



Deep Forward Networks - Introduction

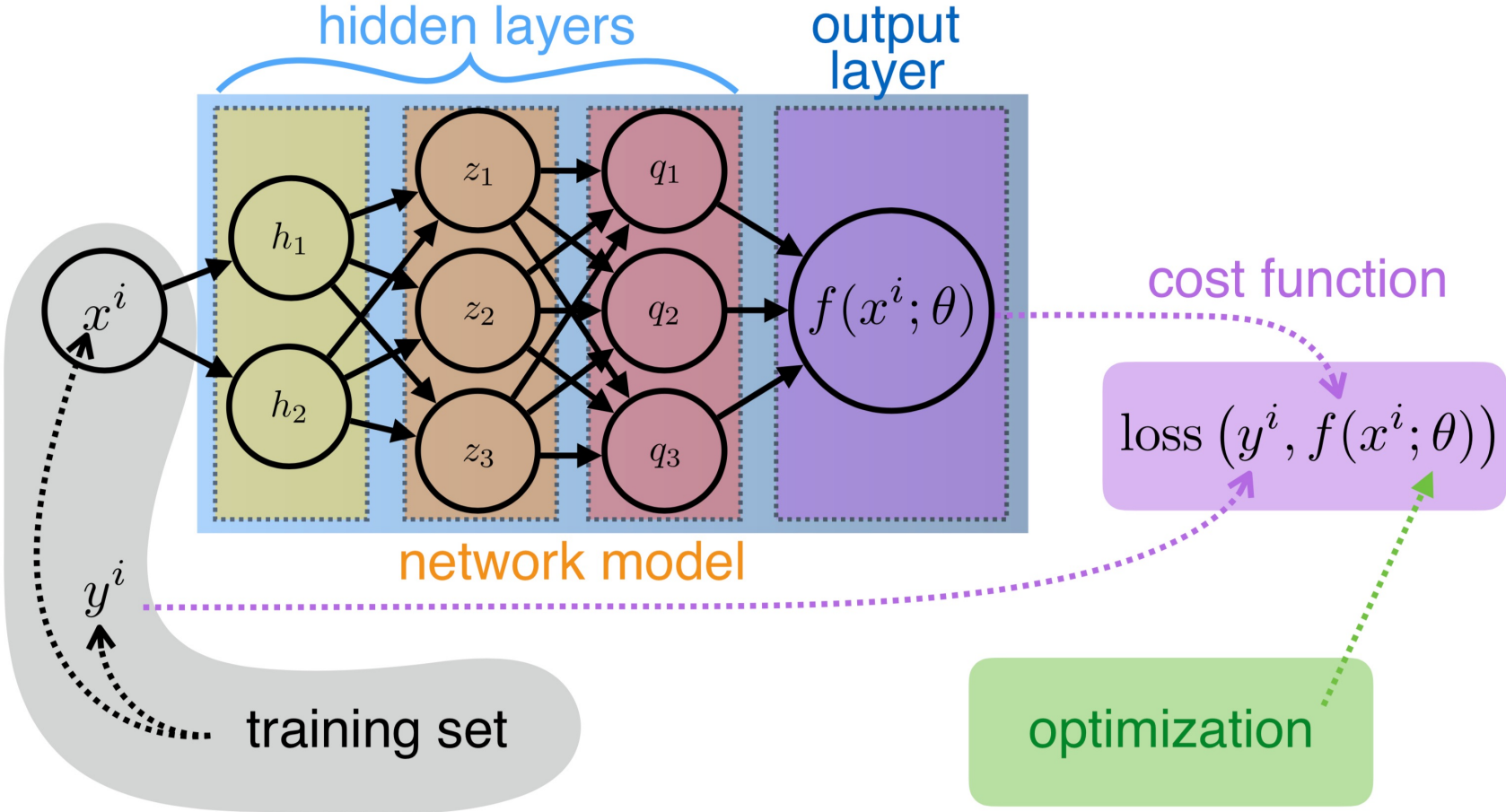
Wednesday
08h00 – 09h00

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

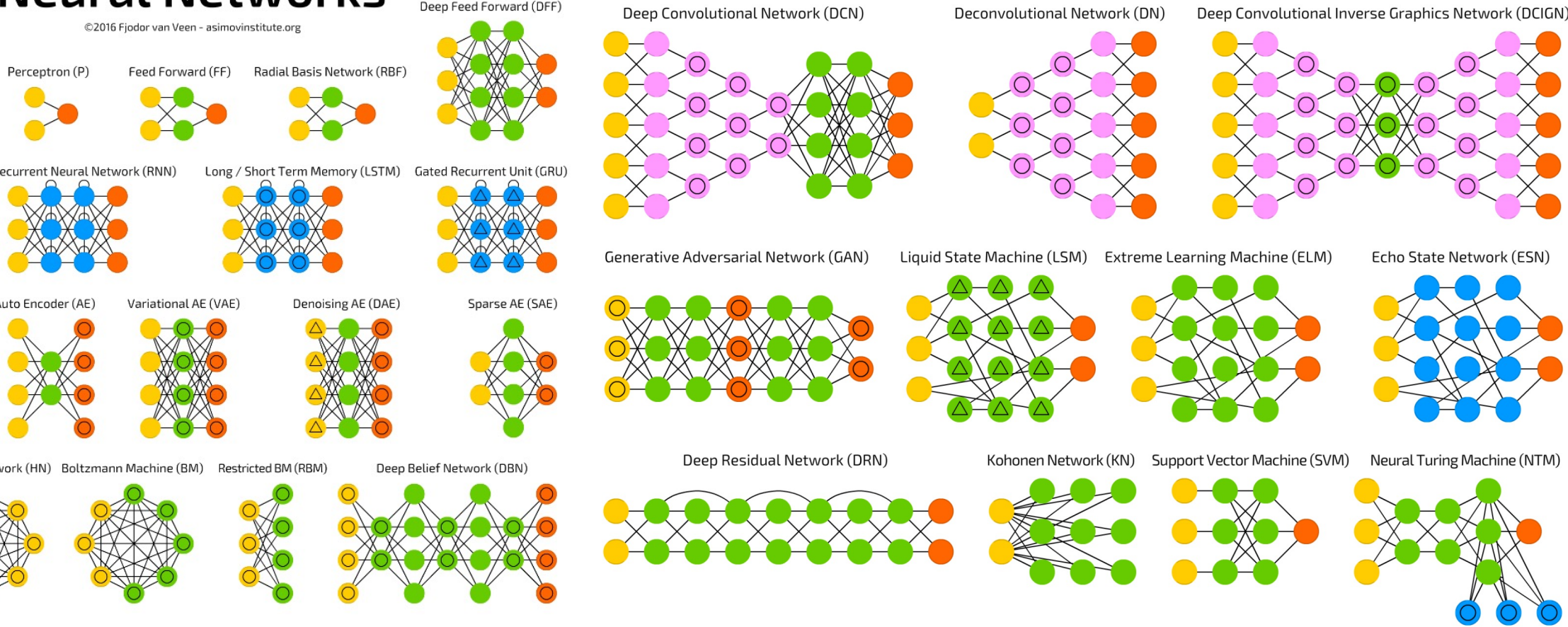


1) Network Model

A mostly complete chart of Neural Networks

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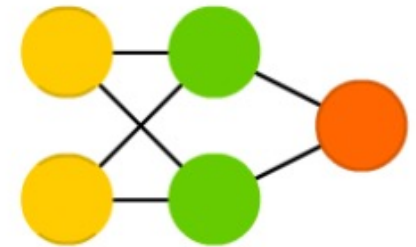
-  Backfed Input Cell
-  Input Cell
-  Noisy Input Cell
-  Hidden Cell
-  Probabilistic Hidden Cell
-  Spiking Hidden Cell
-  Output Cell
-  Match Input Output Cell
-  Recurrent Cell
-  Memory Cell
-  Different Memory Cell
-  Kernel
-  Convolution or Pool



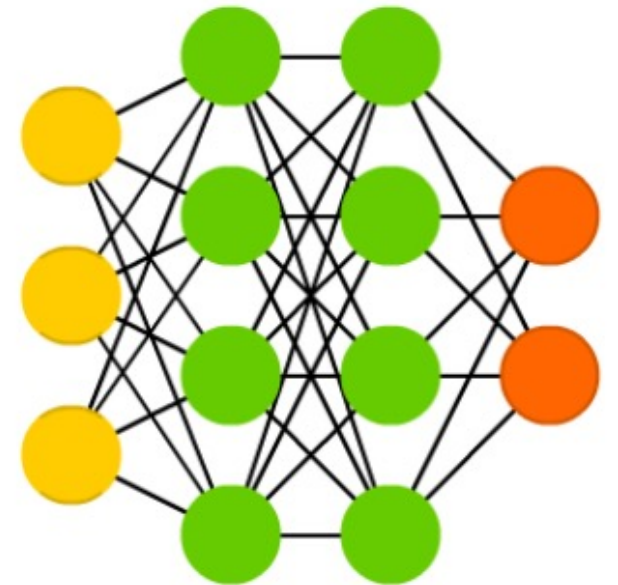
(Deep) Feedforward NN (DFF)

