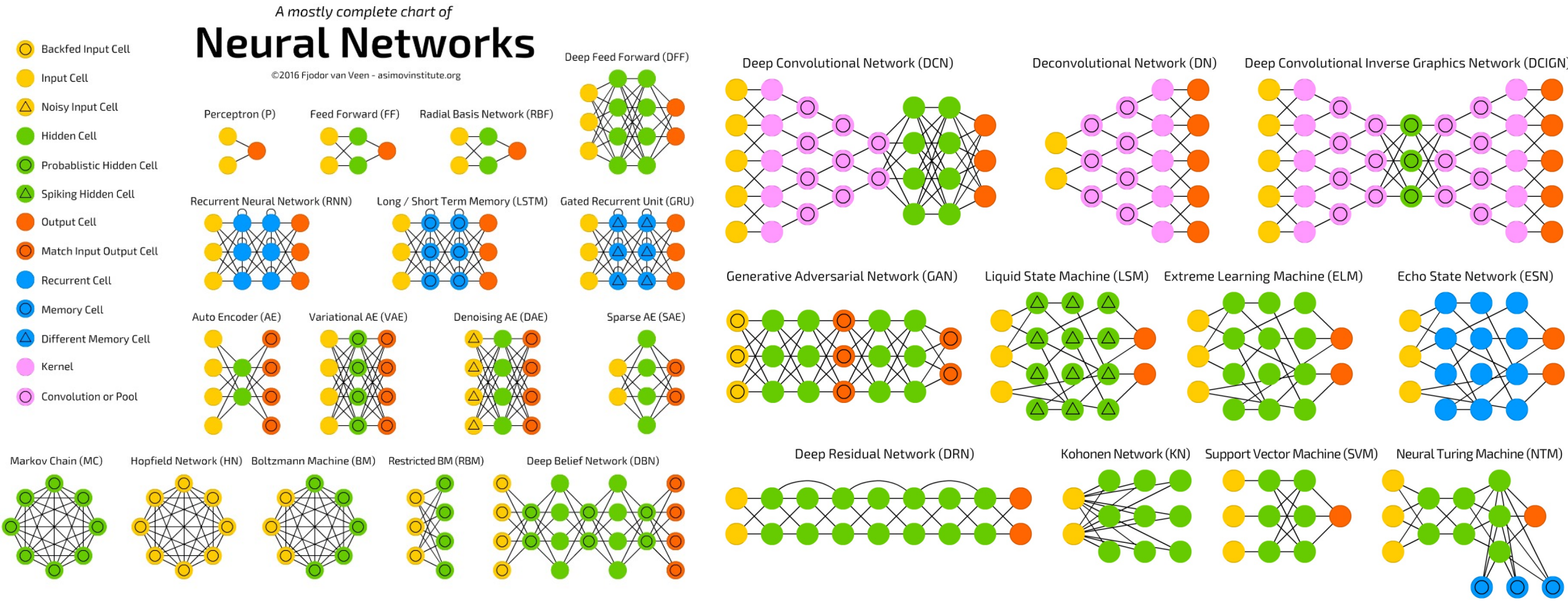
1) **Network model**

2) **Cost function**

3) **Optimization**



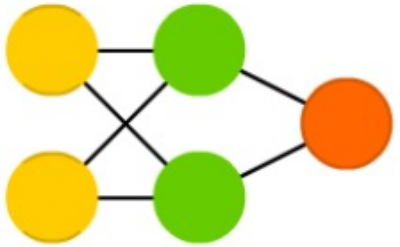
1) Network Model



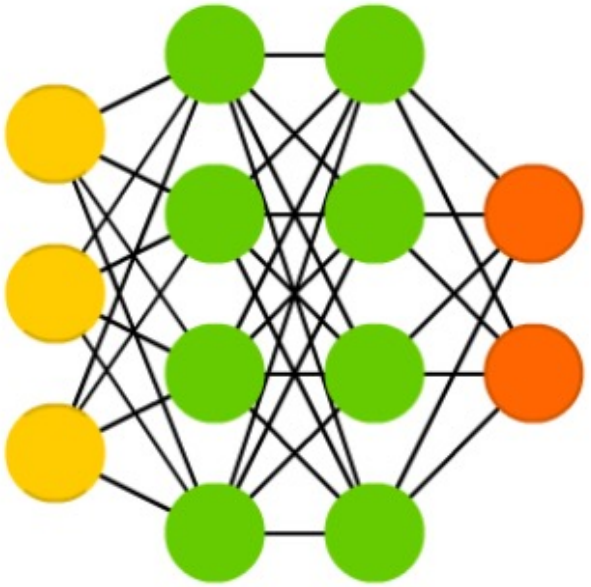
(Deep) Feedforward NN (DFF)

- 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**”

Feed Forward (FF)

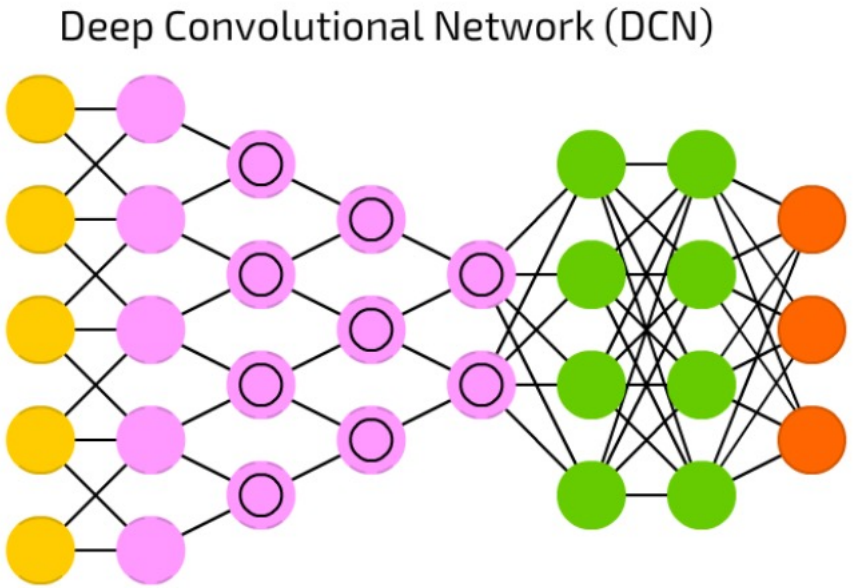


Deep Feed Forward (DFF)



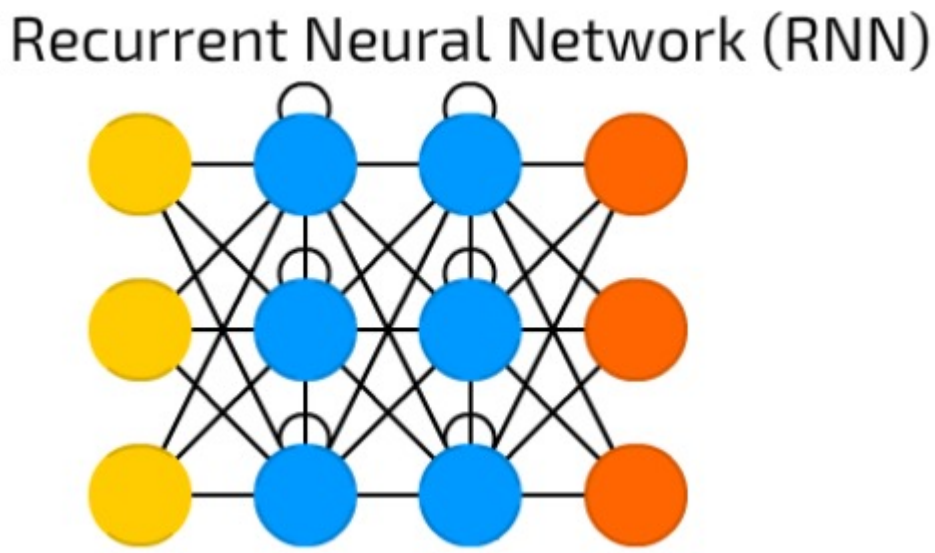
Convolutional Neural Networks (CNN)

- 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



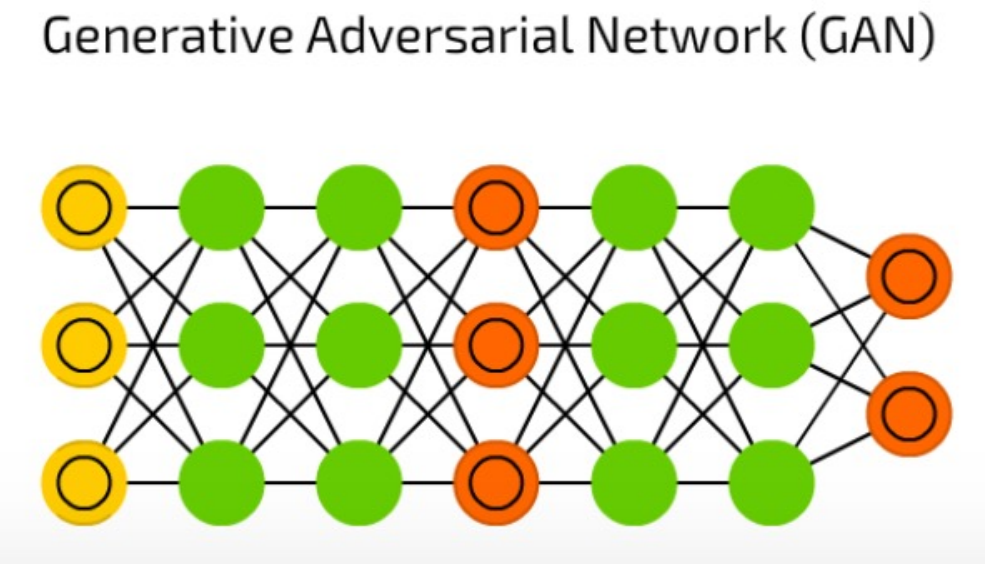
Recurrent Neural Networks (RNN)

