# Deep Network Developments

Lecture #4

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# Requirements

The content of the slides marked by this symbol **will not be included in the exams / tests.**

# Last week - Supervised learning

**Given:** The training sample, a set of (input, label) pairs

$$\{(x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)})\}$$

$$x \in \boldsymbol{X} \subset \mathbb{R}^n,\; y \in \boldsymbol{Y} \subset \mathbb{R}^k$$

**Task:** The estimation of the label (the expected output) from the input

I.e., we search for a (hypothesis-)function $h_\theta$ , for which:

$$h_\theta(x) = \hat{y} \approx y$$

# Last week - Two main tasks in supervised learning

**Regression:** Continuous labels (The label set is infinite)

$$|Y| = \infty$$

**Example:** Number of cars or the age of a person

**Classification:** Discrete labels (The label set is finite)

$$|Y| < \infty$$

**Example:** Categorization of examples

- What is the profession of the person in the image?

# Last week - Example regression tasks

**Example tasks for regression:**

**$x_1$:** Population of a city → **y:** Number of cars in the city

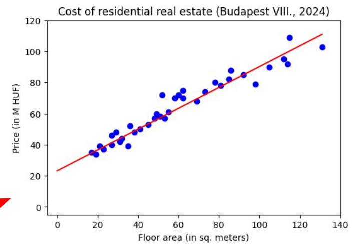
**$x_1$:** Floor area of a flat
**$x_2$:** Distance from city center
→ **y:** Price of the flat

**$x_1$:** Weight of a patient
**$x_2$:** Age of a patient
**$x_3$:** Sex of a patient
→ **y:** Cholesterol levels of the patient

# Last week - Linear regression

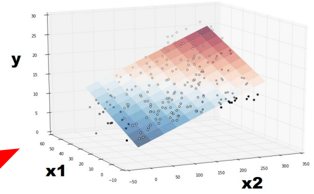
Hypothesis function - **one input variable:**

$$y \approx \hat{y} = h(x) = \theta_1 x + \theta_0$$




Hypothesis function - **two input variables:**

$$y \approx \hat{y} = h(x) = \theta_2 x_2 + \theta_1 x_1 + \theta_0$$




Hypothesis function - **n input variables:**

$$y \approx \hat{y} = h(x) = \theta_n x_n + \theta_{n-1} x_{n-1} + \cdots + \theta_1 x_1 + \theta_0$$

(we cannot visualize the sample space for higher dimensionality…

# Last week - Linear regression

$$\langle x^{(j)}, \theta \rangle = \sum_{i=0}^{n} x_i^{(j)} \theta_i$$

dot product

## Matrix form

$$\theta = \begin{bmatrix} \theta_0 \\ \dots \\ \theta_n \end{bmatrix} \in \mathbb{R}^n$$

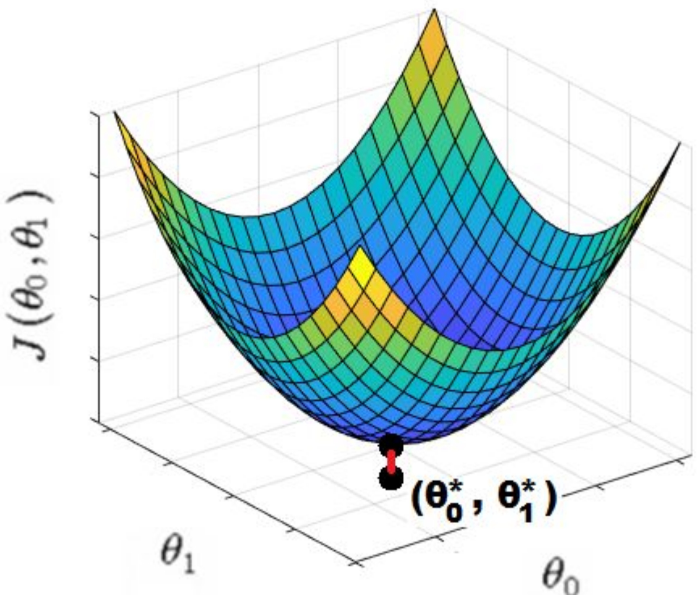
$$x = \begin{bmatrix} 1 & x_1^{(1)} & \dots & x_n^{(1)} \\ \dots & \dots & \dots & \dots \\ 1 & x_1^{(m)} & \dots & x_n^{(m)} \end{bmatrix} \quad \begin{matrix} \langle x^{(1)}, \theta \rangle = \\ \dots \end{matrix} \quad \begin{matrix} \hat{y}^{(1)} \\ \dots \end{matrix} \approx \begin{bmatrix} y^{(1)} \\ \dots \\ y^{(m)} \end{bmatrix} \in \mathbb{R}^m$$

$$h(x) = X\theta = \hat{y} \approx y$$

```
y_pred = np.dot(X, theta)
```

# Last week - Linear regression with least squares

**Goal:** Find parameters where the value of the loss function is minimal!




**Univariate case:**
one input variable, two parameters

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{j=1}^{m} (\theta_1 x^{(j)} + \theta_0 - y^{(j)})^2$$

$$\theta_0^*, \theta_1^* = \underset{\theta_0, \theta_1}{\operatorname{argmin}} J(\theta_0, \theta_1)$$

# Last week - Linear regression with least squares

**Goal:** Find parameters where the value of the loss function is minimal!

**Multivariate case** in matrix form**:**
**n** input variables, **n+1** parameters, **m** data points (examples)

$$J(\Theta) = \frac{1}{2m}||X\theta - y||_2^2 \qquad X \in \mathbb{R}^{m \times n+1},\ \theta \in \mathbb{R}^{n+1}$$

(we cannot visualize the loss function in higher dimensionality, **but it is still quadratic and convex**)

$$\Theta^* = \underset{\Theta}{\operatorname{argmin}}\, J(\Theta)$$

# Last week - Linear regression with least squares

**Gradient descent** - multivariate case

$$
\begin{aligned}
&\text{repeat until convergence} \quad \{ \\
&\quad \text{for i} \leftarrow 1 \ldots \text{n} \quad \{ \\
&\quad\quad grad_i = \frac{\partial}{\partial \theta_i} J(\theta) \\
&\quad \} \\
&\quad \text{for i} \leftarrow 1 \ldots \text{n} \quad \{ \\
&\quad\quad \theta_i = \theta_i - \alpha \, grad_i \\
&\quad \} \\
&\}
\end{aligned}
$$

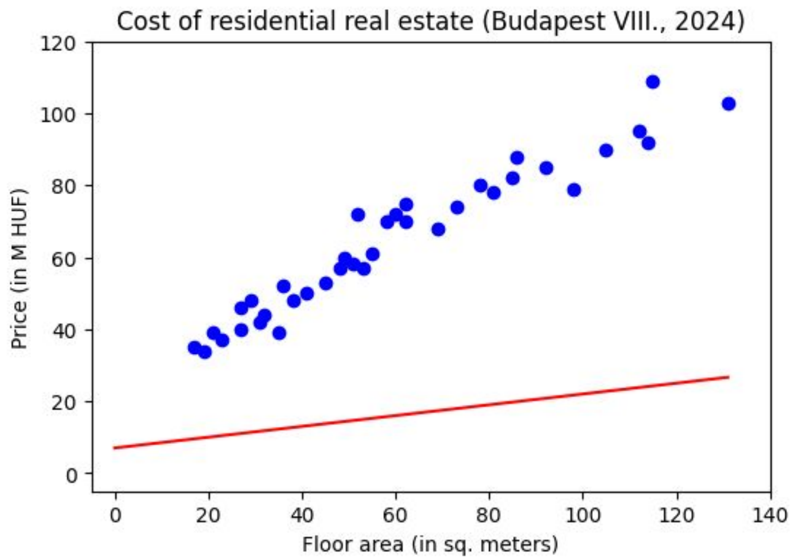
$$\frac{\partial}{\partial \theta_i} J(\theta) = \frac{1}{m} \sum_{j=1}^{m} (\theta_n x_n^{(j)} + \cdots + \theta_0 x_0^{(j)} - y^{(j)}) x_i^{(j)}$$

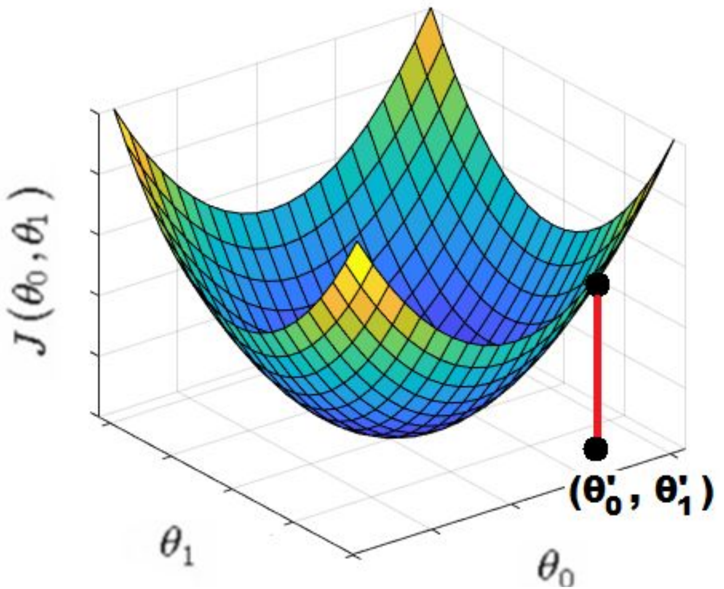
The slope of the tangent in the $\boldsymbol{\theta_i}$ direction