- 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)



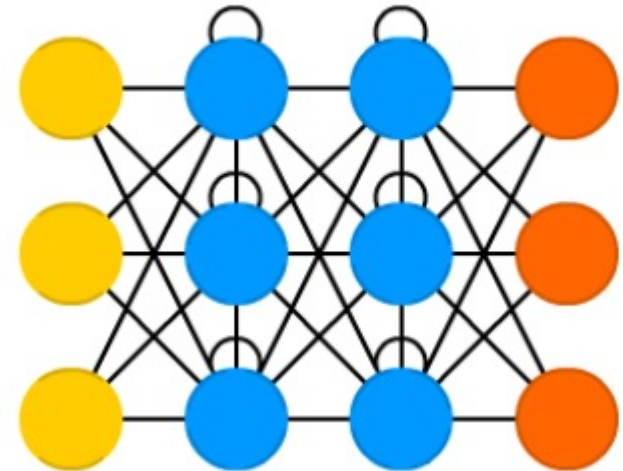
Deep Feed Forward (DFF)



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

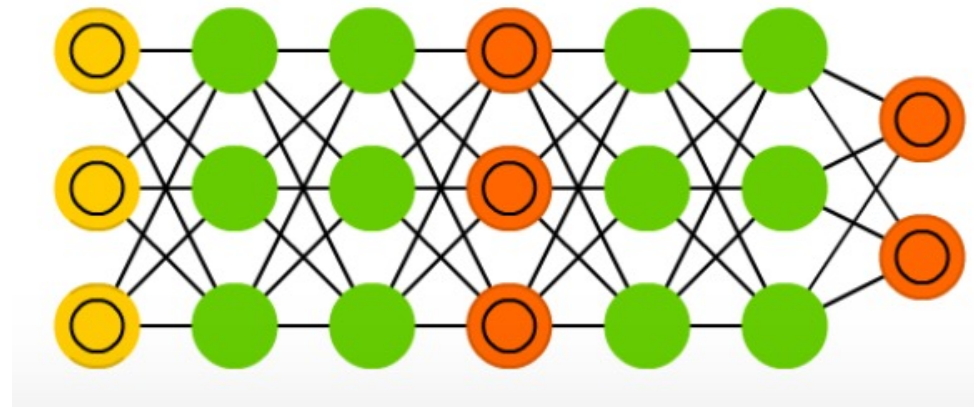
Recurrent Neural Network (RNN)



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

Generative Adversarial Network (GAN)



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

$$\{x^i, y^i\}_{i=1, \dots, m}$$

- Network

$$f(x; \theta)$$

- Cost function

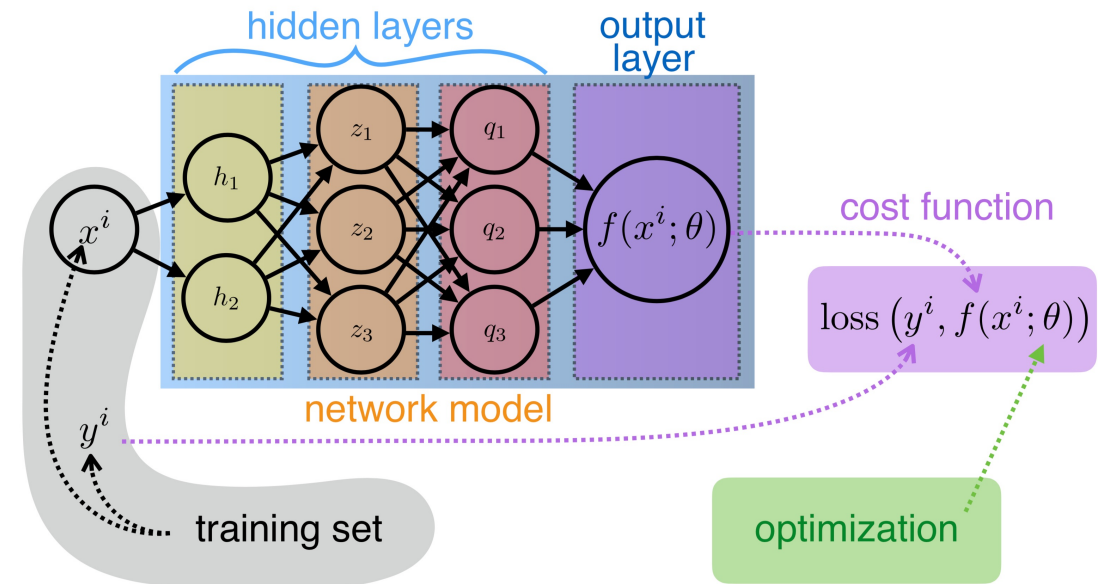
$$J(\theta) = \sum_{i=1}^m \text{loss}(y^i, f(x^i; \theta))$$

- 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):

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

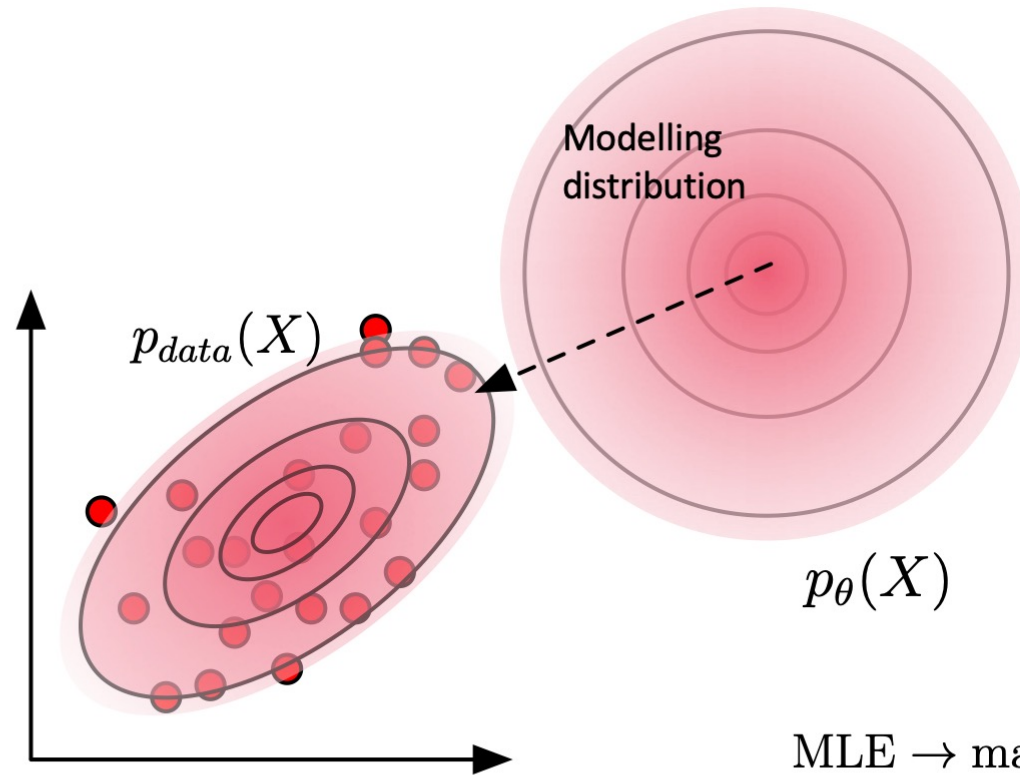
- Mathematical tricks :

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

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

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

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

Loss function choice

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

$$\hat{y} = \sigma(w^\top h + b)$$

$$p(y|\hat{y}) = \hat{y}^y (1 - \hat{y})^{(1-y)}$$

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

(binary classification)

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

$$\hat{y} = W^\top h + b$$

$$p(y|\hat{y}) = N(y; \hat{y})$$

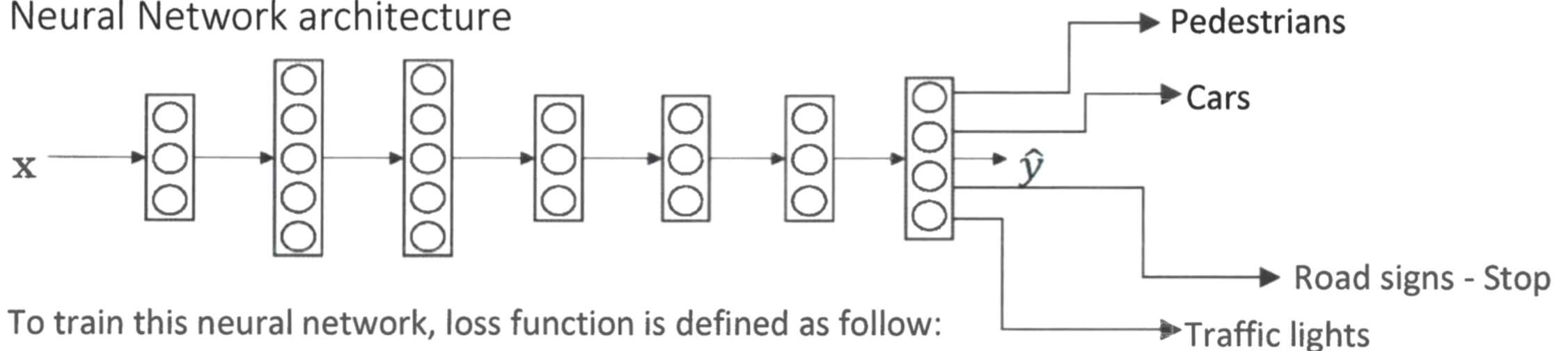
$$L_2(\hat{y}, y) = -\log p(y|\hat{y}) = \sum_{i=0}^m (y^i - \hat{y}^i)^2$$