- 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

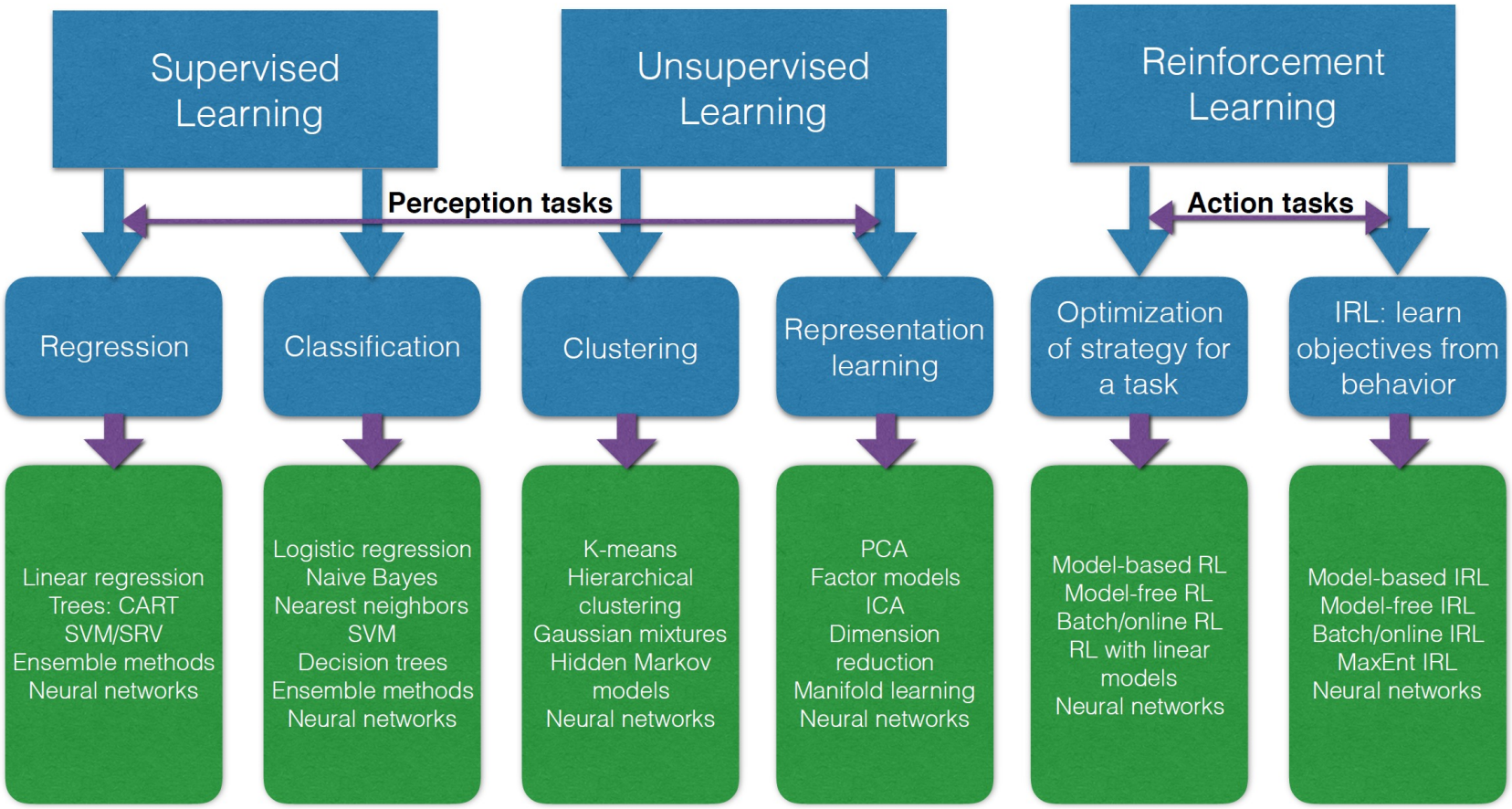


Generative Adversarial Networks (GAN)

- 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

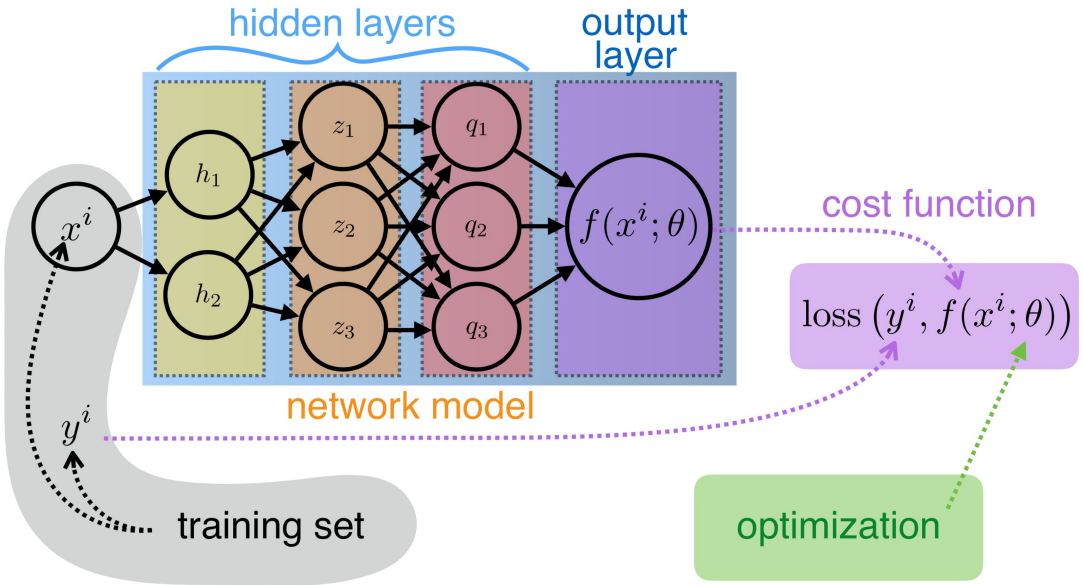
- Loss function $L(\hat{y}^{(i)}, y^{(i)})$, also called error function, measures how different the prediction $\hat{y} = f(x)$ and the desired output y are

- 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):

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

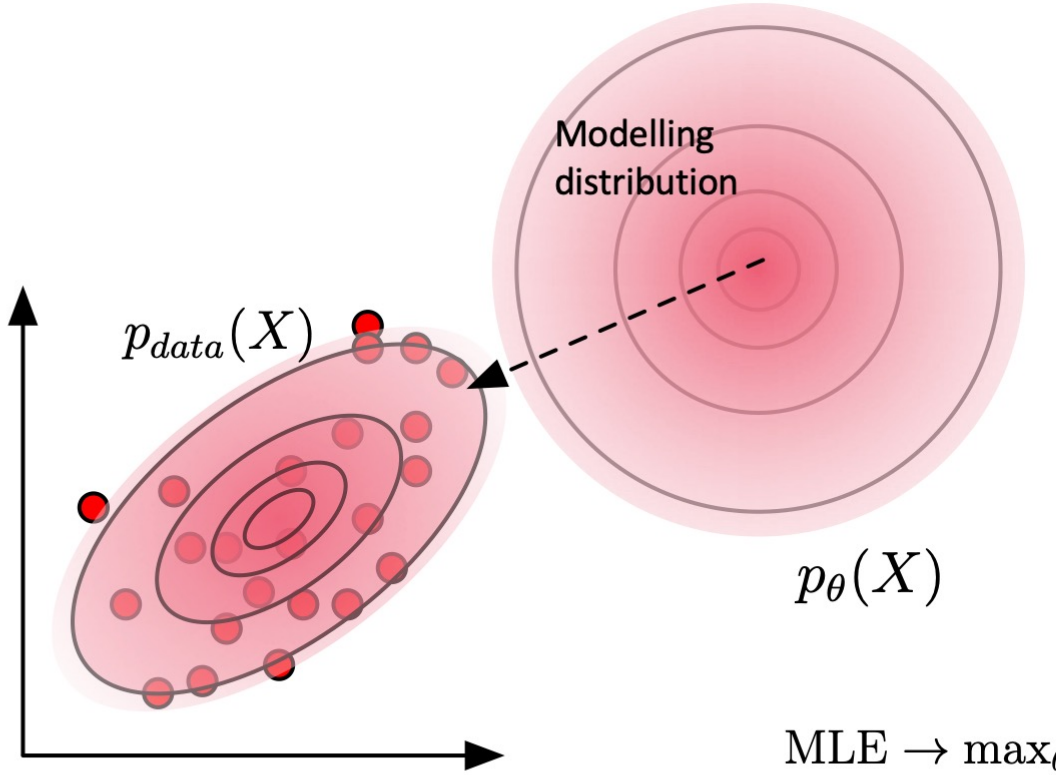
- Mathematical tricks :

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

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

*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

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

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

(binary classification)

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

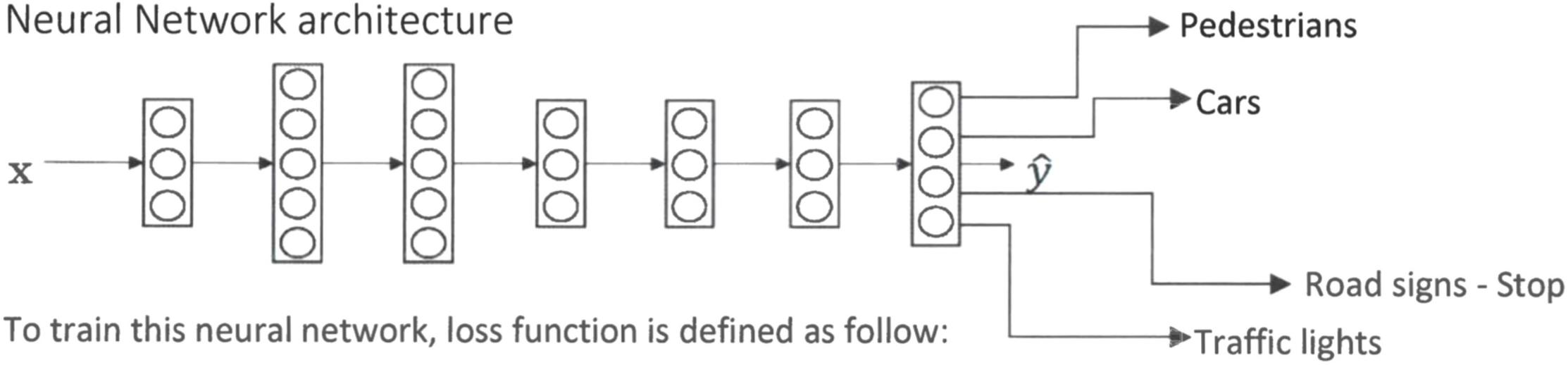
$$\hat{y} = W^\top h + b \qquad p(y|\hat{y}) = \mathrm{N}(y; \hat{y})$$

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

Loss function example

- NN does simultaneously several tasks (multi-task)