(Visualization: univariate case)

# Last week - Linear regression with least squares

## **Applying gradient descent, T = 0** (before taking the first step)

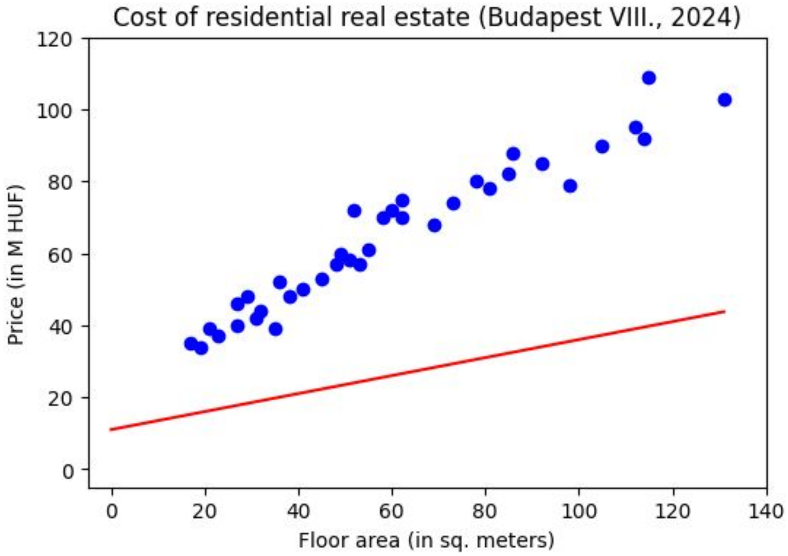


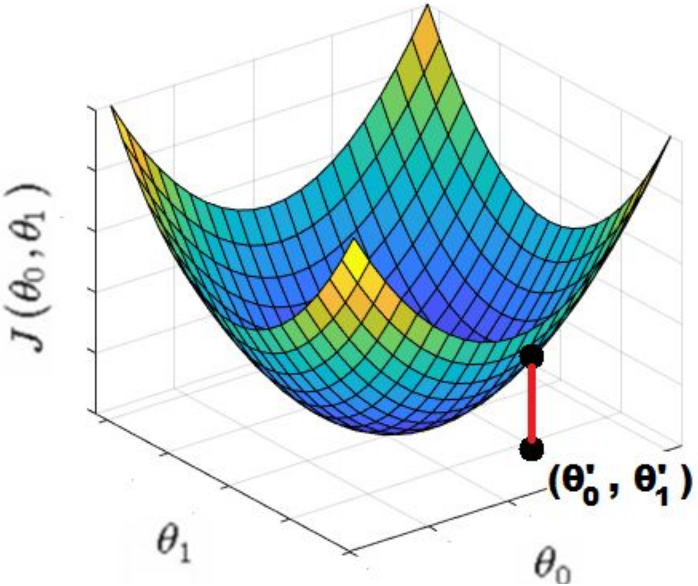




We can choose the initial parameters randomly.

# Last week - Linear regression with least squares

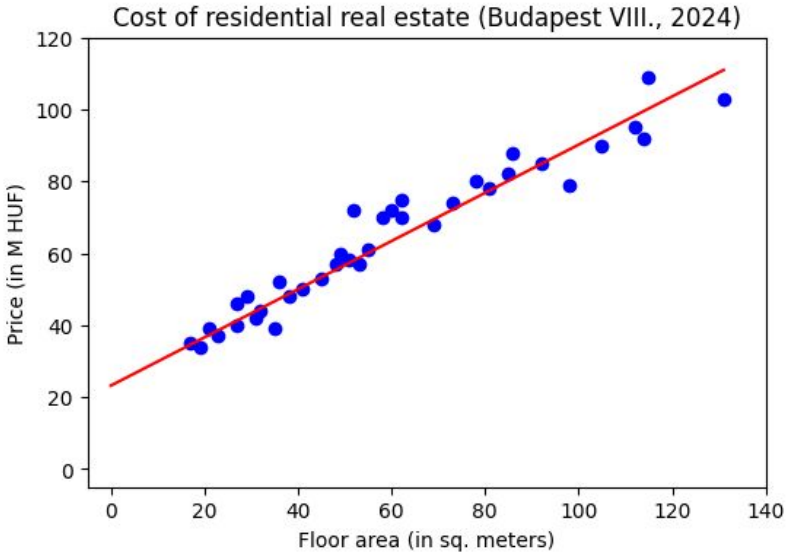
## Applying gradient descent, T = 1

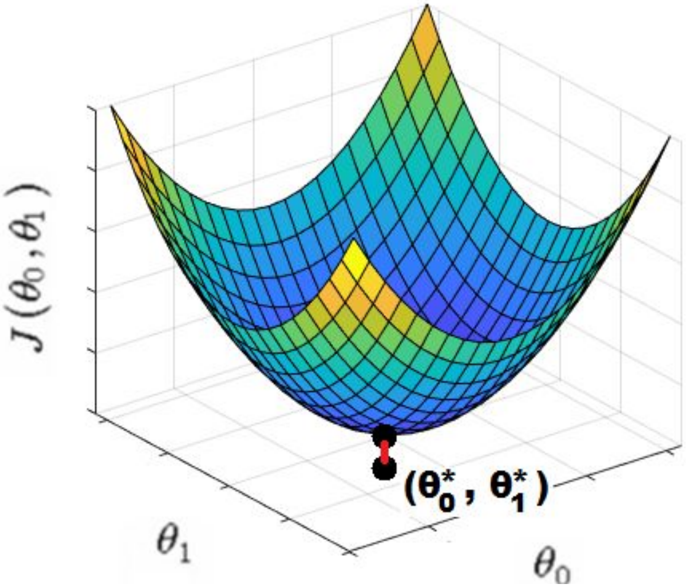


# Last week - Linear regression with least squares

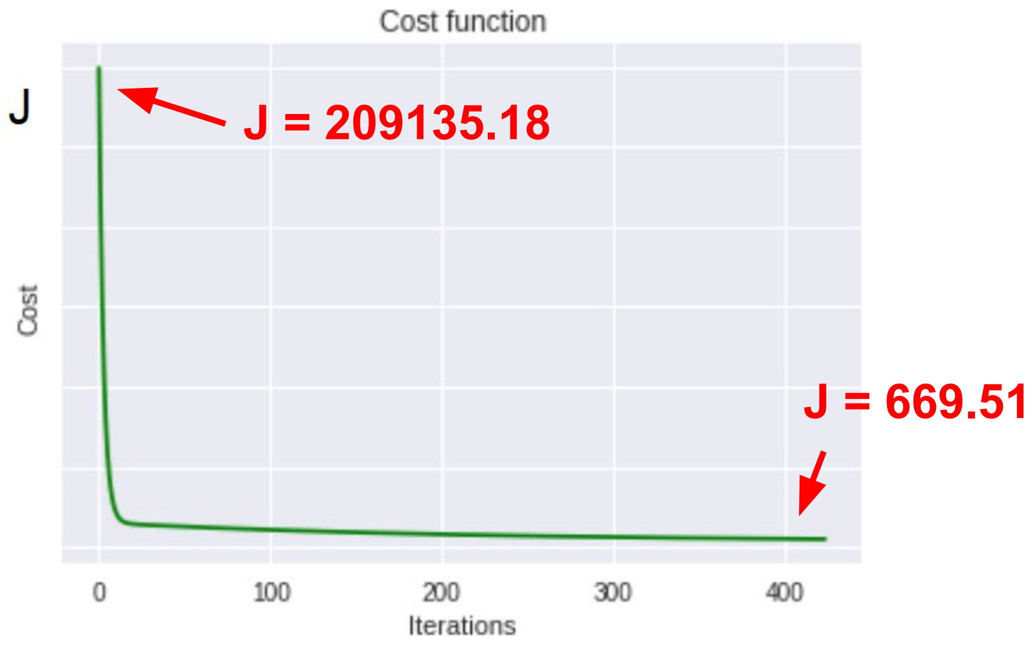
## Applying gradient descent, T = < many >



# Another solution to the least squares method

## Changes in the loss value during the steps of the gradient descent



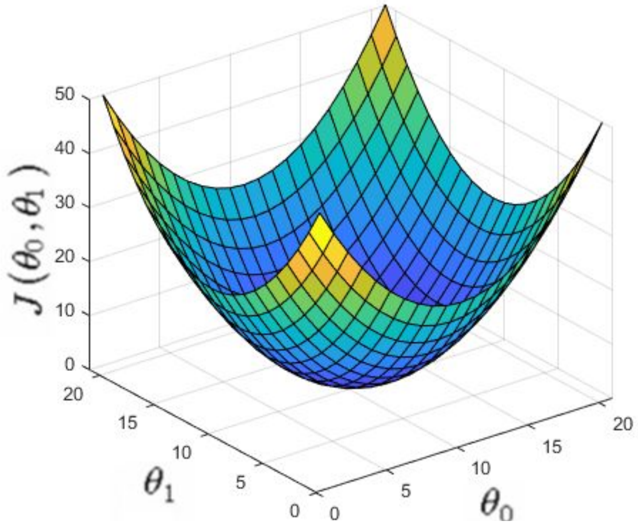
# Another solution to the least squares method