Loss function example

- NN does **simultaneously several tasks (multi-task)**



Neural Network architecture

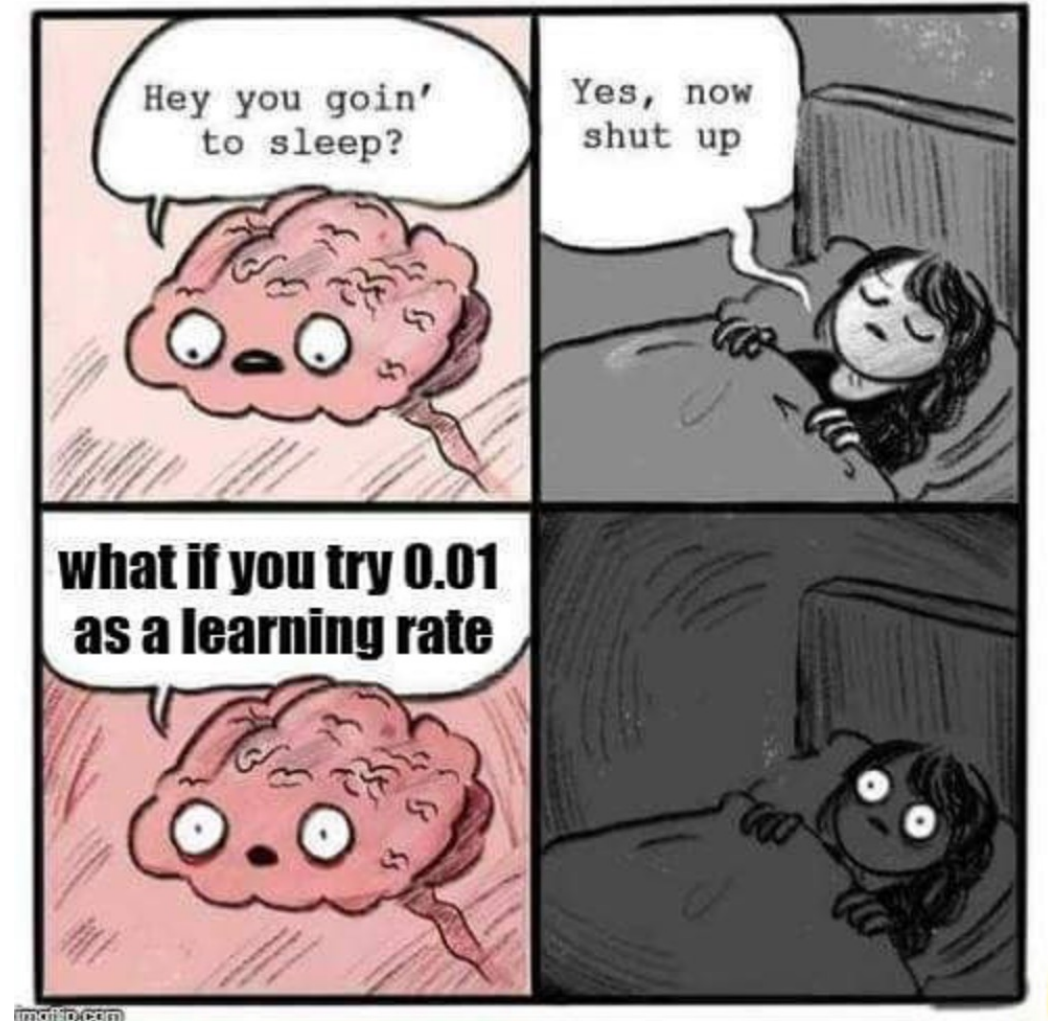


To train this neural network, loss function is defined as follow:

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

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

$$Z = w^T x + b$$
$$A = \sigma(Z)$$



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

epochs

Parameter update
(gradient descent)

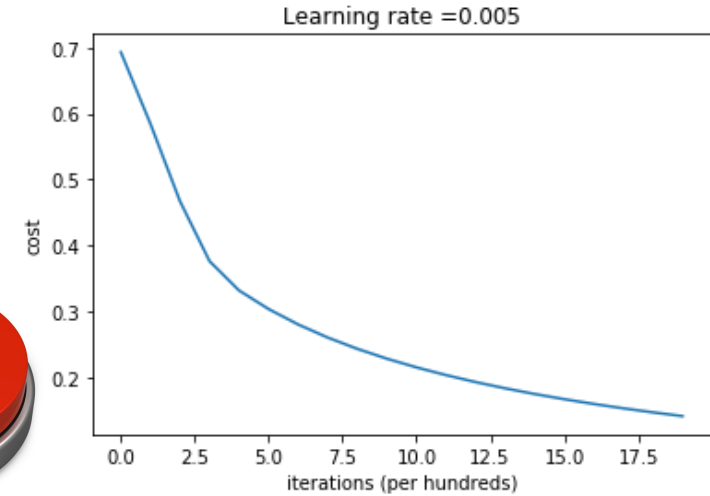
learning rate α

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

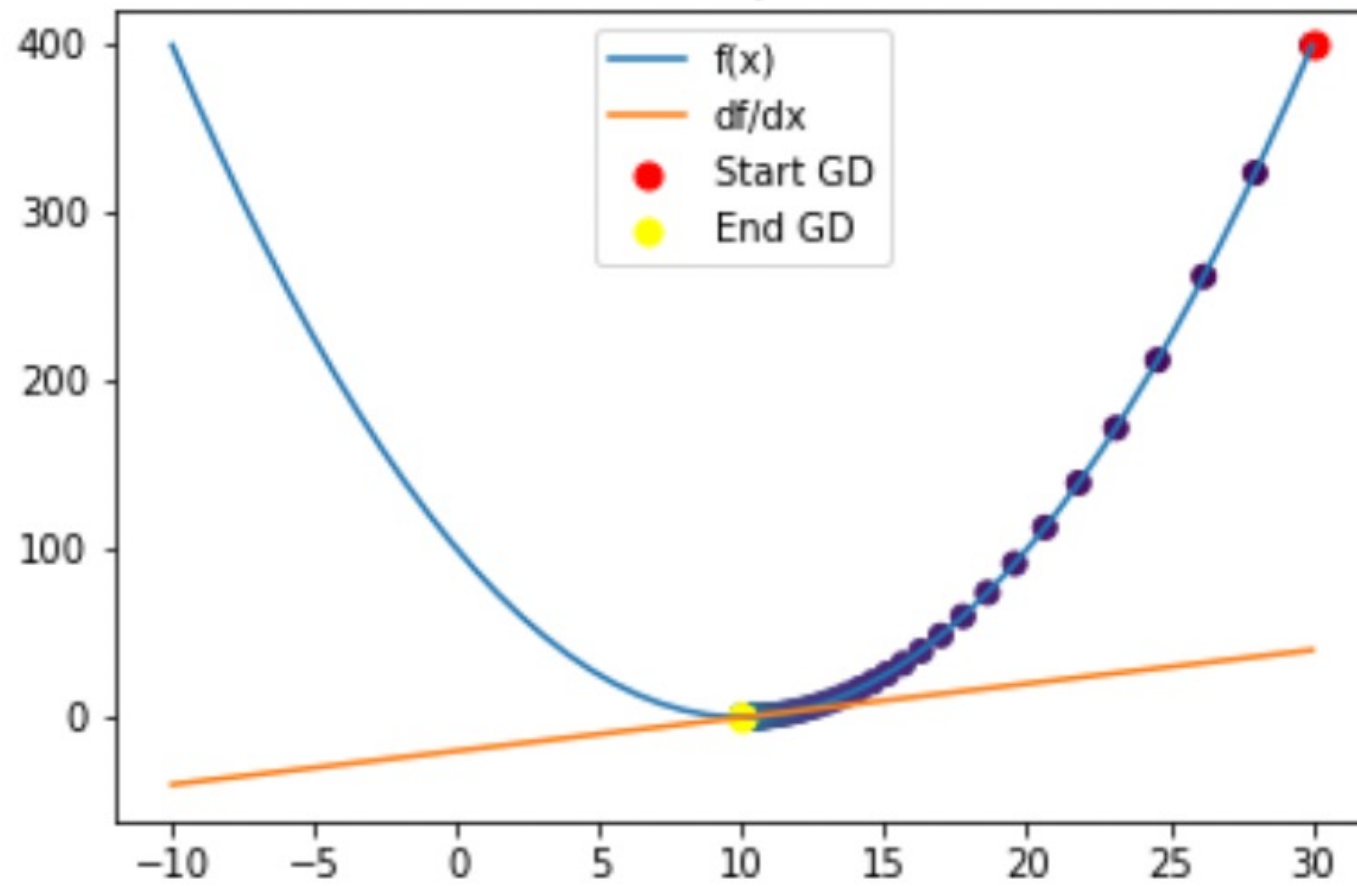


Backward propagation
(dJ/dw , dJ/db)