Neural Network architecture



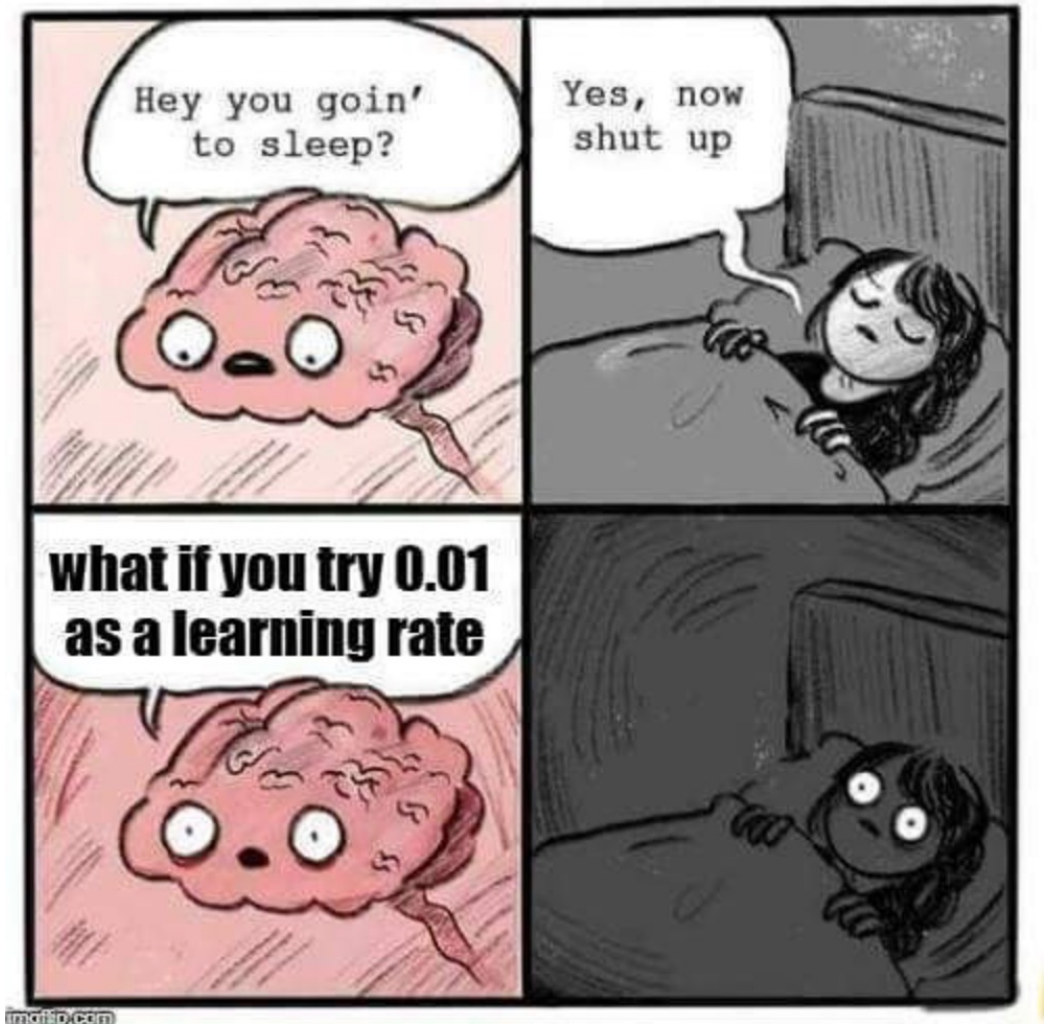
To train this neural network, loss function is defined as follow:

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

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

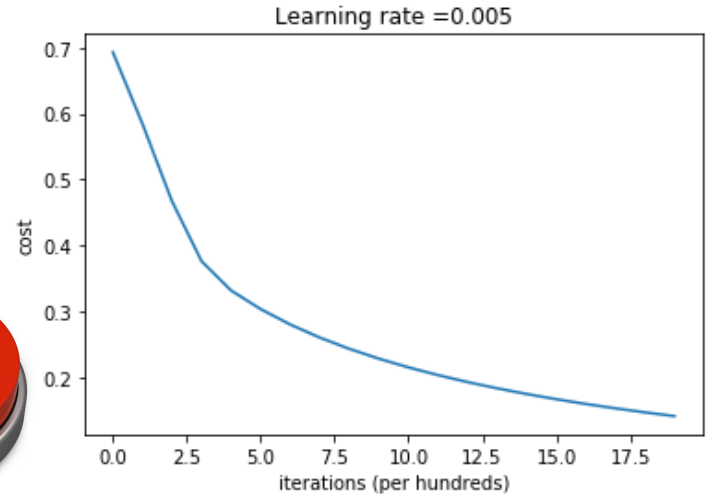
- *Iterative* process

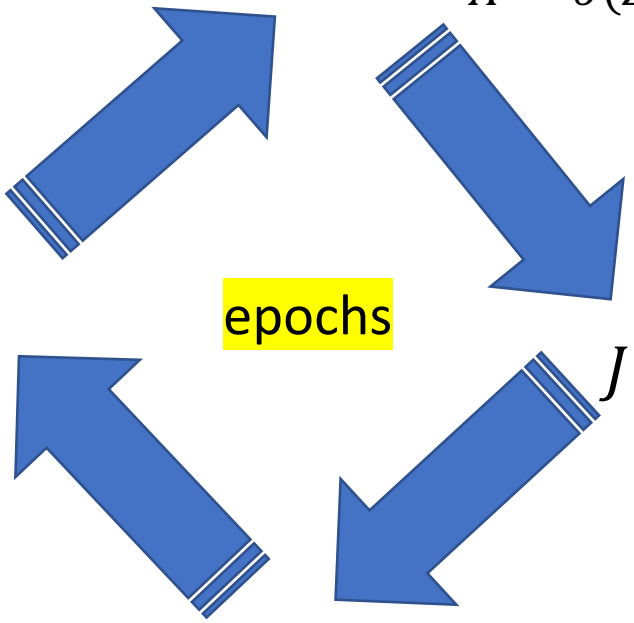
Forward propagation

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

$$A = \sigma(Z)$$

Learning curve





Parameter update
(gradient descent)