## Changes in the loss value during the steps of the gradient descent


We need many iterations and we only approximate the optimal parameters.
**Is there no better way?**

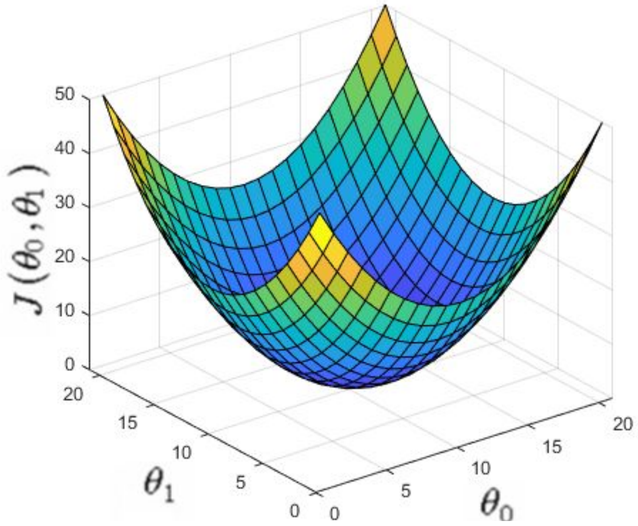
# Another solution to the least squares method

**What do we know about the loss function?**



# Another solution to the least squares method

**What do we know about the loss function?**




- **Quadratic** (second-degree polynomial, may be multivariate)

  → if the second-degree coefficient is positive, then it is **convex**

  → it has a **single** local (and also global) **minimum**

# Another solution to the least squares method

**What do we know about the loss function?**

- **Quadratic** (second-degree polynomial, may be multivariate)

  → if the second-degree coefficient is positive, then it is **convex**

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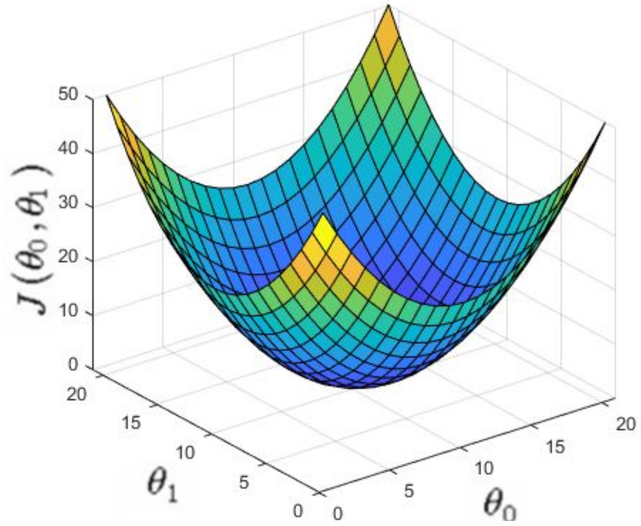



**What can we say about the minimum point** (the optimal parameters)?

# Another solution to the least squares method

$$\forall i = 0 \ldots n : \frac{\partial}{\partial \theta_i} J(\theta) = 0$$

In the minimum of the loss function, **all partial derivatives are zero.**

$$\frac{\partial}{\partial \theta_i} J(\theta) = \frac{1}{m} \sum_{j=1}^{m} (\theta_n x_n^{(j)} + \cdots + \theta_0 x_0^{(j)} - y^{(j)}) x_i^{(j)} = 0$$

# Another solution to the least squares method

$$\forall i = 0 \ldots n : \frac{\partial}{\partial \theta_i} J(\theta) = 0$$

$$\frac{\partial}{\partial \theta_i} J(\theta) = \frac{1}{m} \sum_{j=1}^{m} (\theta_n x_n^{(j)} + \cdots + \theta_0 x_0^{(j)} - y^{(j)}) x_i^{(j)} = 0$$

→ We can write the above equation for each parameter **$\theta_i$** (**n+1 equations**).

→ We are looking for the value of each parameter **$\theta_i$** (**n+1 unknowns**).

Derivation of the normal equation is omitted on this course…

# Another solution to the least squares method

**The normal equation** - an **exact solution** to the least squares problem

$$\theta = (X^T X)^{-1} X^T y$$

$$\theta = X^+ y$$

**Moore-Penrose pseudoinverse**

```
theta = np.matmul(np.linalg.pinv(X), y)
```

# Another solution to the least squares method

**The normal equation** - an **exact solution** to the least squares problem

$$\theta = (X^T X)^{-1} X^T y$$

**We can find the optimal parameters to a linear regression problem**
(with least squares) **in a single step, by using the formula above!**
(X, y are known from the data)

# Another solution to the least squares method

**The normal equation** - an **exact solution** to the least squares problem

$$\theta = (X^T X)^{-1} X^T y$$

**The regularized (L2) least squares solution:**

$$\theta = (X^T X + \boxed{\lambda I})^{-1} X^T y$$

**In practice, we use the regularized version of the normal equation:**
By choosing an appropriate lambda value, we ensure the stability of the solution (and thus a valid input to the inverse operation).

# Last week - Two main tasks in supervised learning

**Regression:** Continuous labels (The label set is infinite)

$$|Y| = \infty$$

**Example:** Number of cars or the age of a person

**Classification:** Discrete labels (The label set is finite)

$$|Y| < \infty$$

**Example:** Categorization of examples

- What is the profession of the person in the image?

# Last week - Example (binary) classification tasks

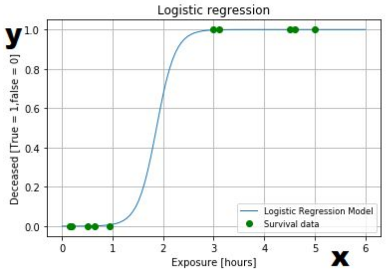
**Example tasks for** (binary) **classification:**

**$x_1$:** Duration of exposure to radiation → **y:** Did the person die?

**$x_1$:** Population of a settlement
**$x_2$:** Annual number of tourists
→ **y:** Is the settlement a town?

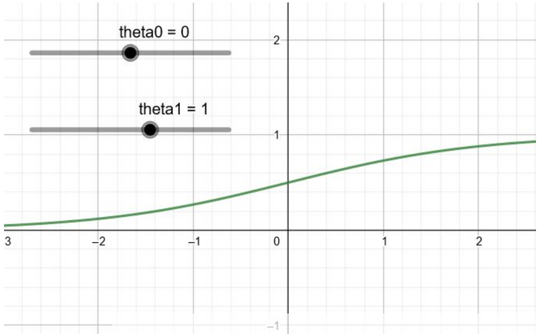
**$x_1$:** Weight of an animal
**$x_2$:** Number of hairballs coughed up
**$x_3$:** Degree of drooling
→ **y:** Is it a dog or a cat?

# Last week - Logistic regression

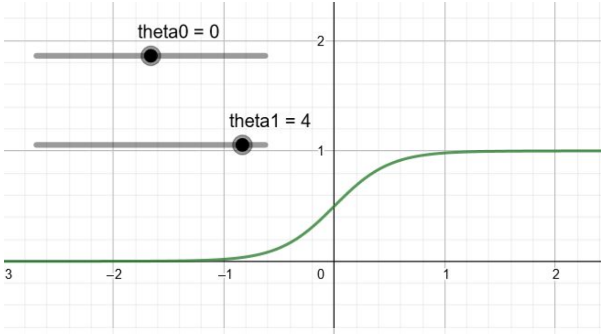



$$h_\theta(x) = g(\theta_0 + \theta_1 x) = \frac{1}{1+e^{-(\theta_0+\theta_1 x)}} = \hat{y}$$

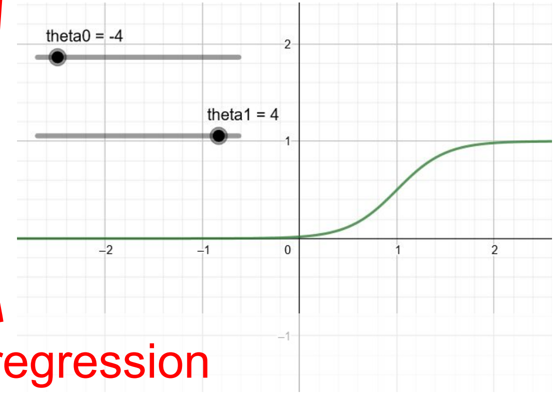
$\theta_0 = 0$
$\theta_1 = 1$




$\theta_0 = 0$
$\theta_1 = 4$




$\theta_0 = -4$
$\theta_1 = 4$

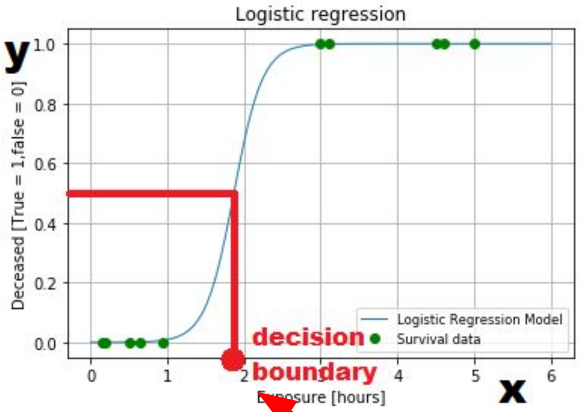



**Logistic regression hypothesis:** Sigmoid ◦ Linear regression

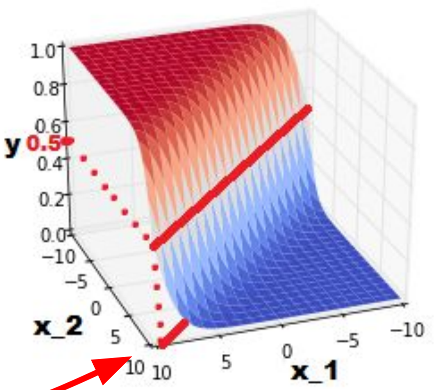
# Last week - Logistic regression

## Logistic regression - **Decision boundary** $\{x \mid \hat{y} = h(x) = 0.5\}$

**Univariate sample**




**Bivariate sample**




...