Learning curve

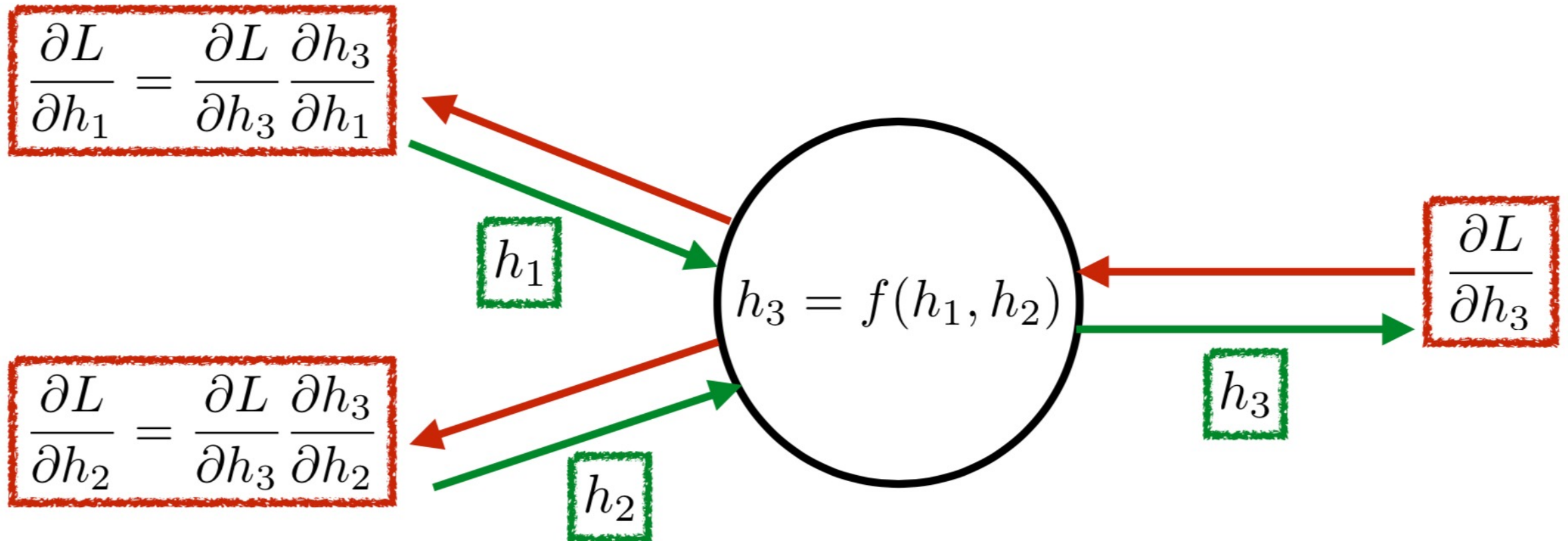


Gradient descent quadratic function

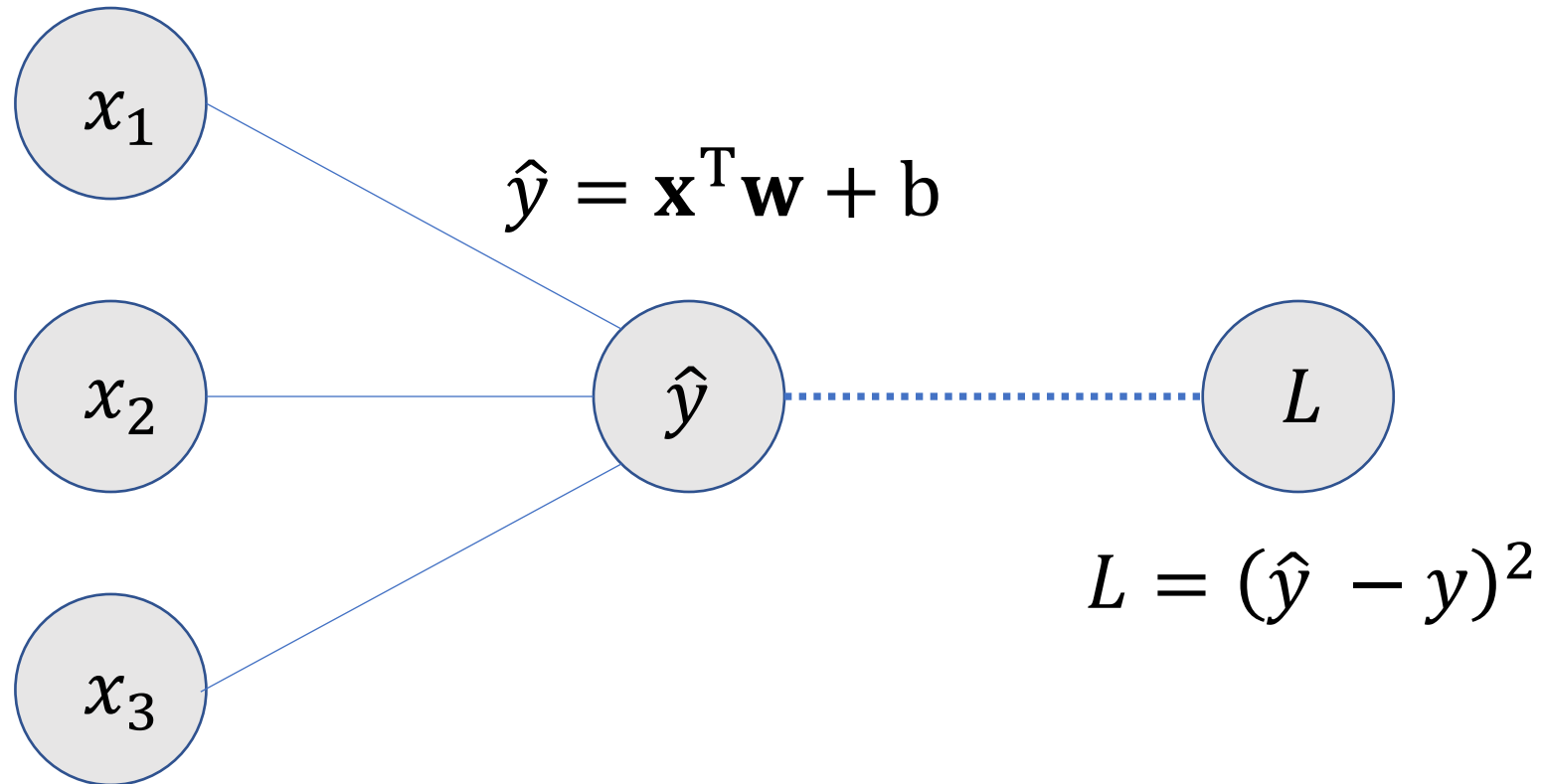


Backpropagation

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



Example



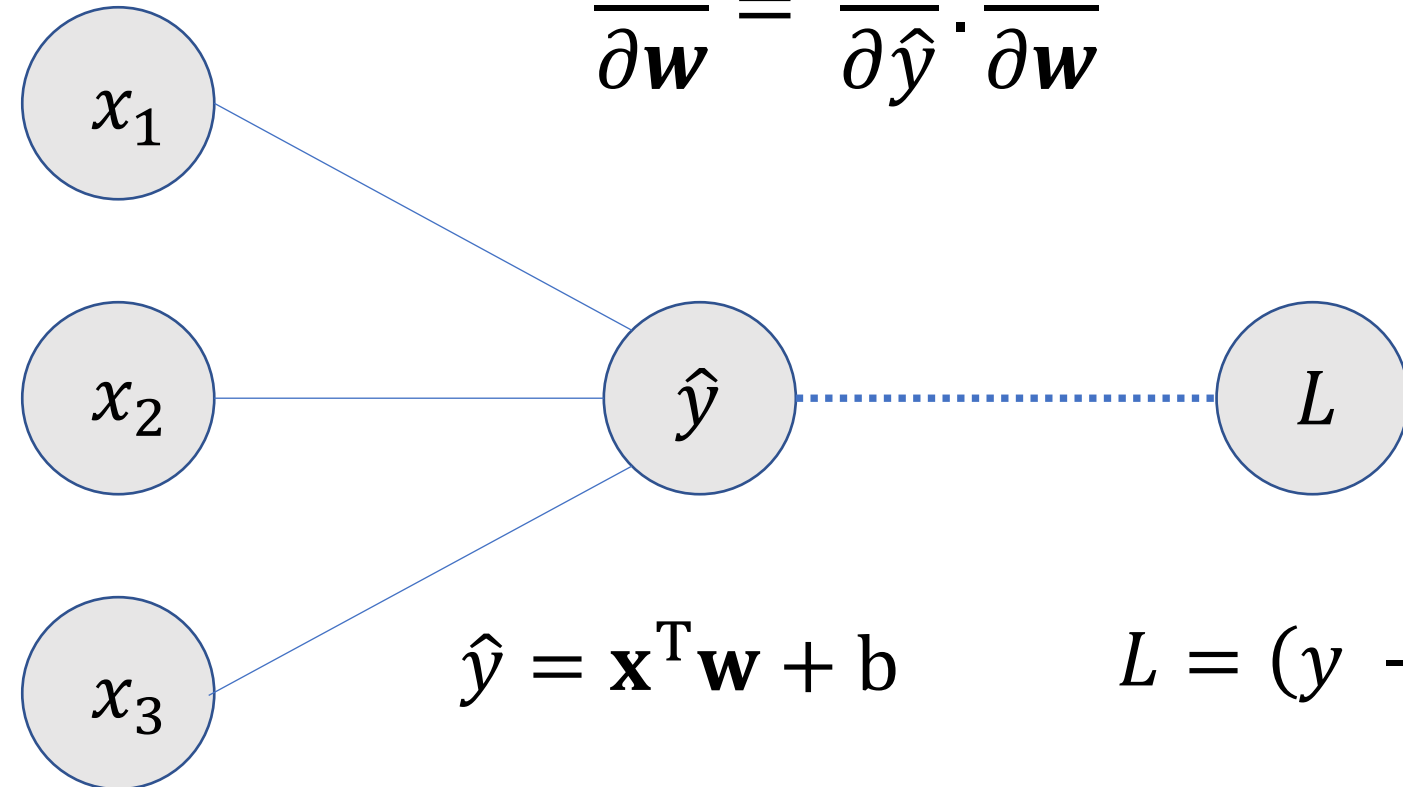
Example

We need to calculate the gradients:

Let's start with this part!

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

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



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

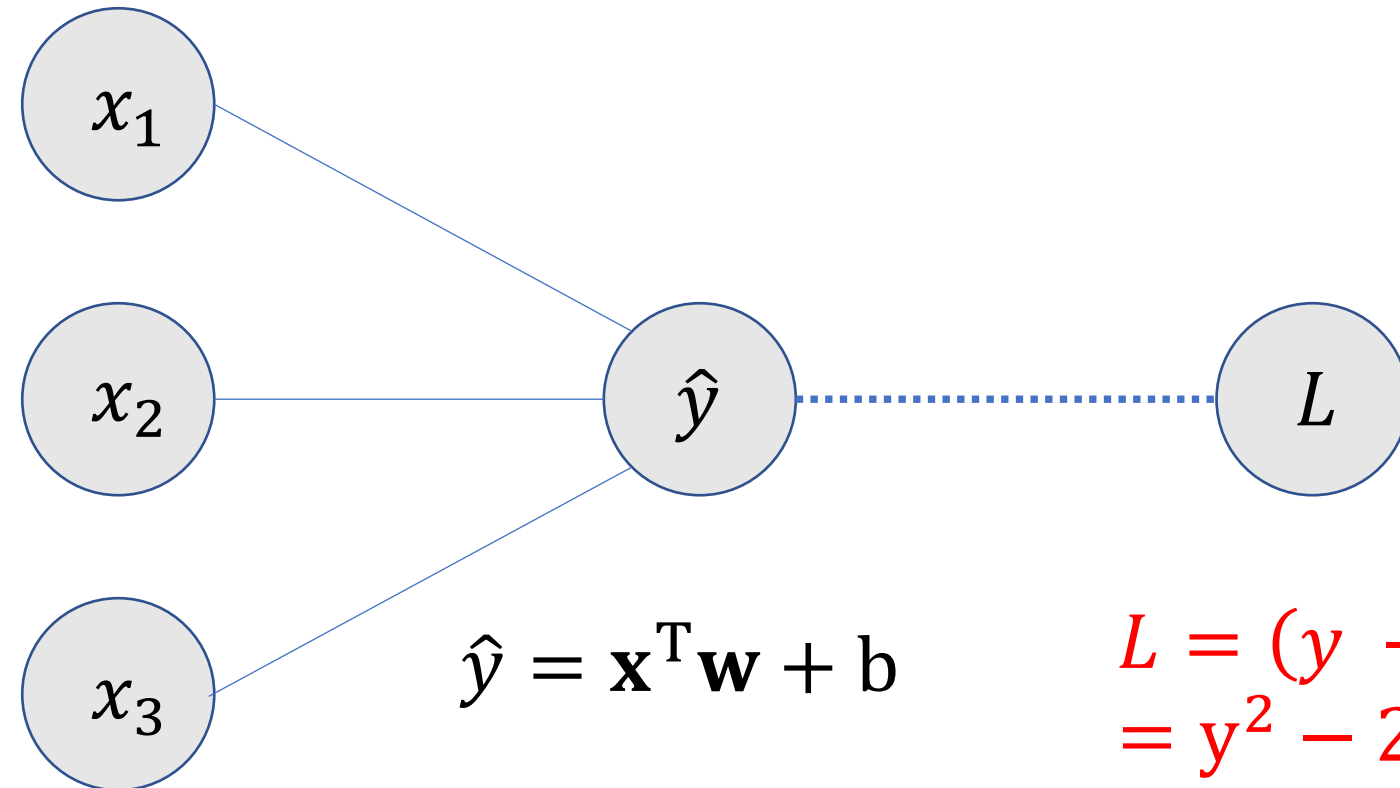
$$L = (y - \hat{y})^2$$

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

Example

First:

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

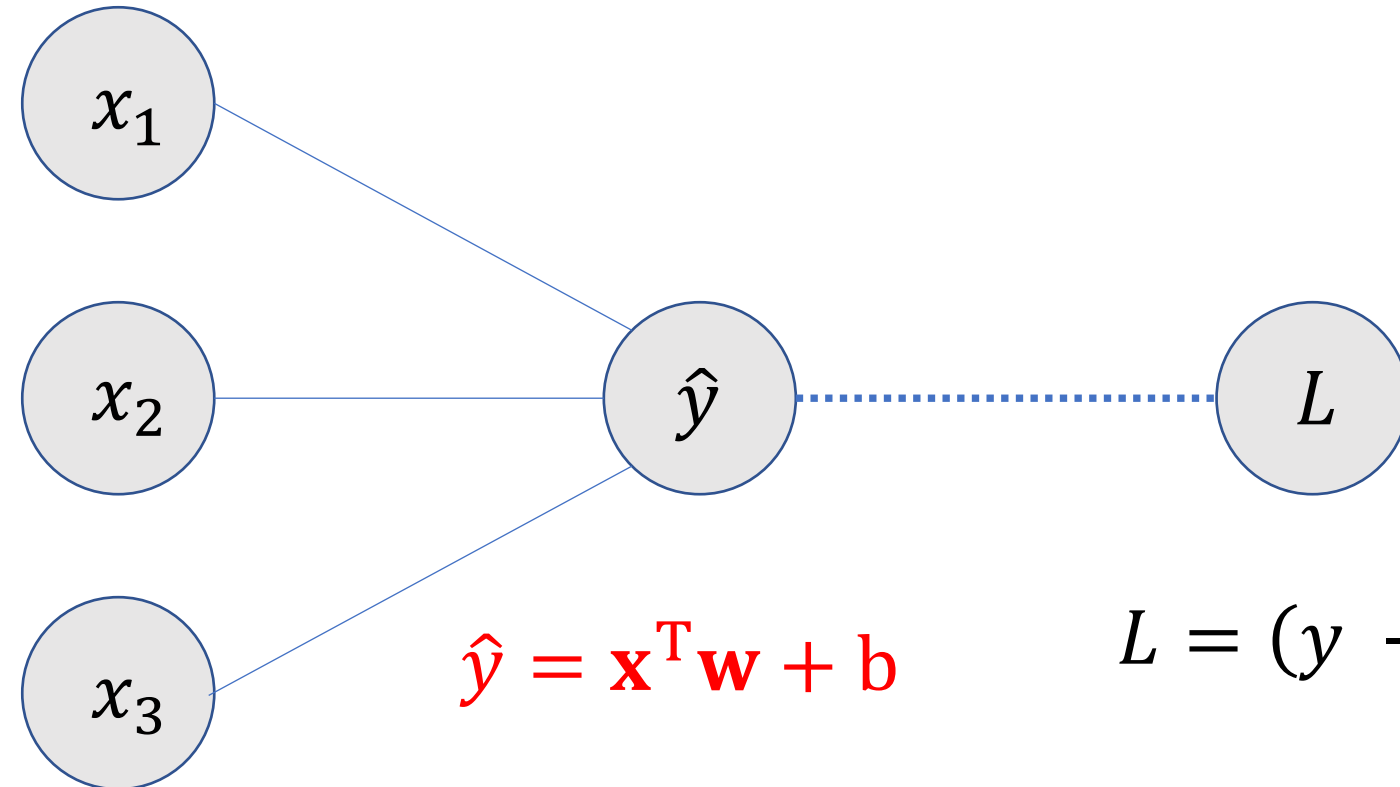


Example

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

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

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



Example

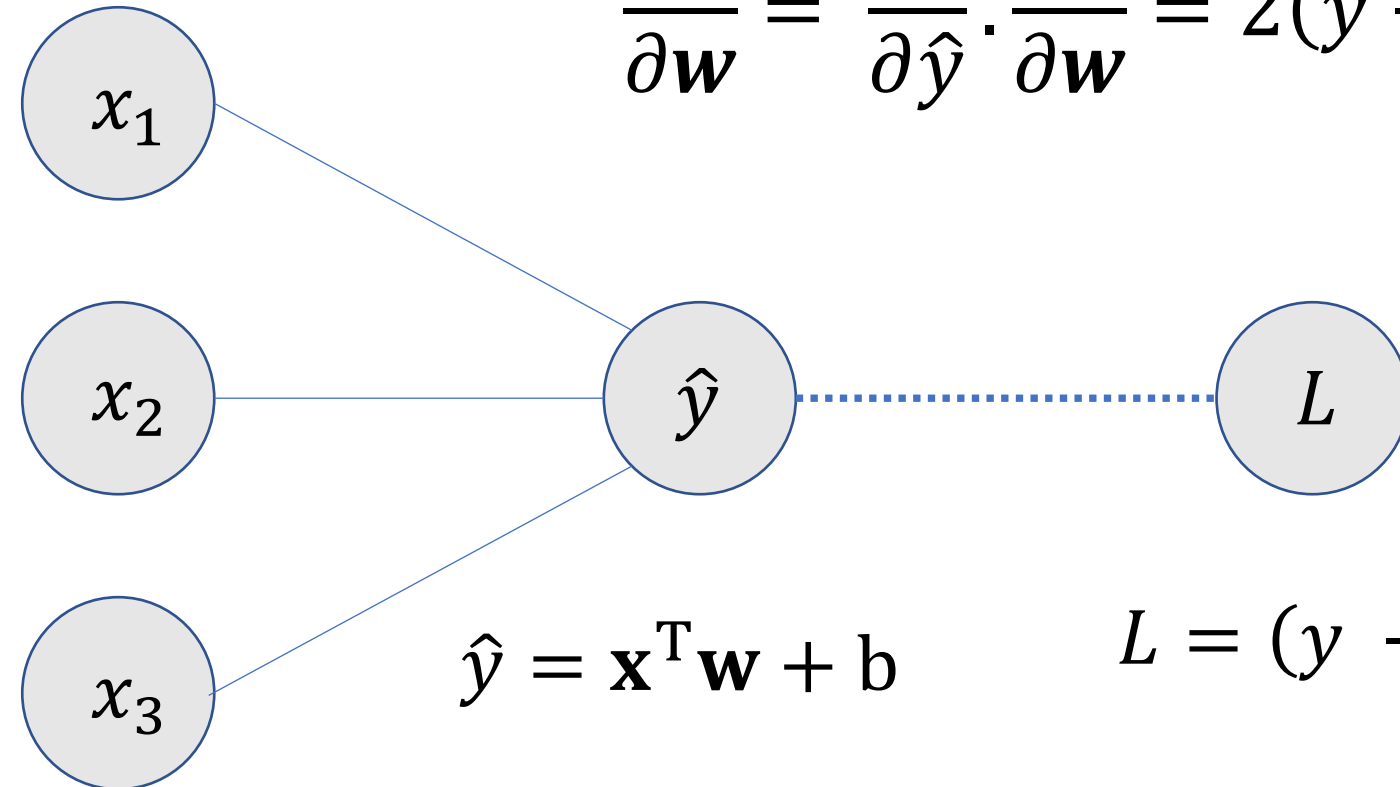
$$\frac{\partial L}{\partial \mathbf{w}} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial \mathbf{w}}$$

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

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

Putting these together:

$$\frac{\partial L}{\partial \mathbf{w}} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial \mathbf{w}} = 2(\hat{y} - y) \cdot \mathbf{x}^T$$



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

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

Example

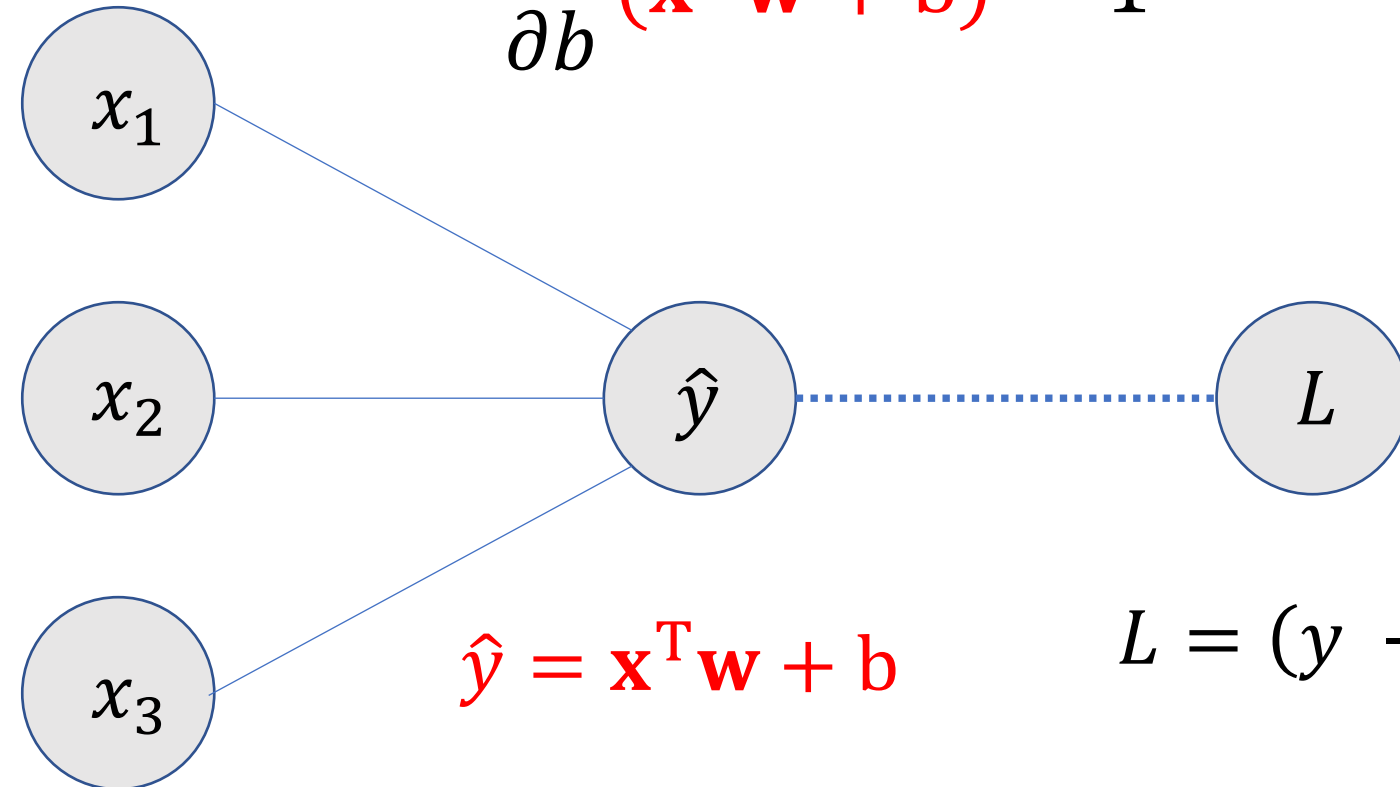
$$\frac{\partial L}{\partial \mathbf{w}} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial \mathbf{w}}$$

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

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

Now for the bias...