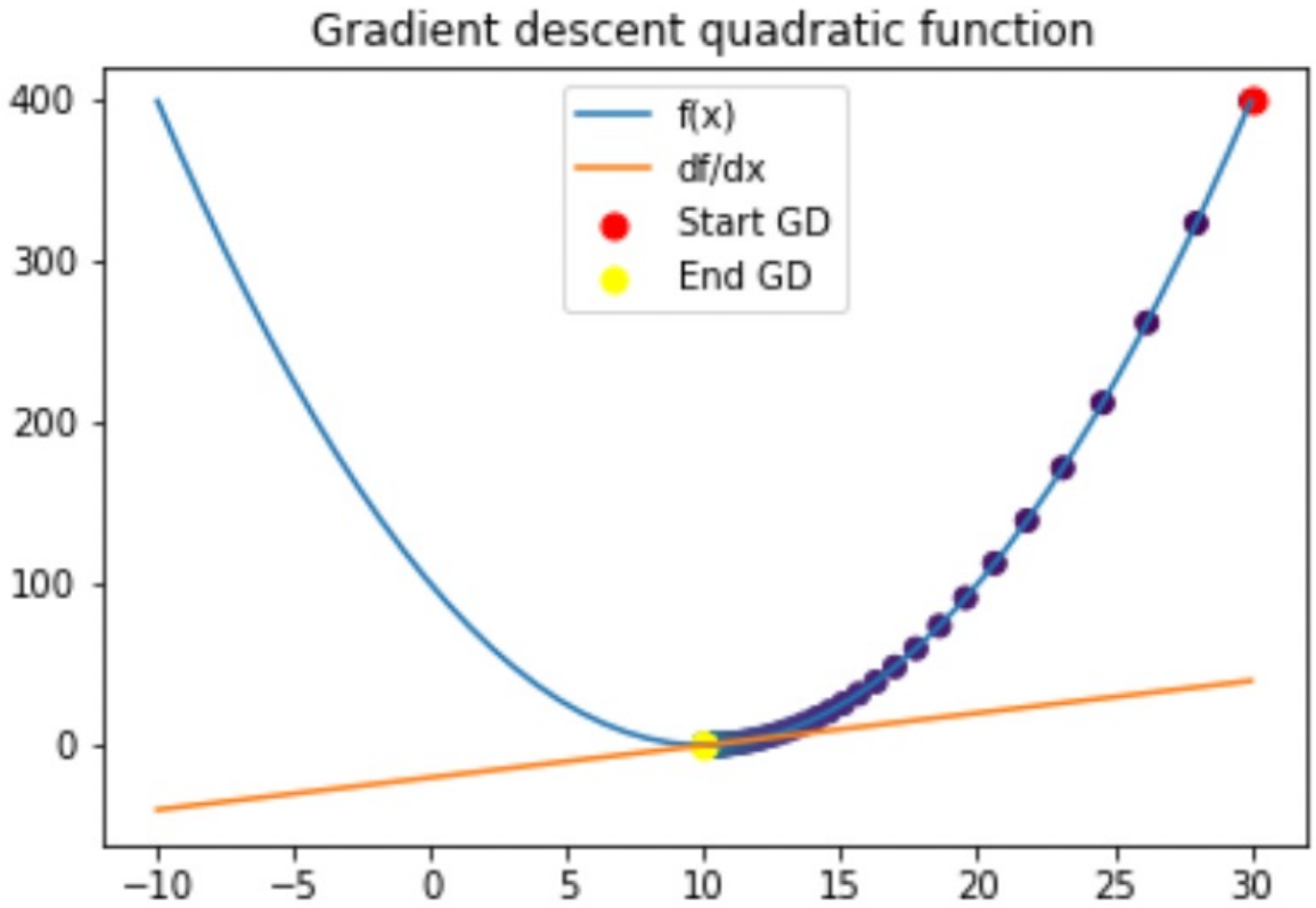
epochs

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

learning rate α

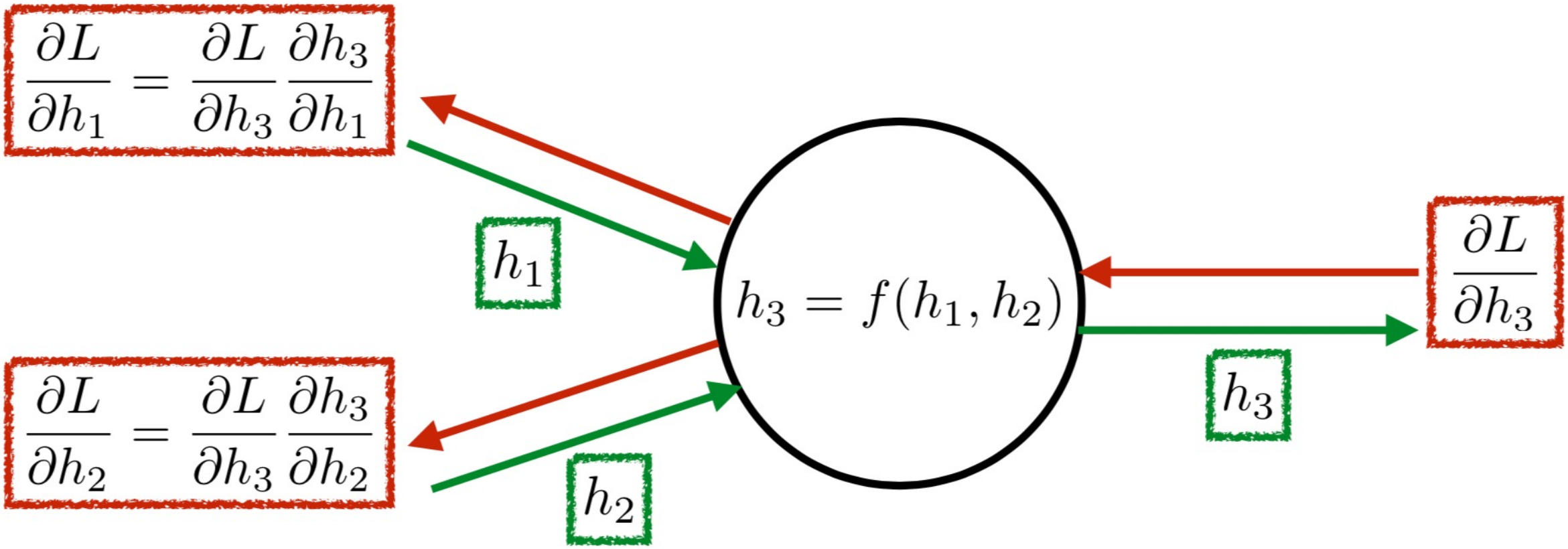
$$\theta_{t+1} = \theta_t - \alpha \nabla J(\theta_t)$$

Backward propagation
(dJ/dw, dJ/db)

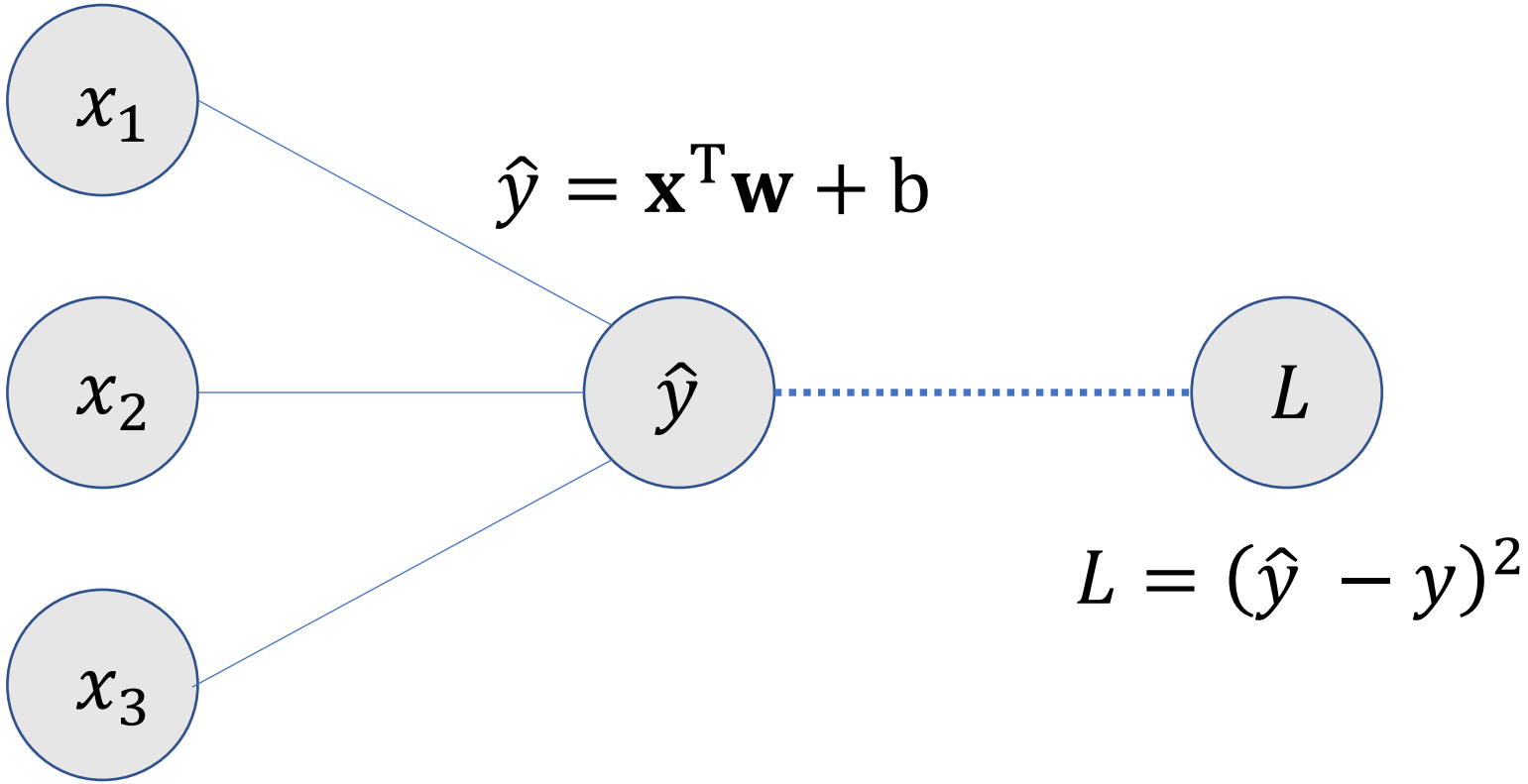

Gradient descent quadratic function
f(x)
df/dx
Start GD
End GD
400
300
200
100
0
−10
−5
0
5
10
15
20
25
30

Backpropagation

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



Example


x_1
x_2
x_3
$\hat{y} = \mathbf{x}^{\mathrm{T}}\mathbf{w} + \mathrm{b}$
$\hat{y}$
L
$L = (\hat{y} - y)^2$

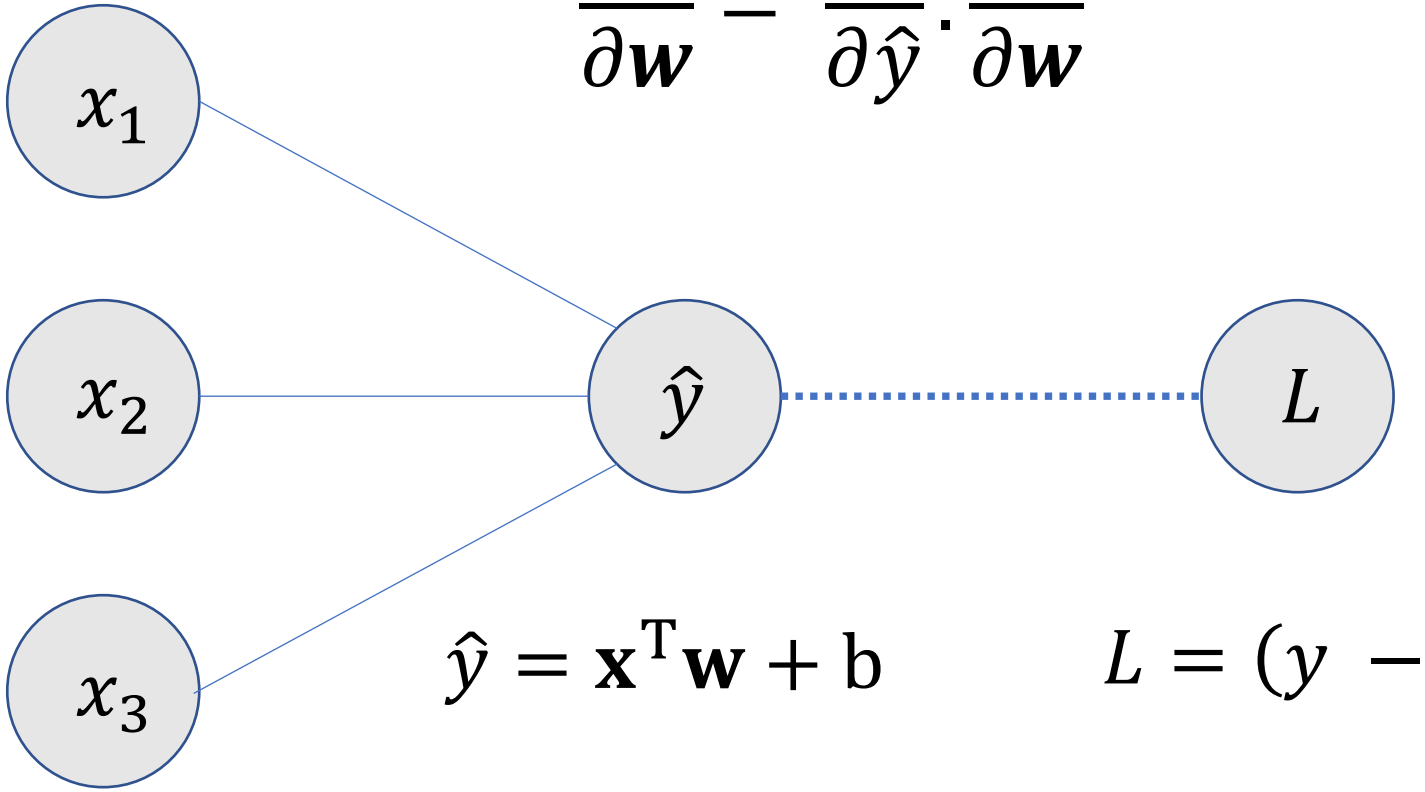
Example

We need to calculate the gradients:

Let's start with this part!