...

**decision boundaries**

# Last week - Logistic regression

**Loss function for logistic regression:** Logistic loss / Binary cross-entropy

$$J(\theta) = \frac{1}{m}\sum_{j=1}^{m}[-y^{(j)}\ log(h_\theta(x^{(j)})) - (1 - y^{(j)})\ log(1 - h_\theta(x^{(j)}))]$$

$$h_\theta(x) = \frac{1}{1+e^{-(\theta_1 x+\theta_0)}}$$

**Logistic loss** (using the logistic regression hypothesis) **is convex**
→ **a single local** (and global) **minimum**
→ **gradient descent will find the globally optimal parameters**

# Logistic regression in NumPy

```
def __sigmoid(self, z):
        return 1 / (1 + np.exp(-z) + self.eps)
```

**sigmoid function** (vectorized)

```
h = self.__sigmoid(np.dot(X, self.theta))
```

**the label prediction** (y hat)

```
loss = np.mean(-y * np.log(h + self.eps) - \\
               (1 - y) * np.log(1 - h + self.eps))
```

**loss value**

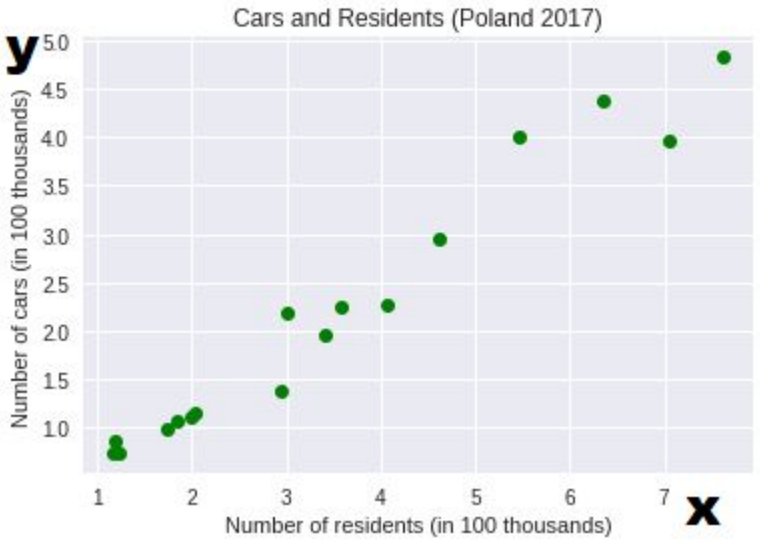
```
gradient = np.dot(X.T, (h - y)) / y.size
self.theta -= self.lr * gradient
```

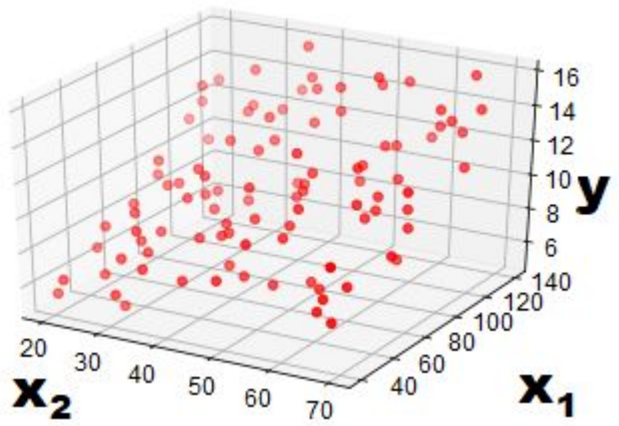
**a single step of gradient descent**

(**eps:** to avoid division by zero)

# Back to regression…

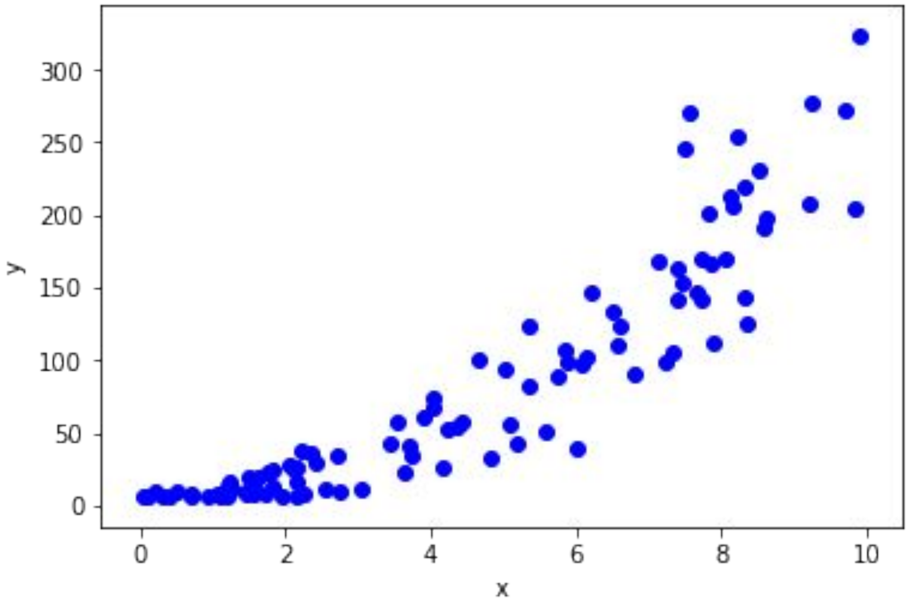
Linear regression worked well on a sample where the **linear combination of variables** closely approximated the label.



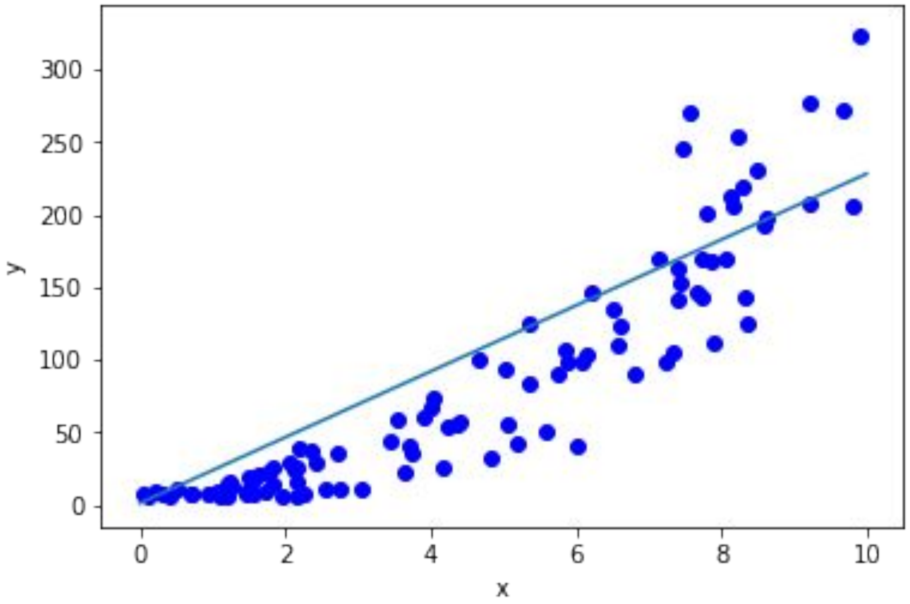
# Back to regression…

**What can we do when a linear approximation is not suitable?**

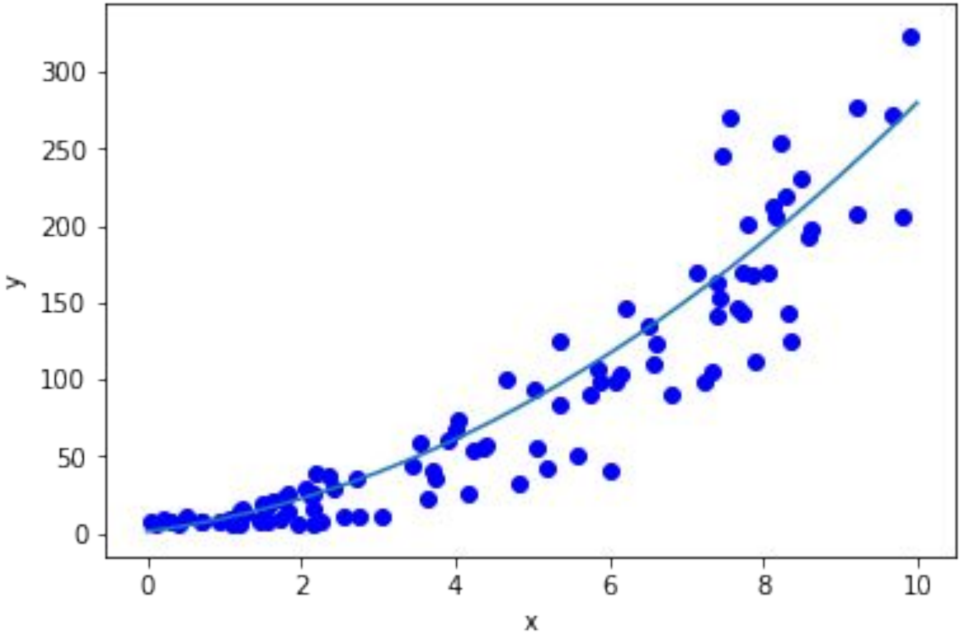


# Back to regression…

**E.g., let's assume** $y \approx ax^2 + bx + c$ . In this case, linear regression does not provide very good results. **What can we do?**