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



Example

Putting these together:

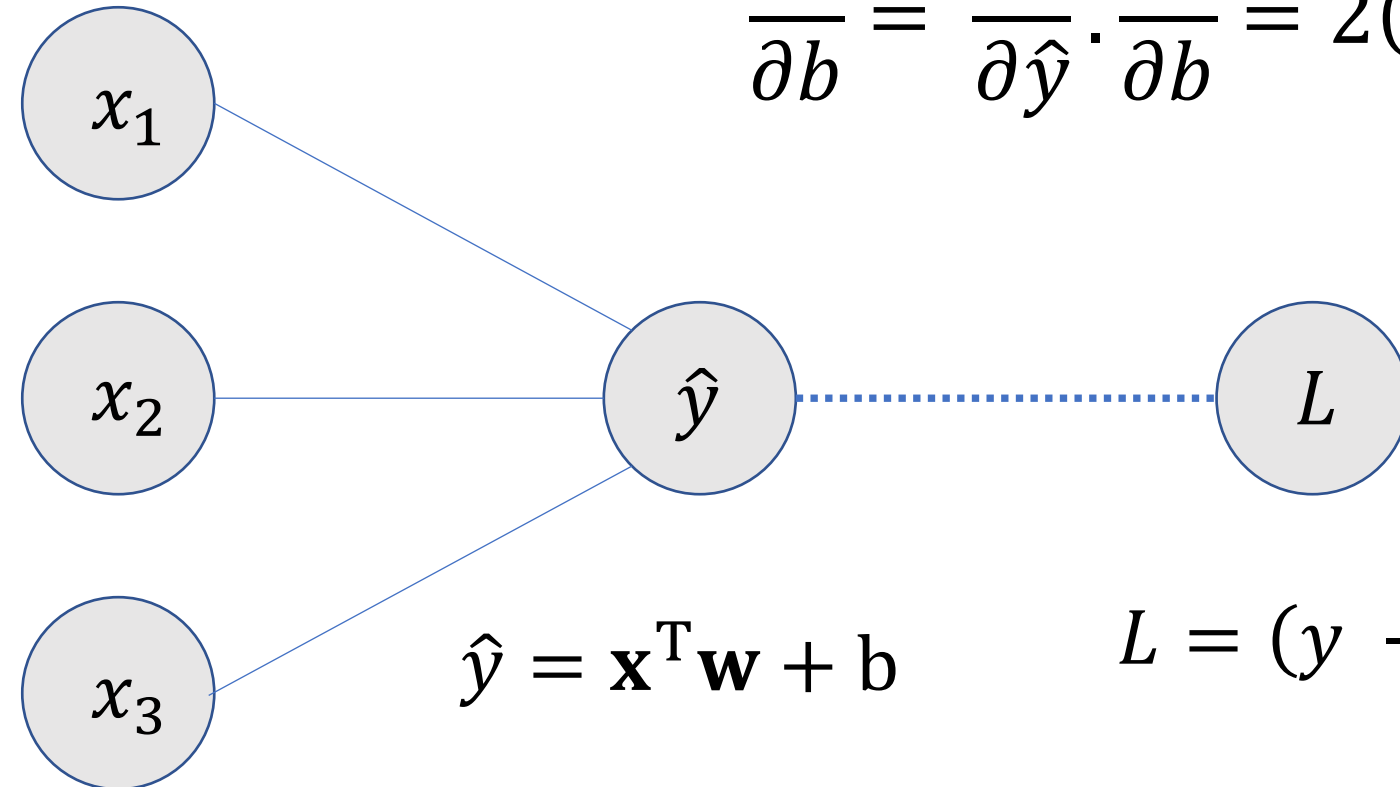
$$\frac{\partial L}{\partial b} = \frac{\partial L}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial b} = 2(\hat{y} - y) \cdot 1$$

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

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

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

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



Example

Finally the updates for the weights:

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \left(\frac{\partial L}{\partial \mathbf{w}} \right)^T = \mathbf{w}_t - 2\alpha(\hat{y} - y)\mathbf{x}$$

And the biases:

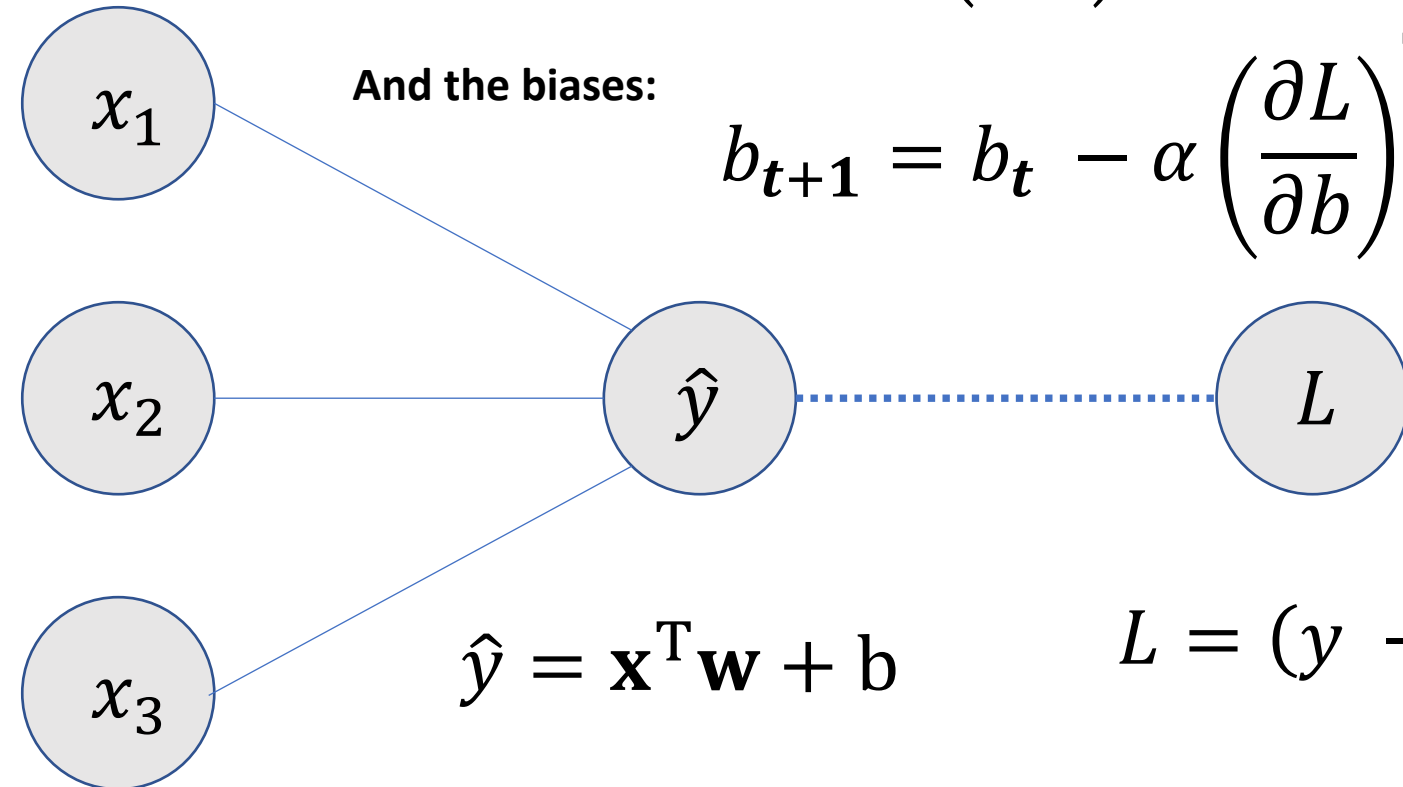
$$b_{t+1} = b_t - \alpha \left(\frac{\partial L}{\partial b} \right)^T = b_t - 2\alpha(\hat{y} - y)$$