$$\frac{\partial L}{\partial \boldsymbol{w}} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial \boldsymbol{w}}$$

$$\frac{\partial L}{\partial b} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial b}$$



$$\hat{y} = \mathbf{x}^{\mathrm{T}}\mathbf{w} + \mathrm{b}$$

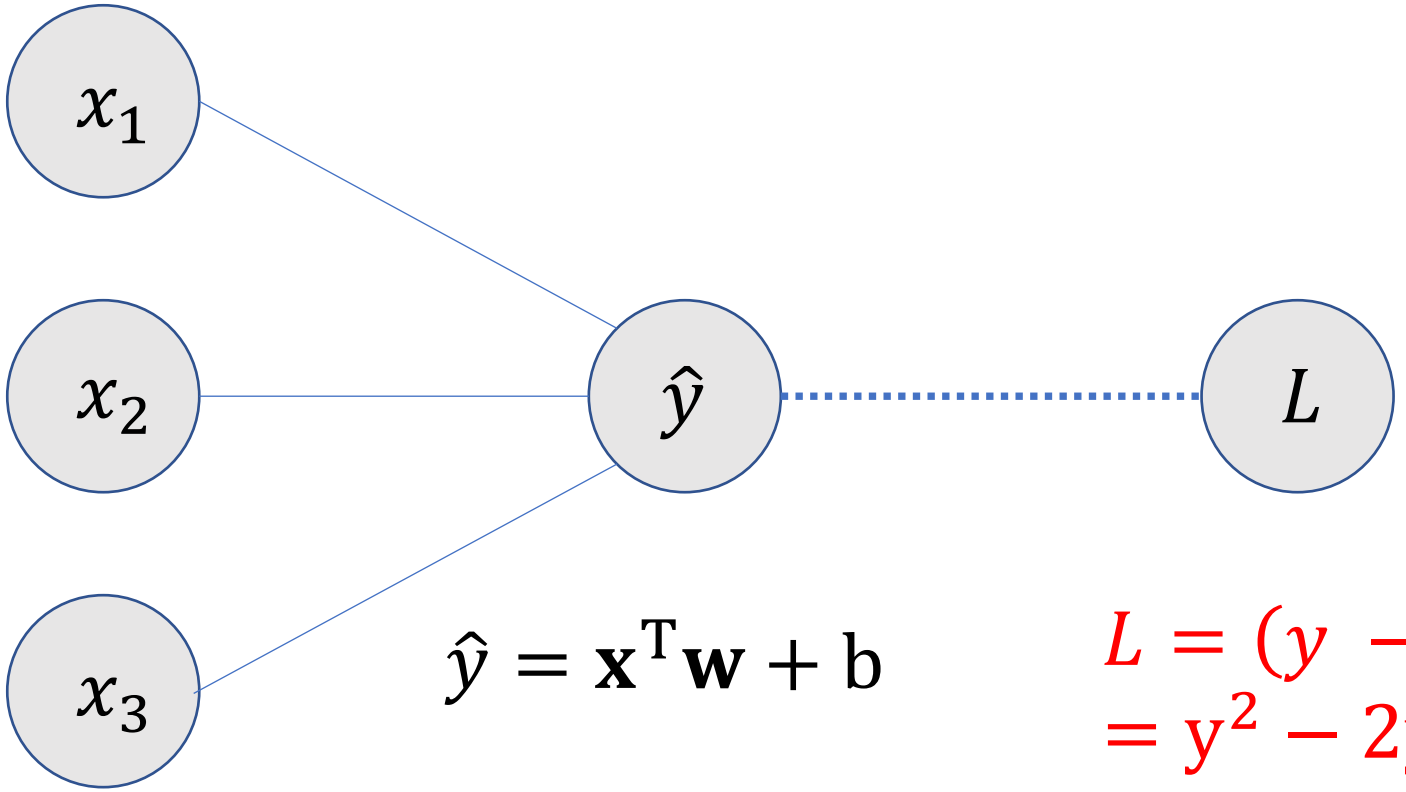
$$L = (y - \hat{y})^2$$

$$\frac{\partial L}{\partial \boldsymbol{w}} = \frac{\partial L}{\partial \hat{y}} . \frac{\partial \hat{y}}{\partial \boldsymbol{w}}$$

Example

First:

$$\frac{\partial L}{\partial \hat{y}} = -2y - 2\hat{y} = 2(\hat{y} - \mathrm{y})$$



$$\hat{y} = \mathbf{x}^{\mathrm{T}}\mathbf{w} + \mathrm{b}$$

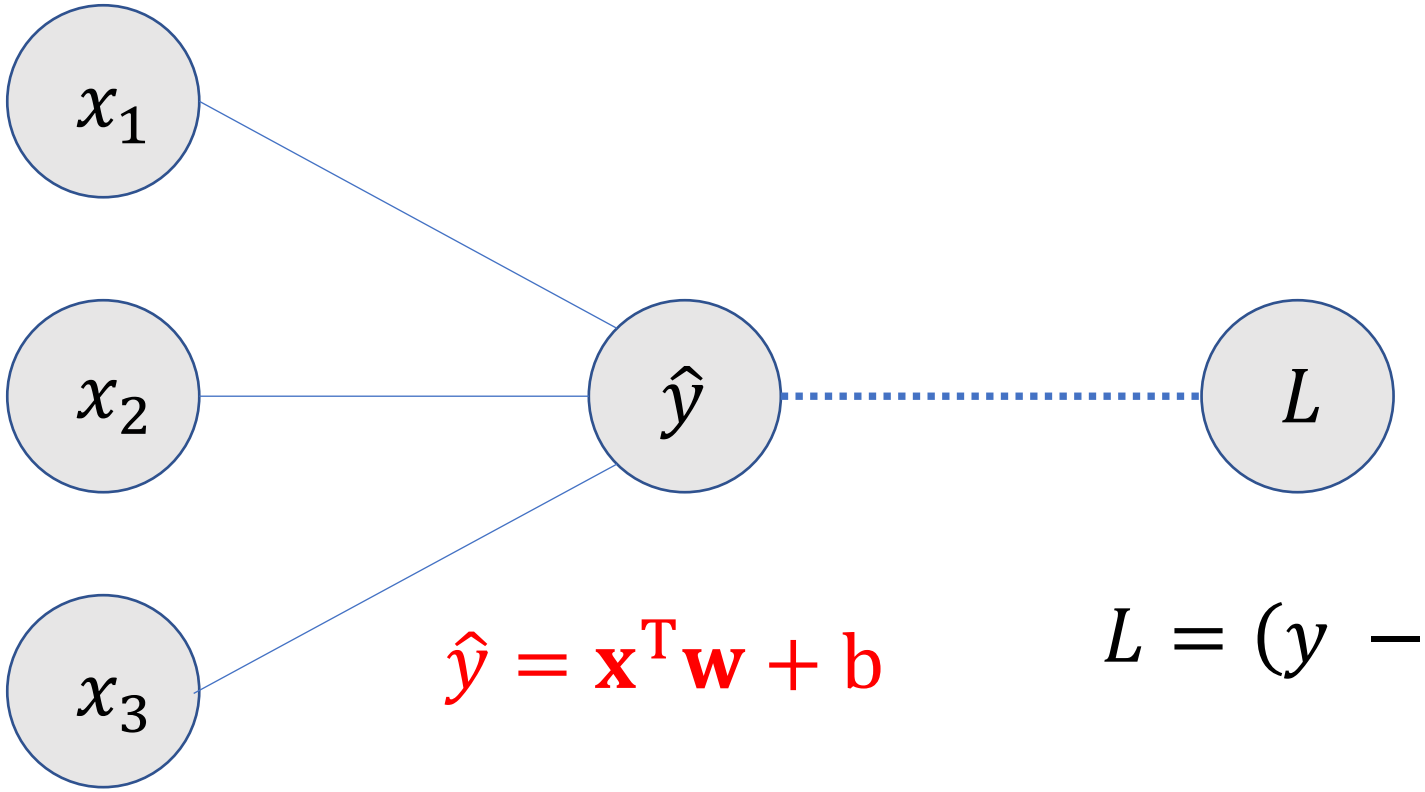
$$L = (y - \hat{y})^2$$
$$= \mathrm{y}^2 - 2\mathrm{y}\hat{y} + \hat{y}^2$$

$$\frac{\partial L}{\partial \boldsymbol{w}} = \frac{\partial L}{\partial \hat{y}} . \frac{\partial \hat{y}}{\partial \boldsymbol{w}}$$

$$\frac{\partial L}{\partial \hat{y}} = -2y - 2\hat{y} = 2(\hat{y} - \mathrm{y})$$

Example

Second: $$\frac{\partial}{\partial \boldsymbol{w}} (\mathbf{x}^{\mathrm{T}}\mathbf{w} + \mathrm{b}) = \boldsymbol{x}^{T} . \frac{\partial}{\partial \boldsymbol{w}} (\mathbf{w}) = \boldsymbol{x}^{T}$$