# Polynomial regression



# Polynomial regression

**Hypothesis function**

Univariate: $h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \ldots$

Multivariate, e.g.,: $h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2 + \theta_5 x_1 x_2 + \ldots$

**Loss function** (MSE):

$$J(\theta) = \frac{1}{2m} \sum_{j=1}^{m} (\overbrace{h_\theta(x^{(j)})}^{\hat{y}^{(j)}} - y^{(j)})^2$$

# Polynomial regression

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2 + \theta_5 x_1 x_2 + \dots$$

$$J(\theta) = \frac{1}{2m} \sum_{j=1}^{m} (h_\theta(x^{(j)}) - y^{(j)})^2$$

**Solution using gradient descent:**

The loss function is differentiable.
→ Gradient descent can be used to find good **θ** coefficients.

# Polynomial regression

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2 + \theta_5 x_1 x_2 + \ldots$$

$$J(\theta) = \frac{1}{2m} \sum_{j=1}^{m} (h_\theta(x^{(j)}) - y^{(j)})^2$$

Now, we have exponents inside
the hypothesis function (and thus the loss).
**Is this a problem?**

**Solution using gradient descent:**

The loss function is differentiable.
→ Gradient descent can be used to find good **θ** coefficients.

# Polynomial regression

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2 + \theta_5 x_1 x_2 + \dots$$

$$J(\theta) = \frac{1}{2m} \sum_{j=1}^{m} (h_\theta(x^{(j)}) - y^{(j)})^2$$

**Solution using gradient descent:**

The loss function is differentiable.
→ Gradient descent can be used to find good **θ** coefficients.

We do not raise **θ** parameters to the power.
→ **J remains quadratic with respect to the θ parameters!**

# Polynomial regression

**Solution in practice:**

- Due to exponents, gradients associated with higher-order coefficients can be extremely large/small.
- As we saw in multivariate linear regression,
  the gradient method is sensitive to this.

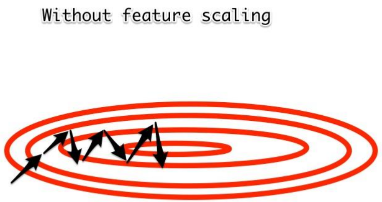
**Solution?**

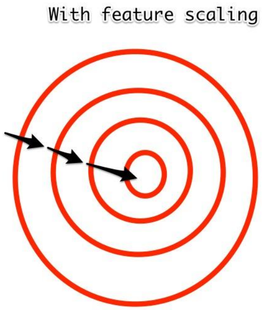
# Polynomial regression

**Solution in practice:**

- Due to exponents, gradients associated with higher-order coefficients can be extremely large/small.
- As we saw in multivariate linear regression, the gradient method is sensitive to this.

**Solution?**



# Polynomial regression

**Solution:**

Treat polynomial regression as if it was linear regression!

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2 + \theta_5 x_1 x_2 + \dots$$

… is **transformed into:**

$$h_\theta(x) = \theta_0 + \theta_1 x_{1'} + \theta_2 x_{2'} + \theta_3 x_{3'} + \theta_4 x_{4'} + \theta_5 x_{5'} + \dots$$

# Polynomial regression

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2 + \theta_5 x_1 x_2 + \dots$$

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$$h_\theta(x) = \theta_0 + \theta_1 x_{1'} + \theta_2 x_{2'} + \theta_3 x_{3'} + \theta_4 x_{4'} + \theta_5 x_{5'} + \dots$$

→ we **substitute** and calculate the powers of the variables in advance.

For example: $x_{4'} := x_2^2$


Finally, we bring the new variables to the same order of magnitude using feature scaling and solve the problem as a **linear regression**.

# Polynomial regression

**Univariate case:** Vandermonde matrix

$$x = \begin{bmatrix} 1 & x^{(1)} & (x^{(1)})^2 & \dots & (x^{(1)})^n \\ \dots & \dots & \dots & \dots & \\ 1 & x^{(m)} & (x^{(m)})^2 & \dots & (x^{(m)})^n \end{bmatrix} \in \mathbb{R}^{m \times n}$$

$$\theta = \begin{bmatrix} \theta_0 \\ \dots \\ \theta_n \end{bmatrix} \in \mathbb{R}^n \qquad y = \begin{bmatrix} y^{(1)} \\ \dots \\ y^{(m)} \end{bmatrix} \in \mathbb{R}^m$$

**Feature scaling:**
We treat x, $x^2$, …, $x^n$ as separate variables and scale them independently of each other.

$$h(x) = X\theta = \hat{y} \approx y$$

# Polynomial regression

**Multivariate case,** for example:

$$x = \begin{bmatrix} 1 & x_1^{(1)} & x_2^{(1)} & (x_1^{(1)})^2 & (x_1^{(1)})^3(x_2^{(1)})^2 & \dots \\ \dots & \dots & \dots & \dots & & \\ 1 & x_1^{(m)} & x_2^{(m)} & (x_1^{(m)})^2 & (x_1^{(m)})^3(x_2^{(m)})^2 & \dots \end{bmatrix} \in \mathbb{R}^{m \times n}$$

$$\theta = \begin{bmatrix} \theta_0 \\ \dots \\ \theta_n \end{bmatrix} \in \mathbb{R}^n \qquad y = \begin{bmatrix} y^{(1)} \\ \dots \\ y^{(m)} \end{bmatrix} \in \mathbb{R}^m$$

**Feature scaling:**
We treat $x_1$, $x_2$, $x_1^2$, … as separate variables and scale them independently of each other.

$$h(x) = X\theta = \hat{y} \approx y$$

# Splitting the sample

The life cycle of the model:

1. We train the model on the **training set**
2. We evaluate the model on the **test set**

The two sets must be **disjoint**!

# Splitting the sample

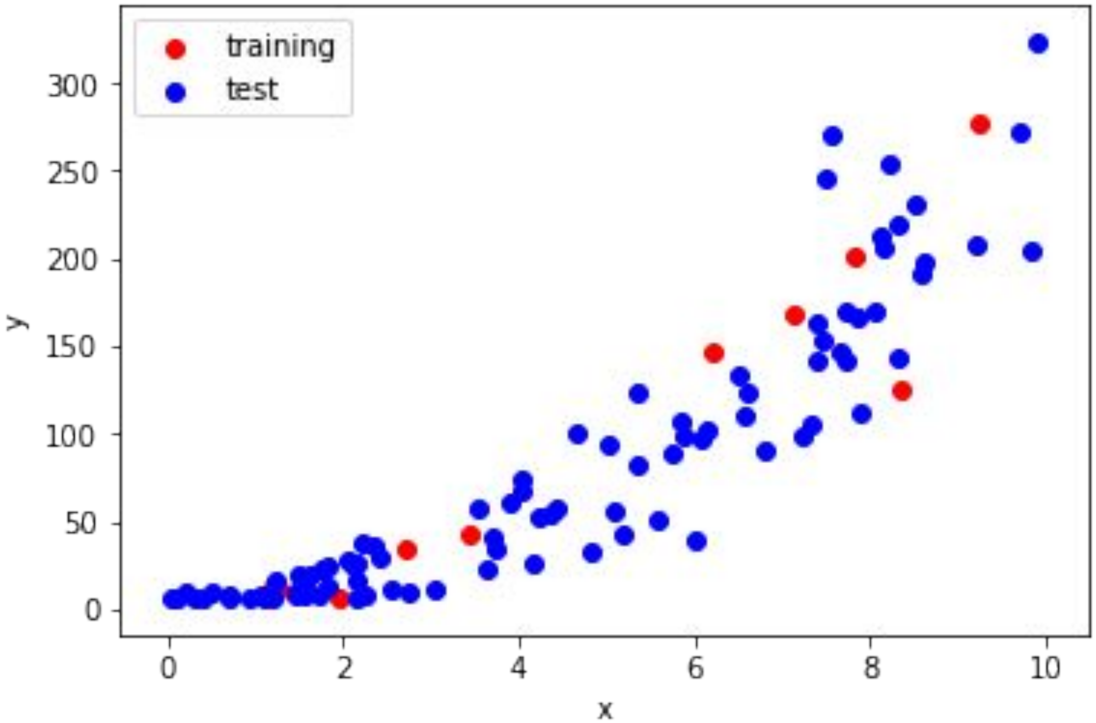
The life cycle of the model:

1. We train the model on the **training set**
2. We evaluate the model on the **test set**

The two sets must be **disjoint**!