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

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

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

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



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

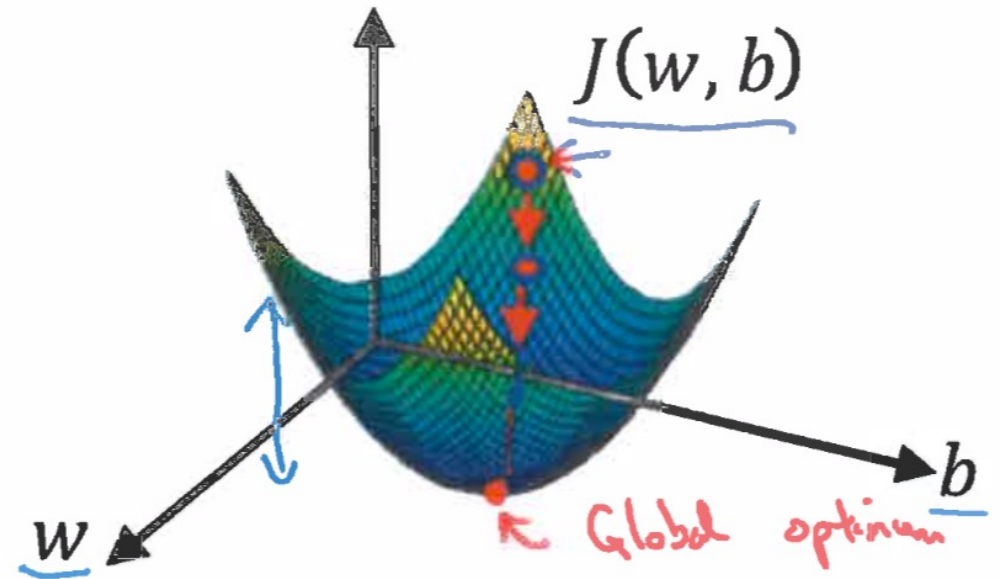
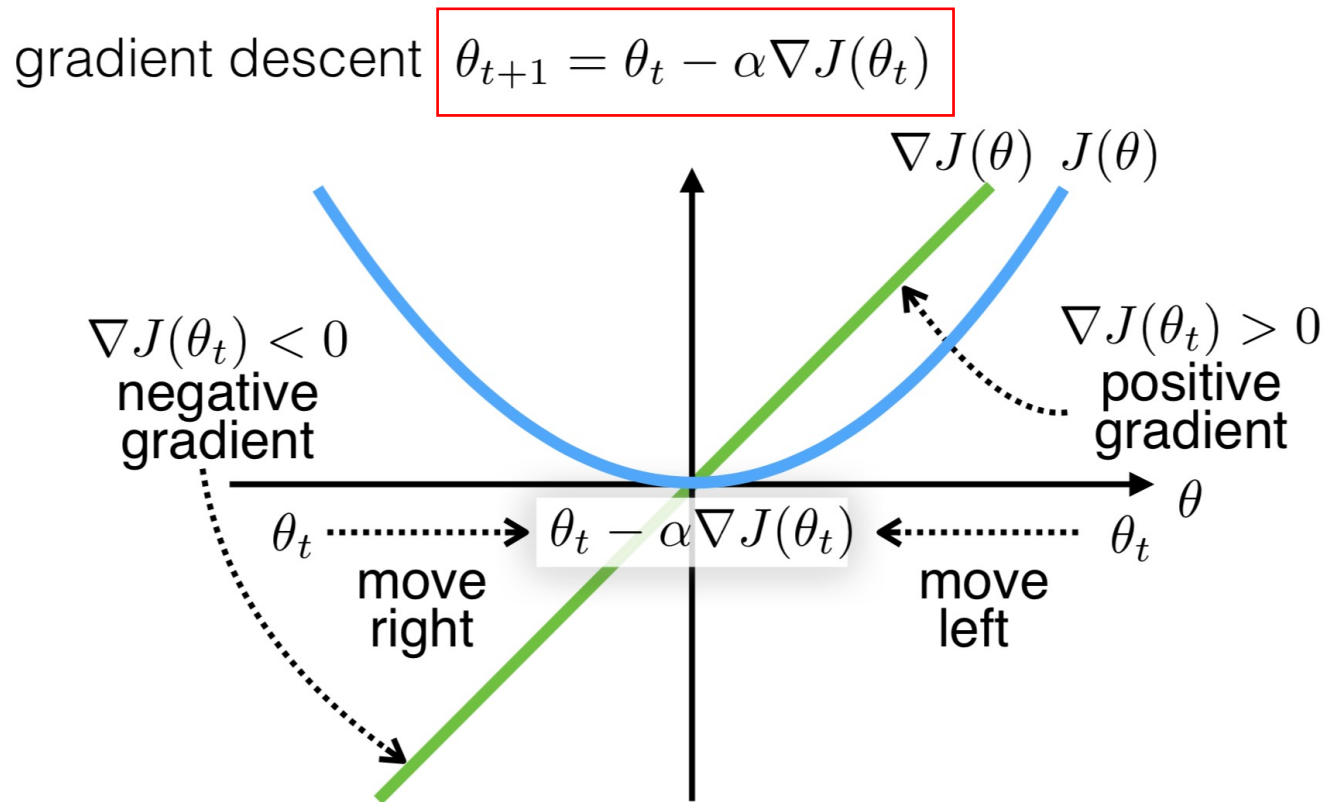
$$L = (y - \hat{y})^2$$

Gradient Descent Illustration



Gradient Descent

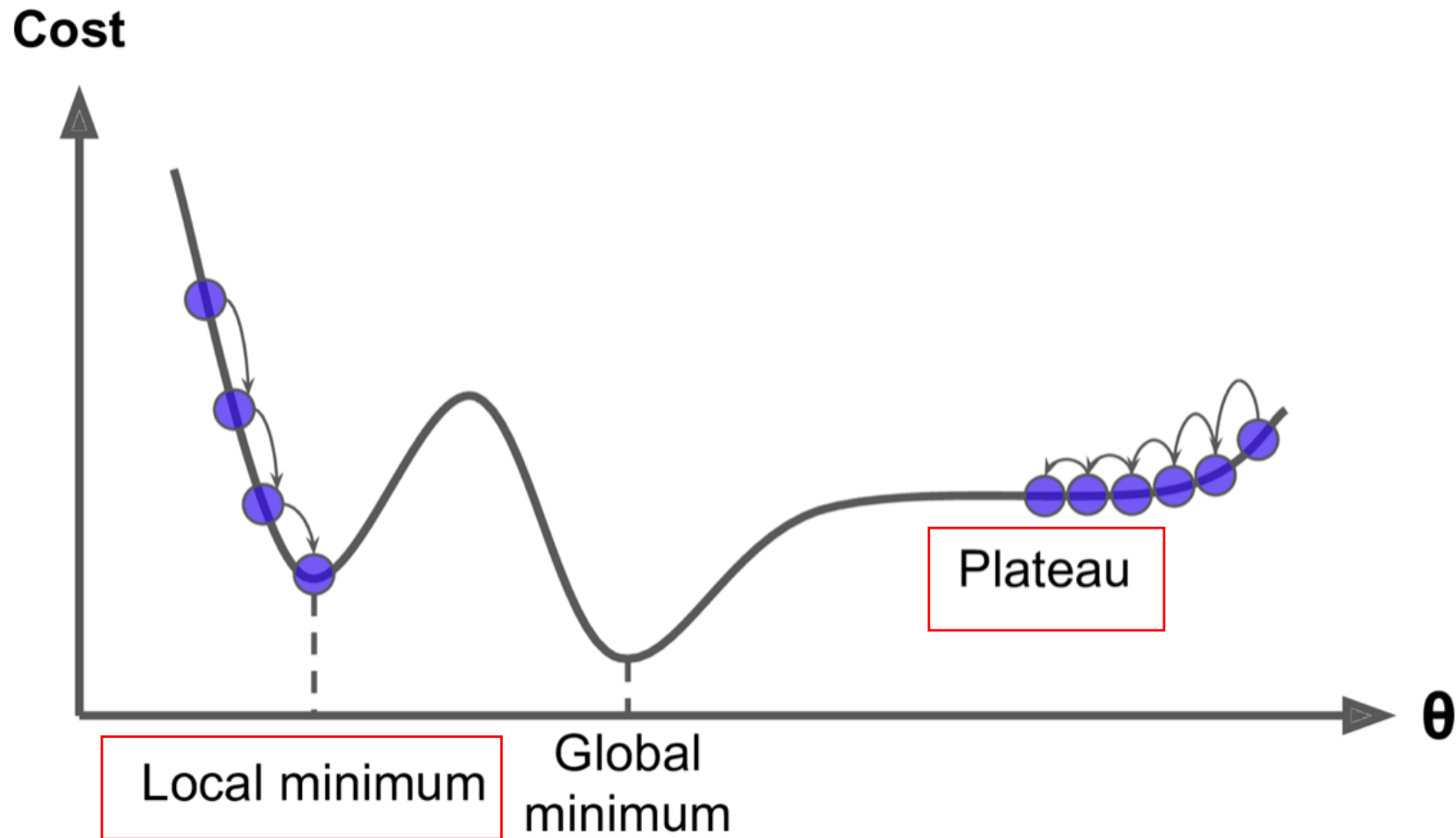
- **Iterative method** to find the parameters $\theta = (w, b)$ that minimize $J(\theta)$



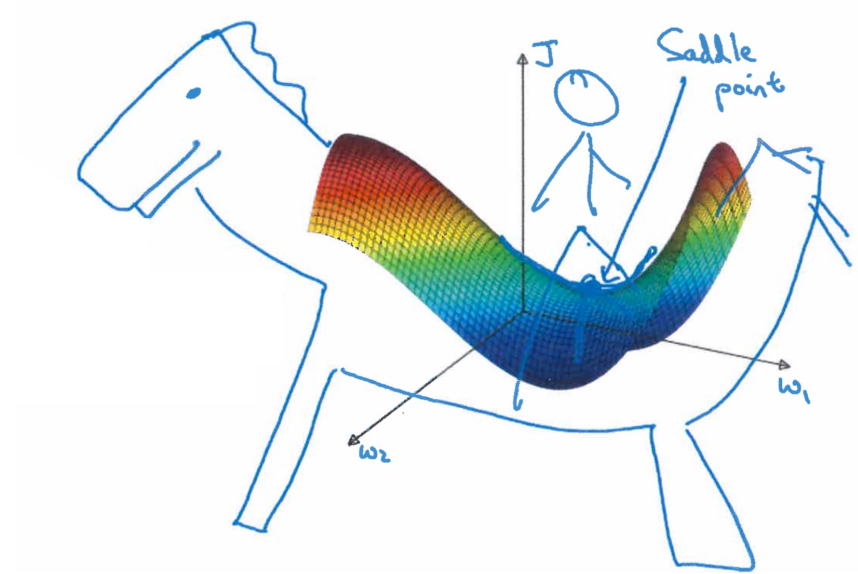
$$\nabla J(w) = \frac{dJ(w, b)}{dw}$$

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

Optimization pitfalls



Saddle point



Tutorial / Practical