$$\hat{y} = \mathbf{x}^{\mathrm{T}}\mathbf{w} + \mathrm{b}$$

$$L = (y - \hat{y})^2$$

Example

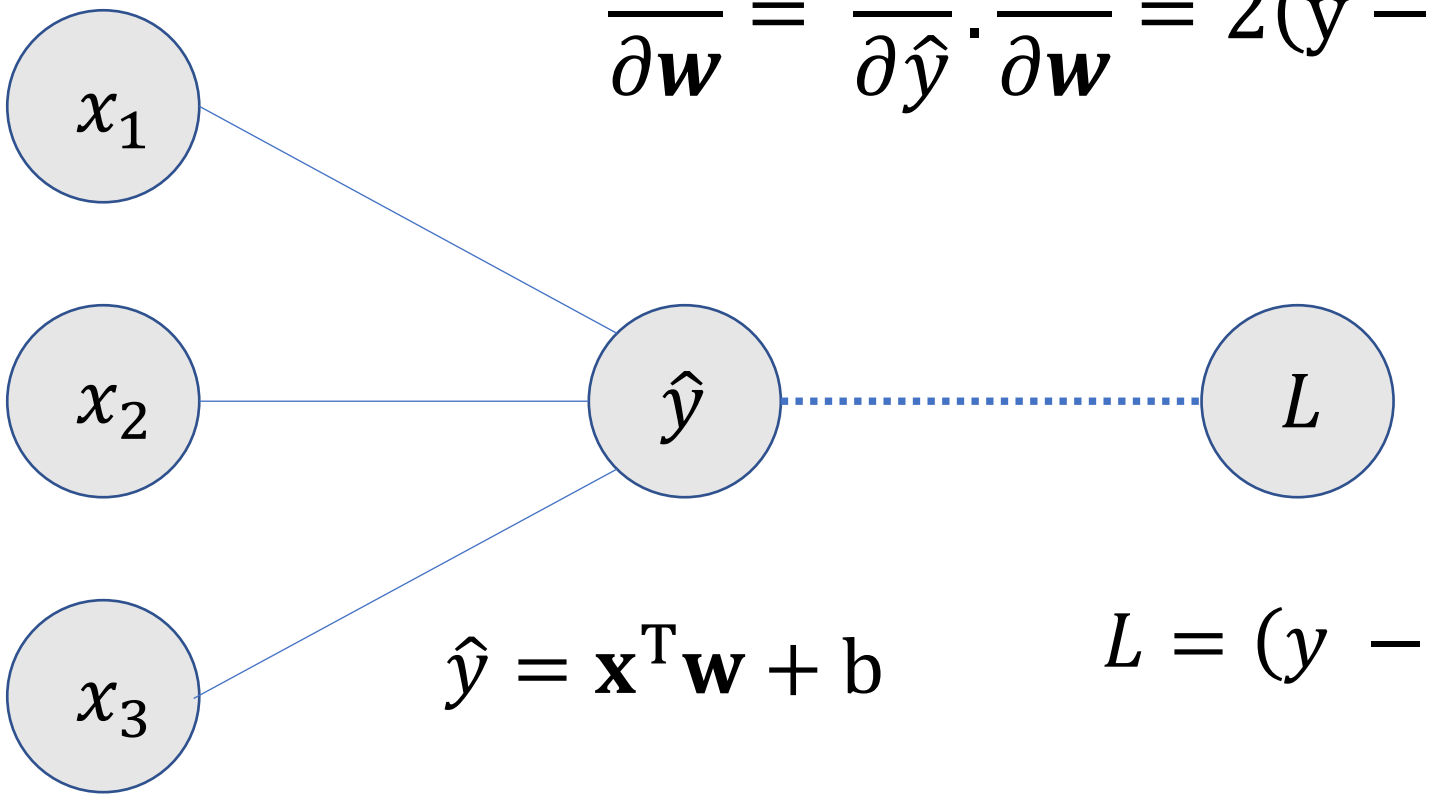
$$\frac{\partial L}{\partial \boldsymbol{w}} = \frac{\partial L}{\partial \hat{y}} . \frac{\partial \hat{y}}{\partial \boldsymbol{w}}$$

$$\frac{\partial L}{\partial \hat{y}} = -2y \ - 2\hat{y} = 2(\hat{y} - \mathrm{y})$$

$$\frac{\partial}{\partial \boldsymbol{w}} (\mathbf{x}^{\mathrm{T}}\mathbf{w} + \mathrm{b}) = \boldsymbol{x}^{T}$$

Putting these together:

$$\frac{\partial L}{\partial \boldsymbol{w}} = \frac{\partial L}{\partial \hat{y}} . \frac{\partial \hat{y}}{\partial \boldsymbol{w}} = 2(\mathrm{y} - \hat{y}) . \boldsymbol{x}^{T}$$



$$\hat{y} = \mathbf{x}^{\mathrm{T}}\mathbf{w} + \mathrm{b}$$

$$L = (y \ - \ \hat{y})^2$$

Example

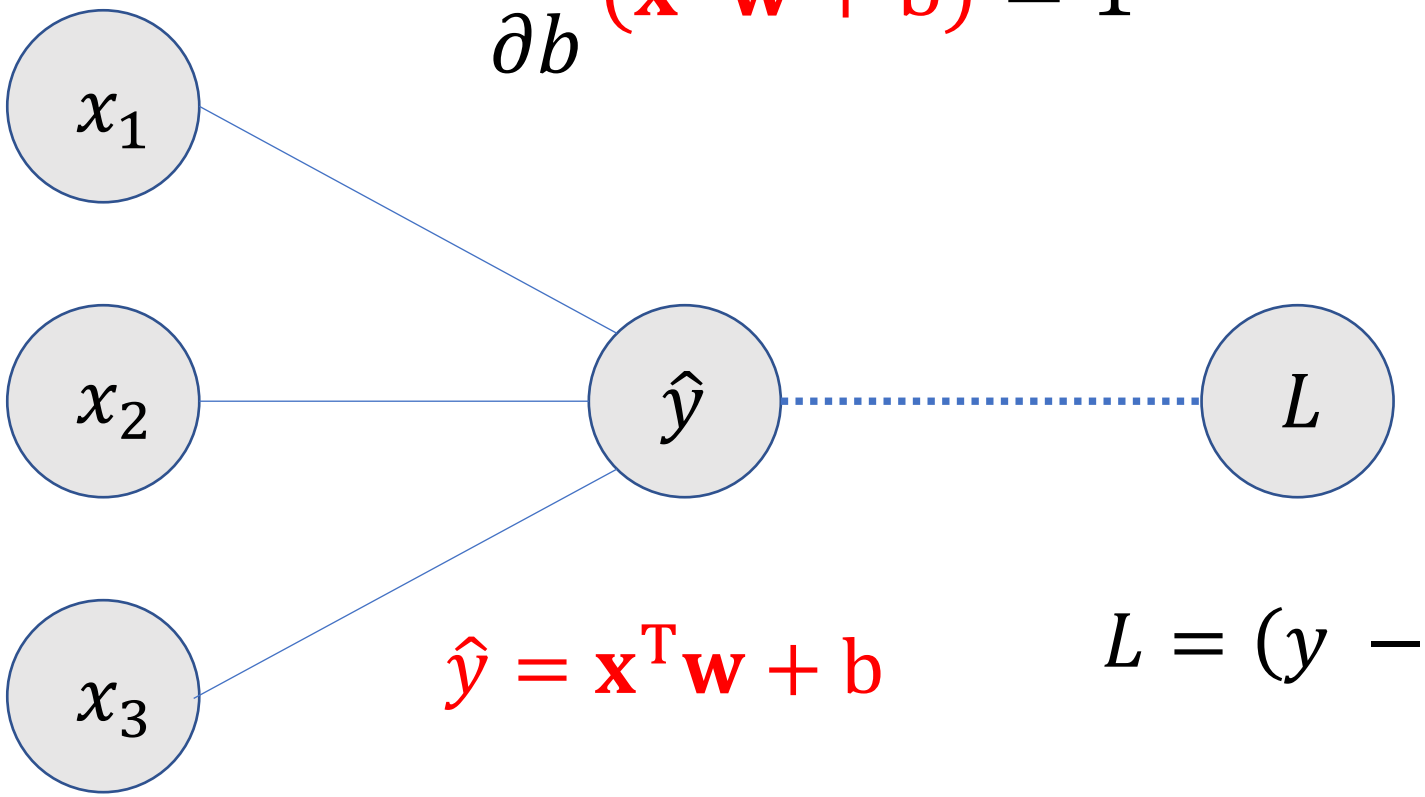
$$\frac{\partial L}{\partial \boldsymbol{w}} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial \boldsymbol{w}}$$

$$\frac{\partial L}{\partial \hat{y}} = -2y\ - 2\hat{y} = 2(\hat{y} - \mathrm{y})$$

$$\frac{\partial}{\partial \boldsymbol{w}}(\mathbf{x}^{\mathrm{T}}\mathbf{w} + \mathrm{b}) = \boldsymbol{x}^{T}$$

Now for the bias…

$$\frac{\partial}{\partial b}(\mathbf{x}^{\mathrm{T}}\mathbf{w} + \mathrm{b}) = 1$$



$$\hat{y} = \mathbf{x}^{\mathrm{T}}\mathbf{w} + \mathrm{b}$$

$$L = (y\ -\ \hat{y})^2$$

Example

$$\frac{\partial L}{\partial \boldsymbol{w}} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial \boldsymbol{w}}$$

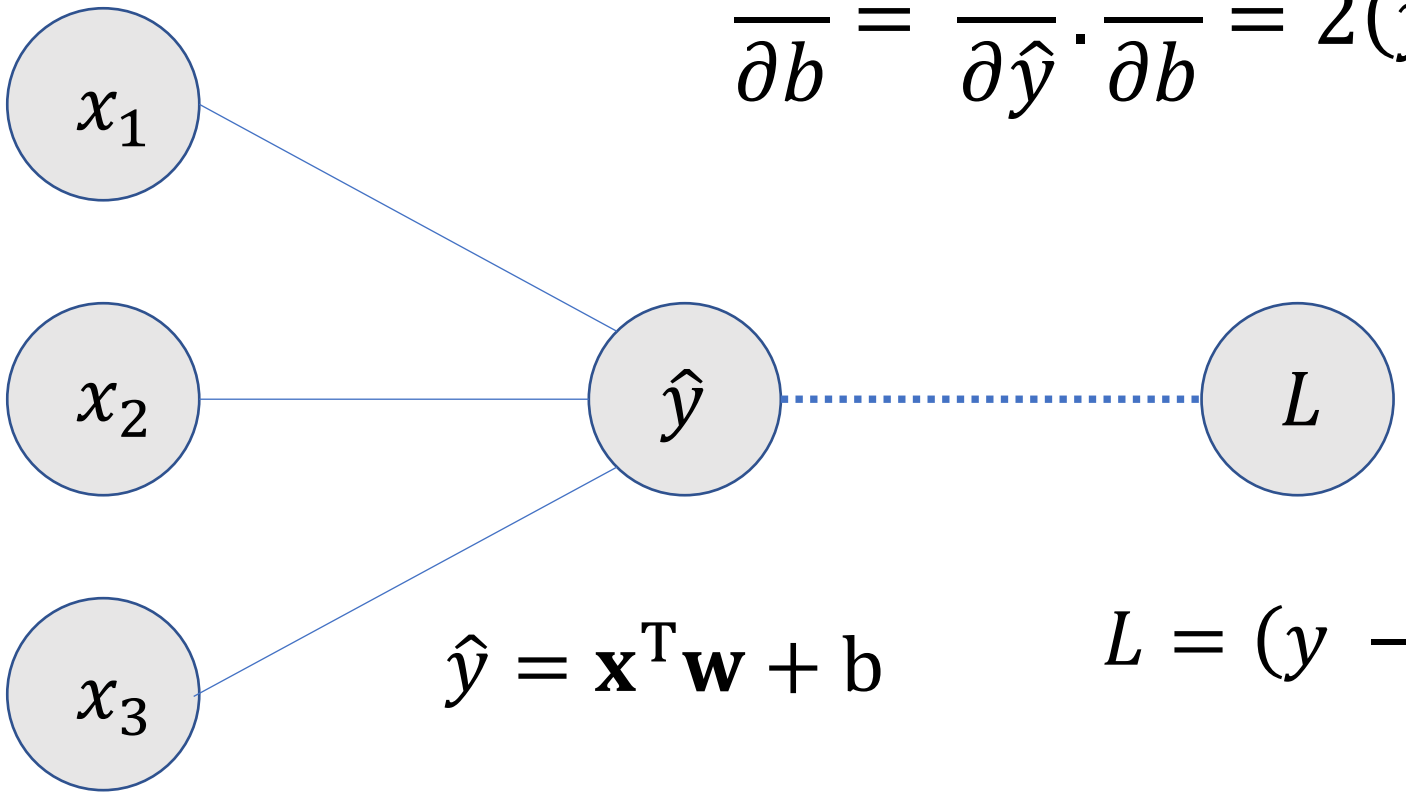
$$\frac{\partial L}{\partial \hat{y}} = -2y\ - 2\hat{y} = 2(\hat{y} - \mathrm{y})$$

$$\frac{\partial}{\partial \boldsymbol{w}}(\mathbf{x}^{\mathrm{T}}\mathbf{w} + \mathrm{b}) = \boldsymbol{x}^{T}$$

$$\frac{\partial}{\partial b}(\mathbf{x}^{\mathrm{T}}\mathbf{w} + \mathrm{b}) = 1$$