**Do not use the test set for learning!**
We use the test set to estimate how our trained model will perform on new data points, not seen during training.

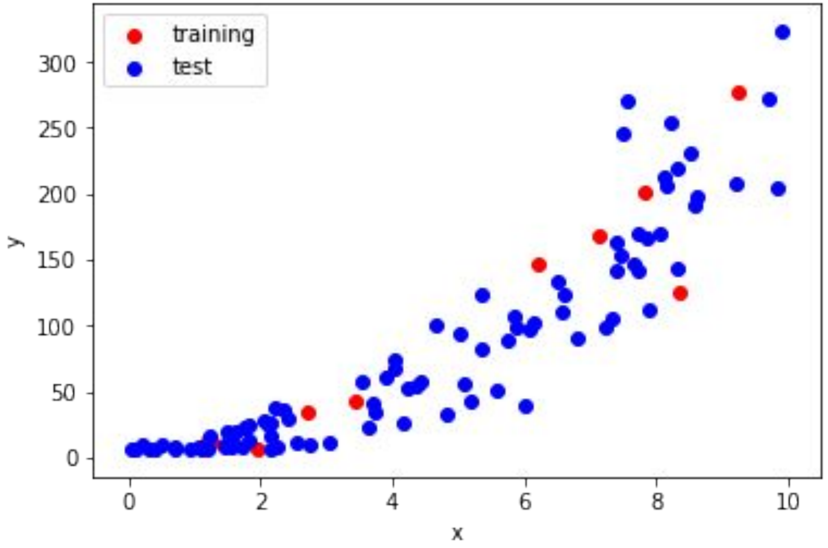
# Splitting the sample



# Observing the loss curve during training

Perform polynomial regression on the following sample!

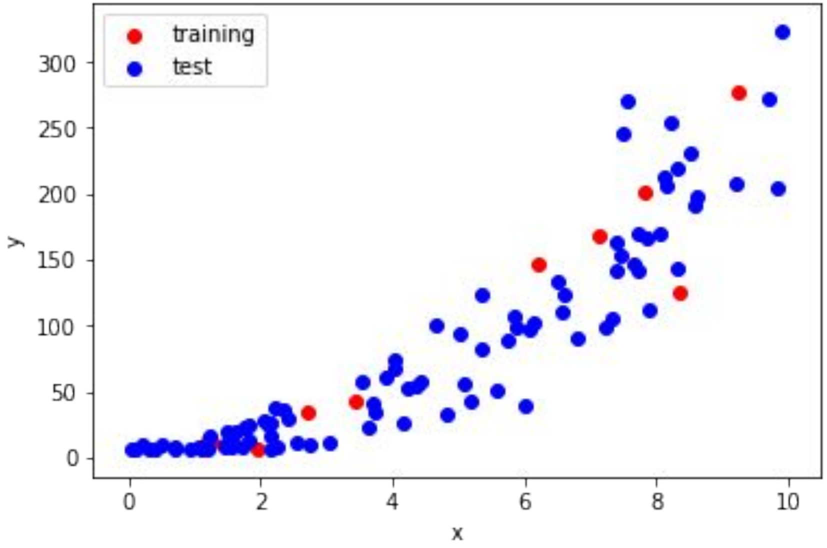
**What degree polynomial should we fit?**



# Observing the loss curve during training

Perform polynomial regression on the following sample!

**What degree polynomial should we fit?**



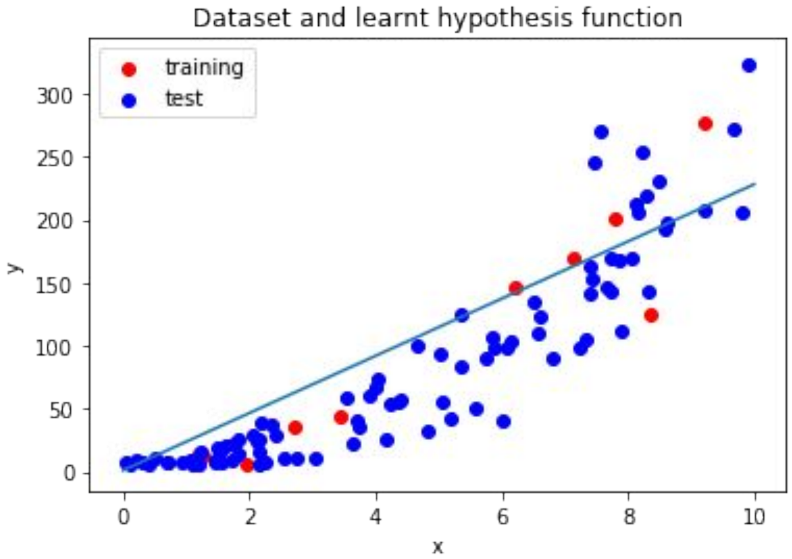

With a single variable, it is clear from looking at the graph that a second-degree polynomial fits the sample well.

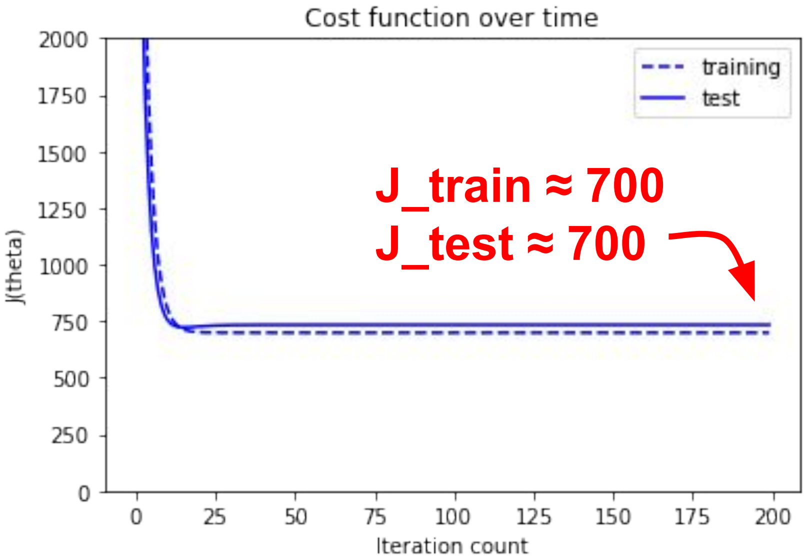
Unfortunately, we cannot visualize the data like this with more than two variables. Therefore, without additional experimentation, we cannot tell what degree polynomial would be ideal.

# Observing the loss curve during training: **underfitting**

$$h_\theta(x) = \theta_0 + \theta_1 x$$

**The training and test losses are both** (similarly) **large.**



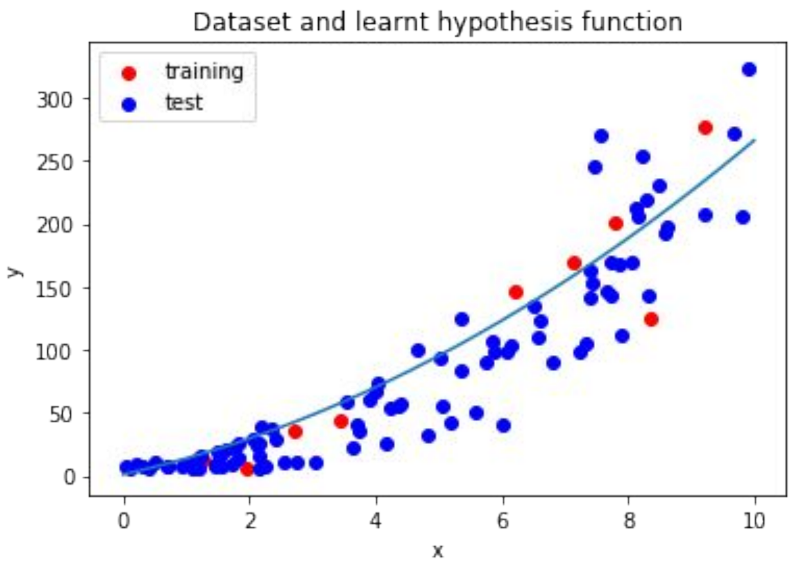



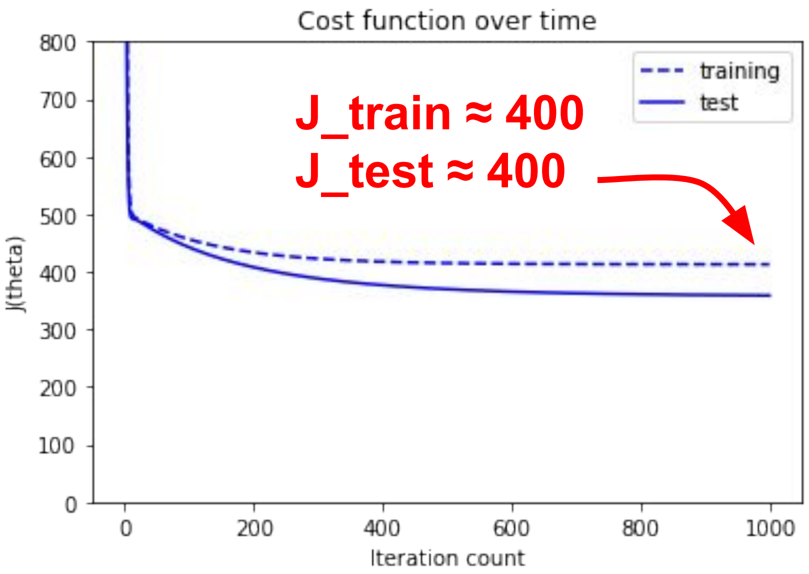

“high bias, low variance”

# Observing the loss curve during training: **“just right”**

$$h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2$$

**Both the training and the test losses are small and both decrease over time.**



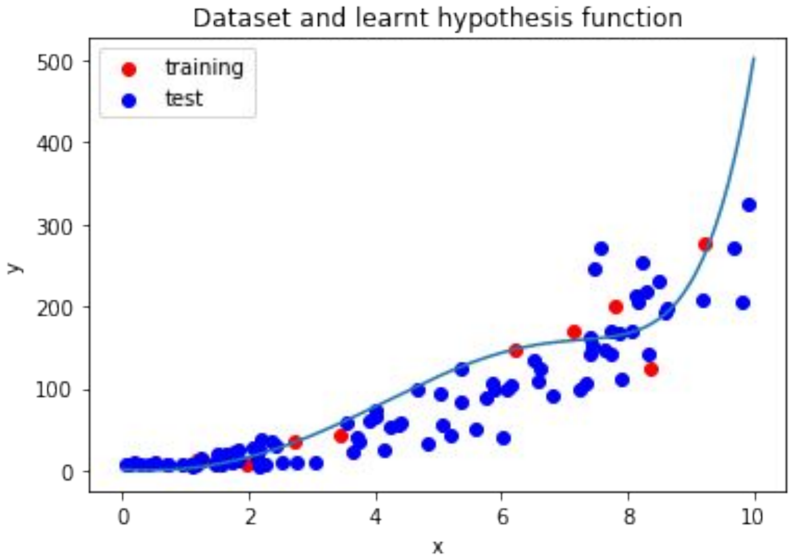



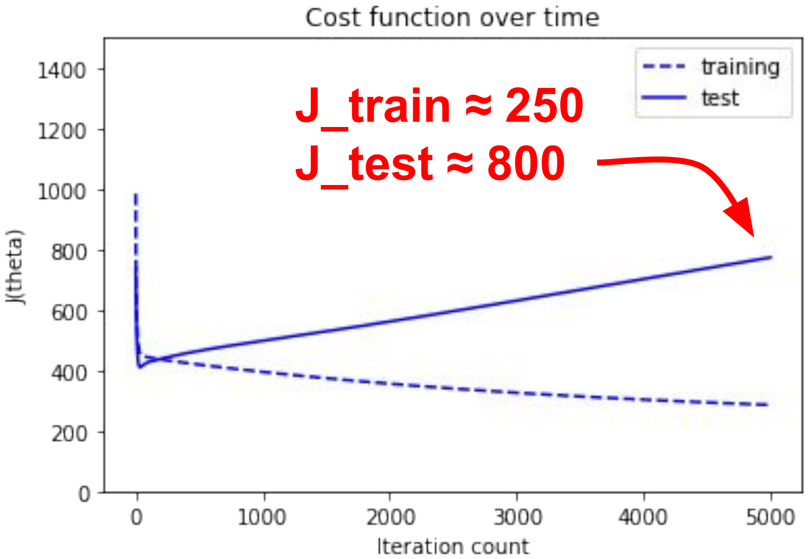

“balancing bias & variance”

# Observing the loss curve during training: **overfitting**

$$h_\theta(x) = \theta_0 + \theta_1 x + \cdots + \theta_9 x^9$$

**The training loss decreases, but the test loss increases.**

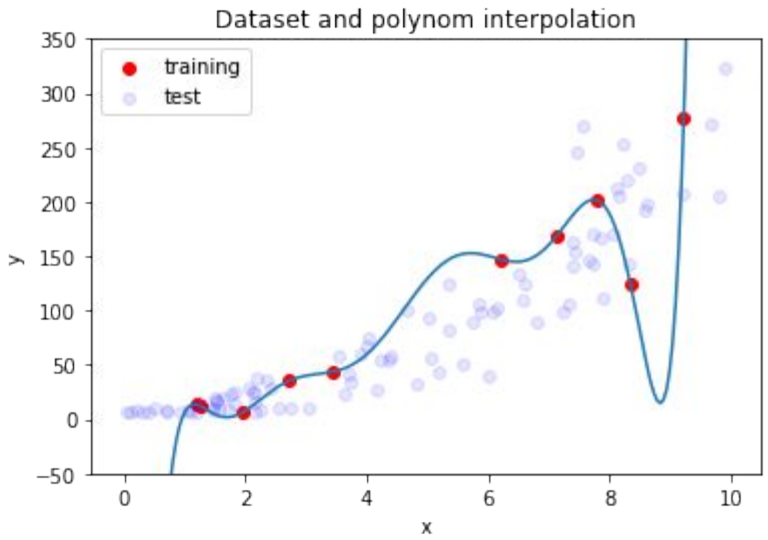



“low bias, high variance”

# **Detour:** Polynomial interpolation

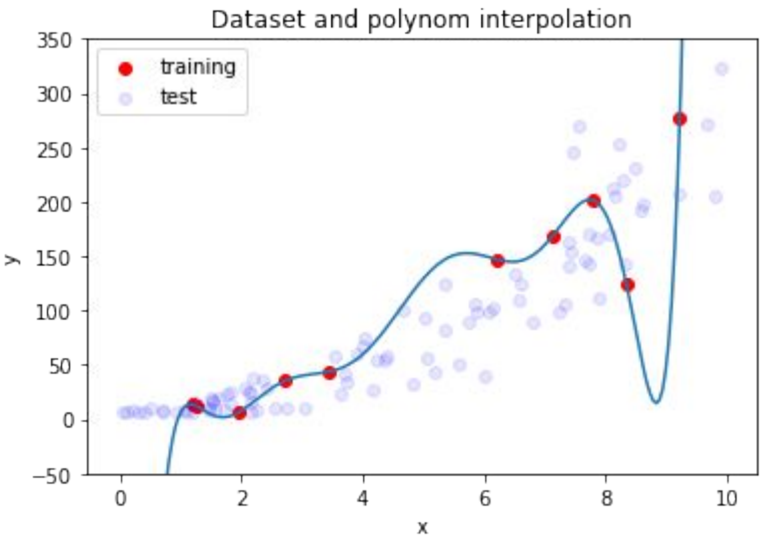
**With polynomial interpolation, we can even fit a polynomial exactly to the training set.**




**J_train = 0**
**J_test ≈ 252507.67**

# **Detour:** Polynomial interpolation

**With polynomial interpolation, we can even fit a polynomial exactly to the training set.** However, this is not useful in machine learning!




**J_train = 0**
**J_test ≈ 252507.67**

A ninth-degree polynomial can be fitted to ten points without any error.
If there is enough training data and the hypothesis function is sufficiently complex, a precise fit can be achieved, but this will be very far from the test data.
→ **"Extreme overfitting"**