Putting these together:

$$\frac{\partial L}{\partial b} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial b} = 2(\hat{y} - y).1$$



$$\hat{y} = \mathbf{x}^{\mathrm{T}}\mathbf{w} + \mathrm{b}$$

$$L = (y\ -\ \hat{y})^2$$

Example

$$\frac{\partial L}{\partial \boldsymbol{w}} = \frac{\partial L}{\partial \hat{y}} . \frac{\partial \hat{y}}{\partial \boldsymbol{w}}$$

$$\frac{\partial L}{\partial \hat{y}} = -2y - 2\hat{y} = 2(\hat{y} - \mathrm{y})$$

$$\frac{\partial}{\partial \boldsymbol{w}}(\mathbf{x}^{\mathrm{T}}\mathbf{w} + \mathrm{b}) = \boldsymbol{x}^{T}$$

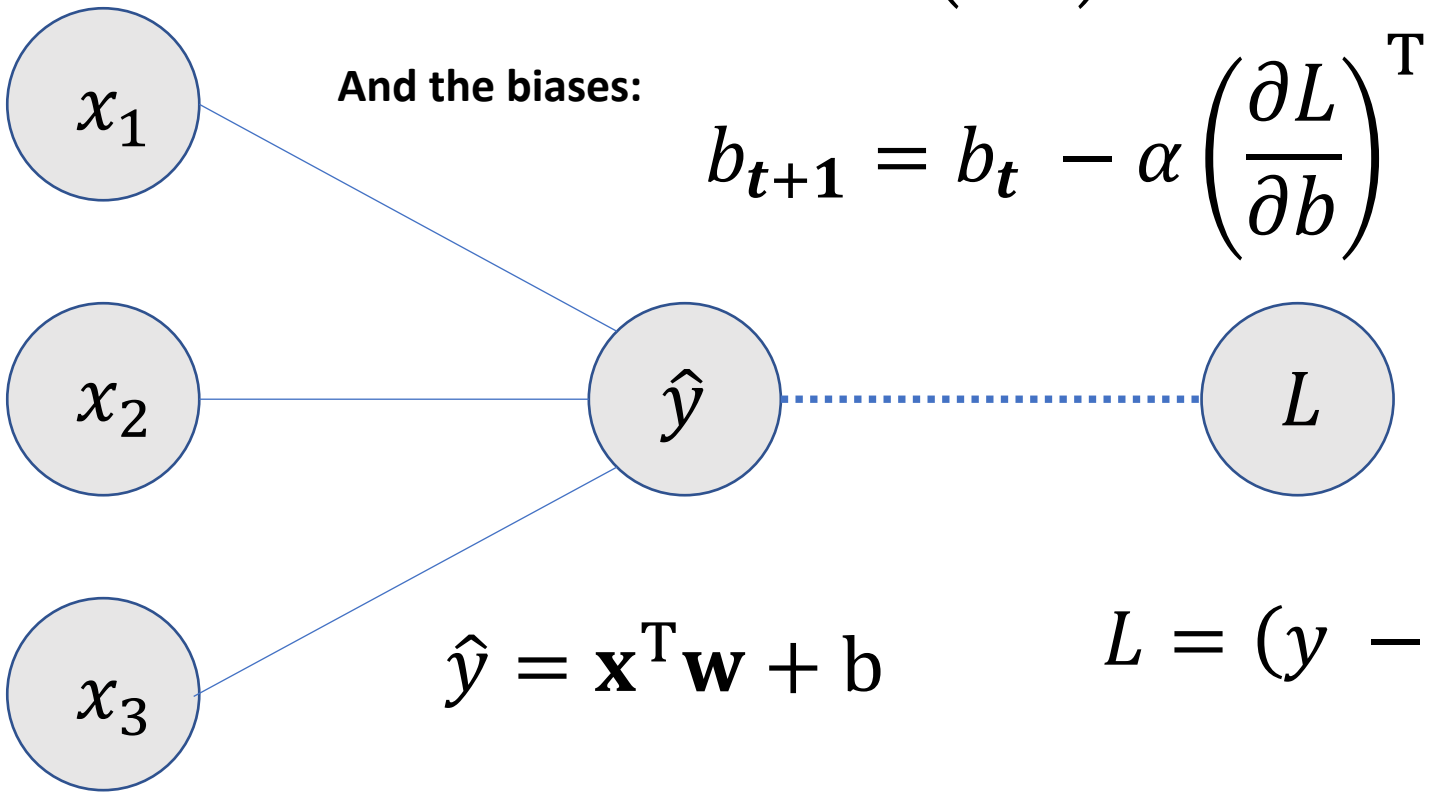
$$\frac{\partial}{\partial b}(\mathbf{x}^{\mathrm{T}}\mathbf{w} + \mathrm{b}) = 1$$

Finally the updates for the weights:

$$\boldsymbol{w_{t+1}} = \boldsymbol{w_t} - \alpha \left(\frac{\partial L}{\partial \boldsymbol{w}}\right)^{\mathrm{T}} = \boldsymbol{w_t} - 2\alpha(\hat{y} - y)\boldsymbol{x}$$

And the biases:

$$b_{\boldsymbol{t+1}} = b_{\boldsymbol{t}} - \alpha \left(\frac{\partial L}{\partial b}\right)^{\mathrm{T}} = b_{\boldsymbol{t}} - 2\alpha(\hat{y} - y)$$



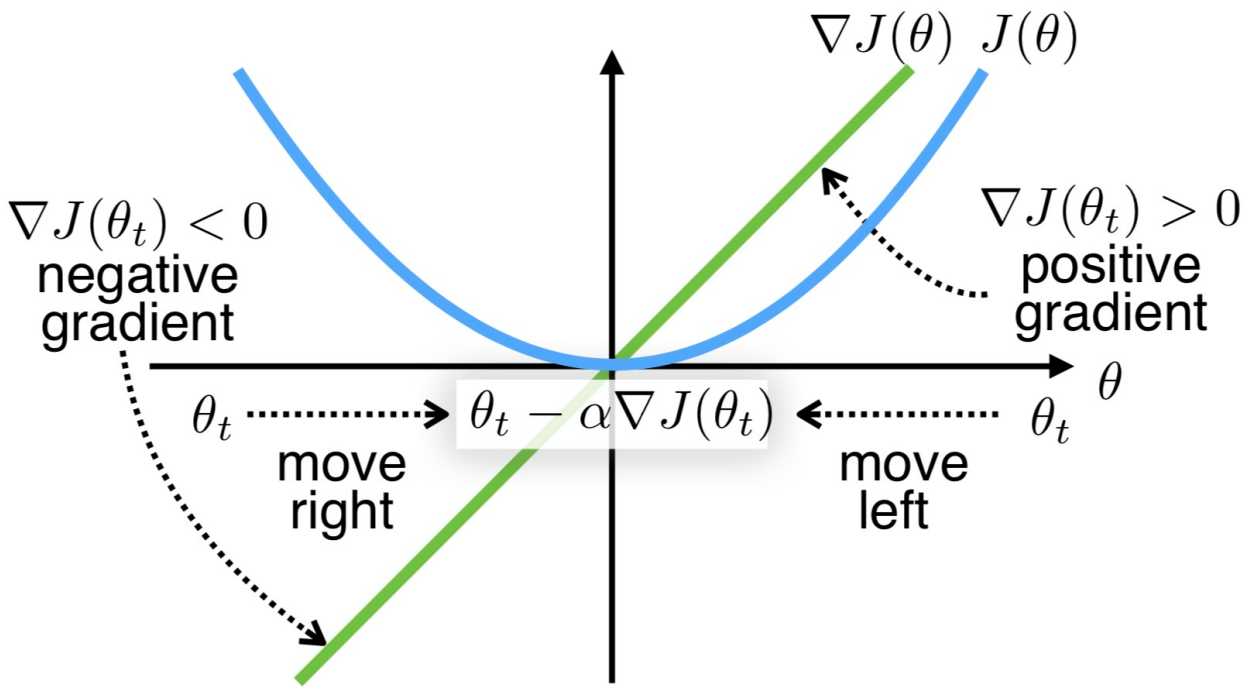
$$\hat{y} = \mathbf{x}^{\mathrm{T}}\mathbf{w} + \mathrm{b}$$

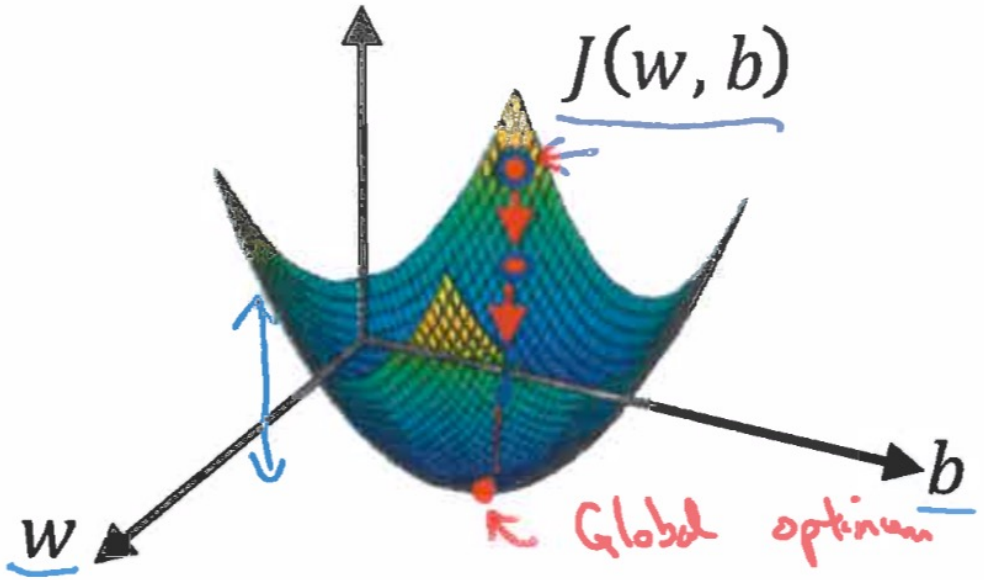
$$L = (y - \hat{y})^2$$

Gradient Descent

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

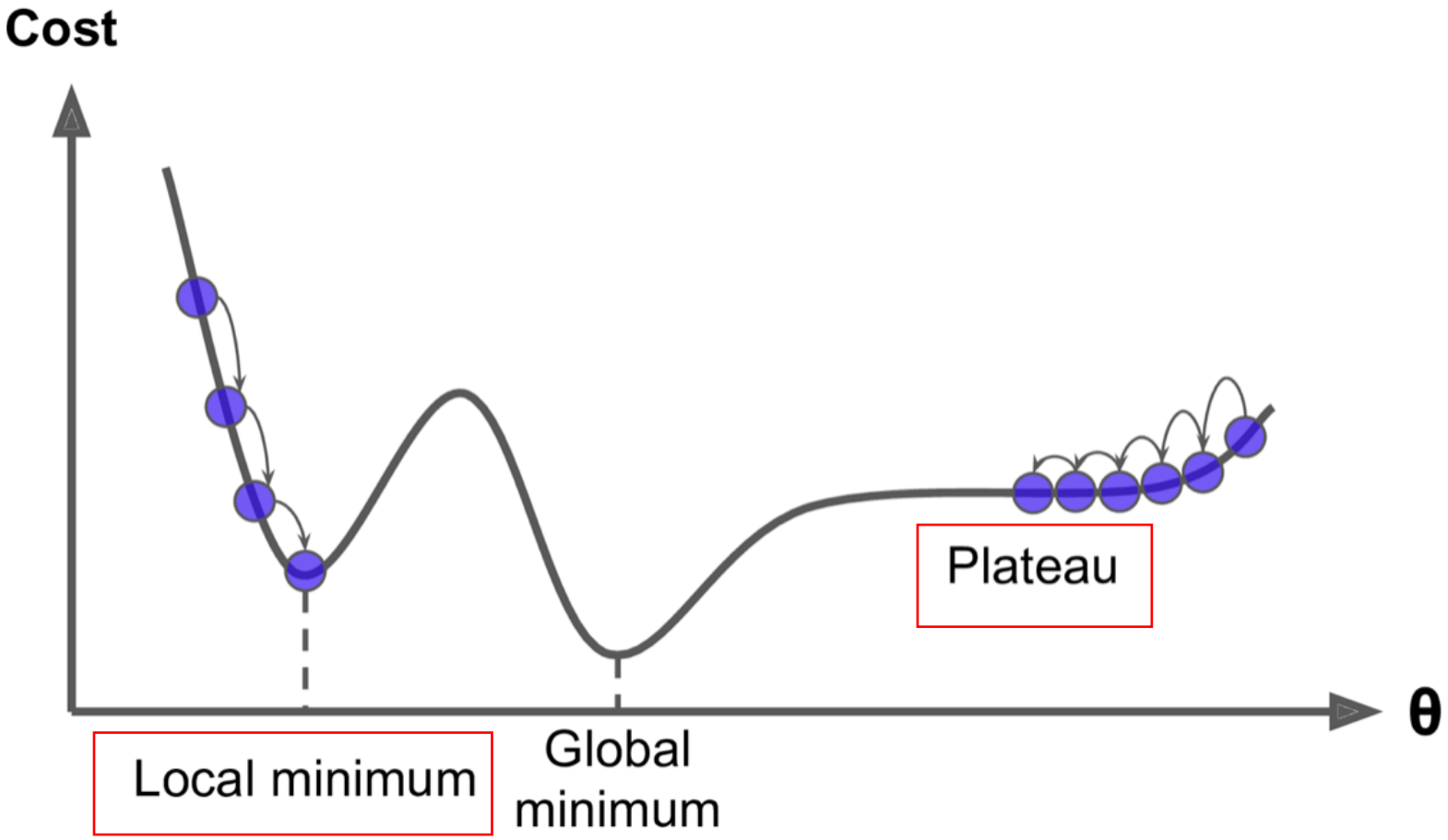
gradient descent $\theta_{t+1} = \theta_t - \alpha \nabla J(\theta_t)$



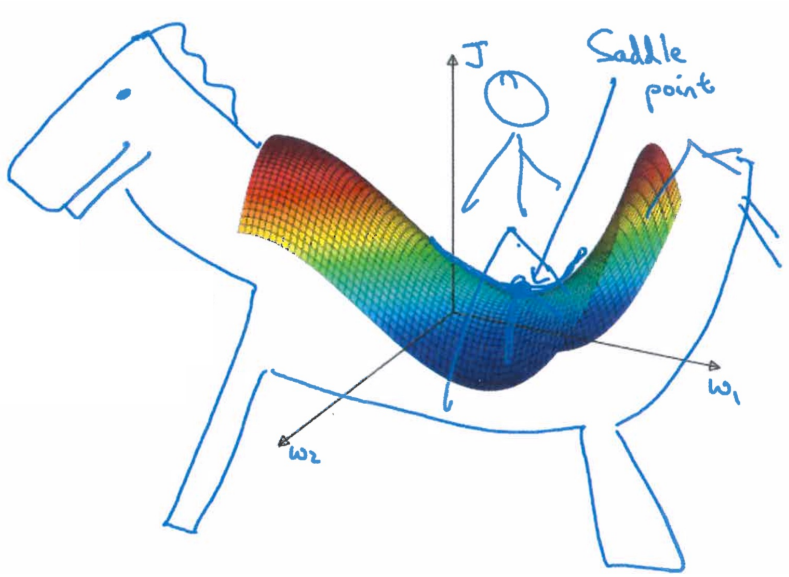


$$\nabla J(w) = \frac{dJ(w,b)}{dw} \qquad \nabla J(b) = \frac{dJ(w,b)}{db}$$

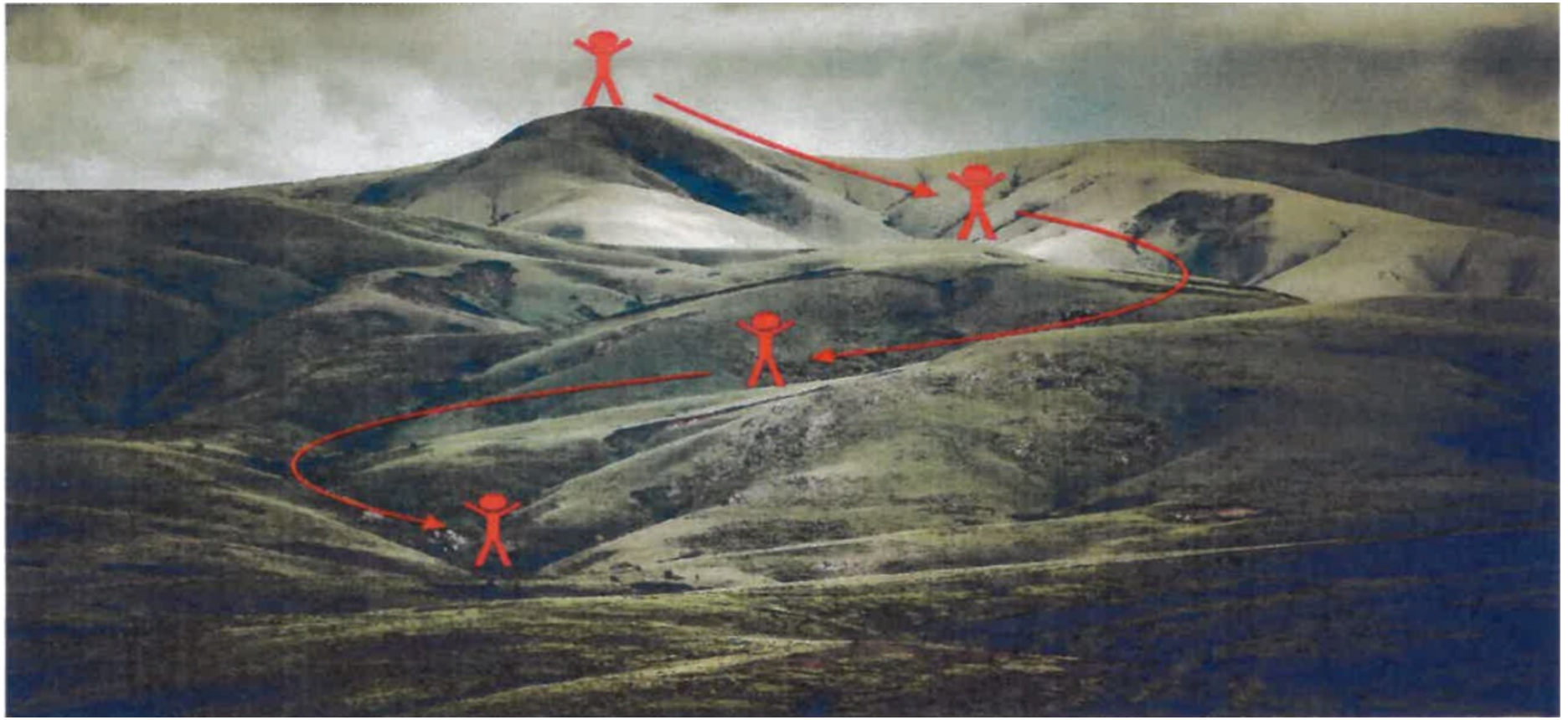
Optimization pitfalls



Saddle point



Gradient Descent Illustration



Tutorial / Practical