Image source: Andrew Ng Machine learning video series

# Under- and overfitting in case of classification

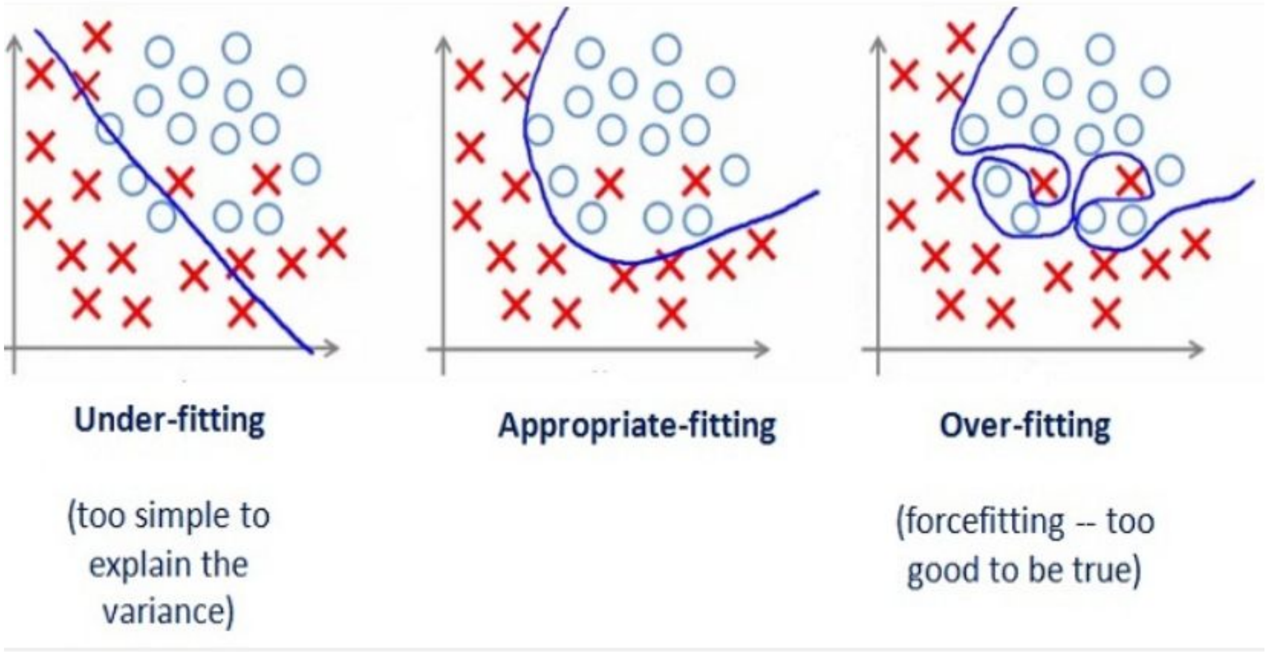
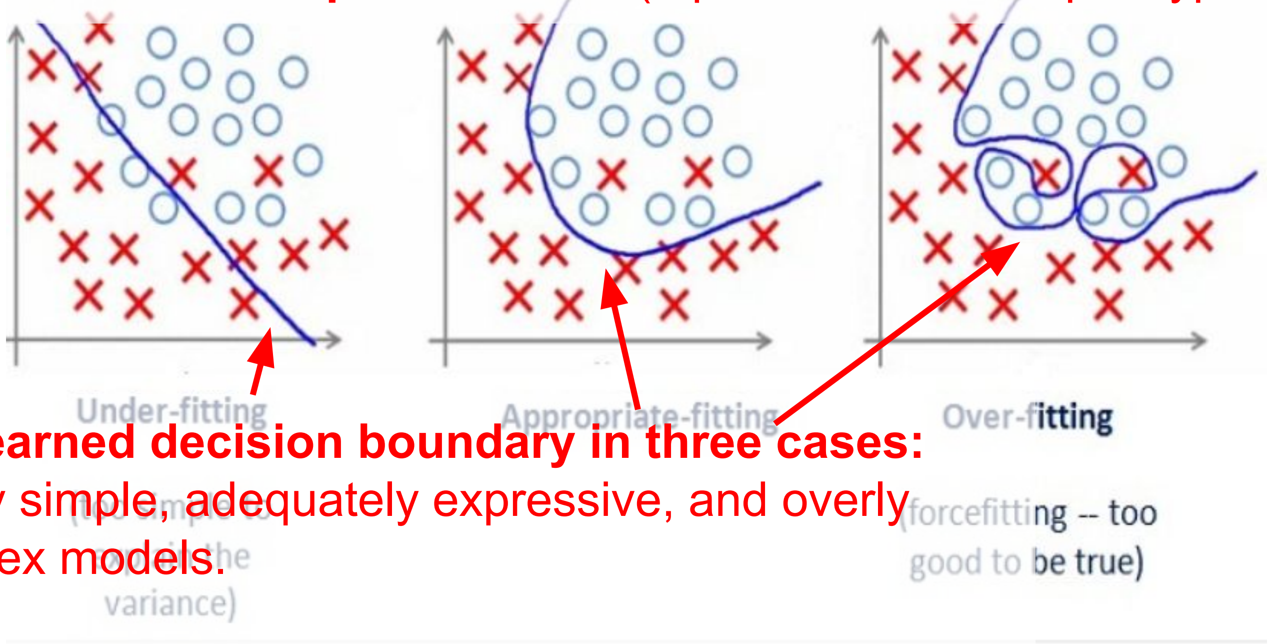


Image source: Andrew Ng Machine learning video series

# Under- and overfitting in case of classification

**Classification with two input variables** (top view of the sample/hypothesis graph)

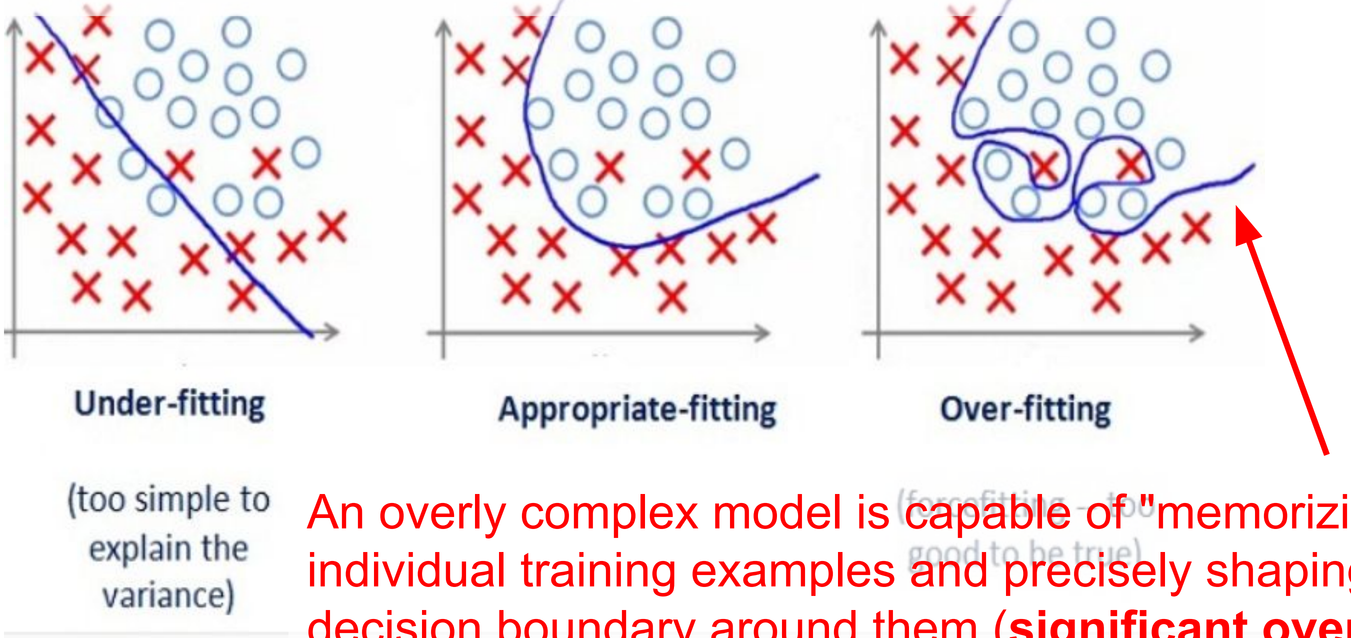



**The learned decision boundary in three cases:**
Overly simple, adequately expressive, and overly complex models.

Image source: Andrew Ng Machine learning video series

# Under- and overfitting in case of classification

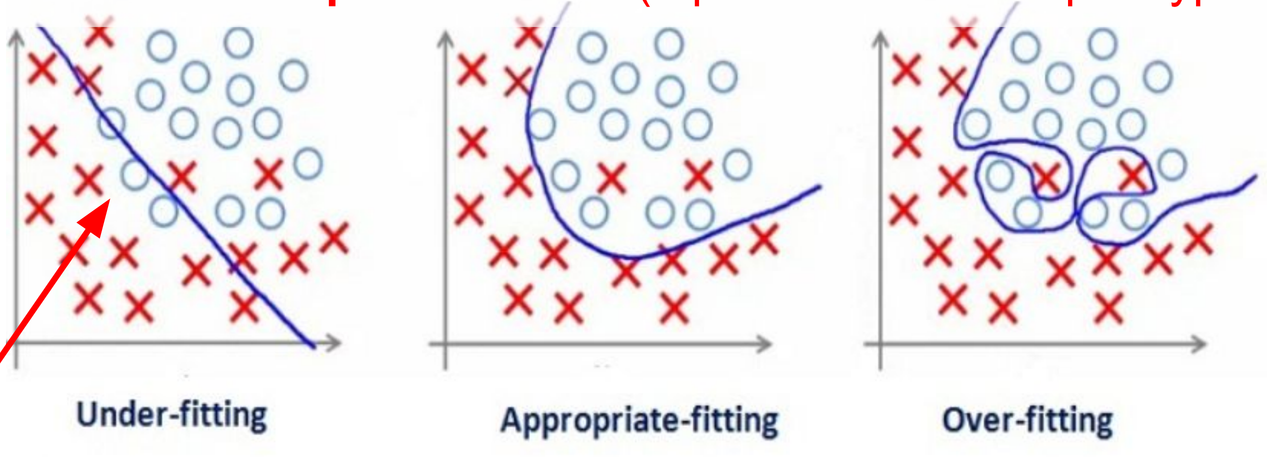
**Classification with two input variables** (top view of the sample/hypothesis graph)




An overly complex model is capable of "memorizing" individual training examples and precisely shaping the decision boundary around them (**significant overfitting**).

# Under- and overfitting in case of classification

**Classification with two input variables** (top view of the sample/hypothesis graph)




**Logistic regression learns a linear decision surface,**
thus overfitting is not expected
(unless the training set size is minimal).

Image source: sastanin @ Stack Exchange

# Overfitting in deep neural networks

**Example:** Categorizing photos

If the deep network is powerful enough and has enough learnable parameters, it may learn the task in an undesirable way.

Image source: sastanin @ Stack Exchange

# Overfitting in deep neural networks

**Example:** Categorizing photos

If the deep network is powerful enough and has enough learnable parameters, it may learn the task in an undesirable way.

For example, **it "memorizes" every single image in the training set** with a specific pattern.
...even a unique JPEG compression artifact!

# Avoiding underfitting and overfitting

Our goal is to ensure that our model does not underfit or overfit. Instead, we want to find the "just right" model!

**How can we avoid underfitting and overfitting?**

# Avoiding underfitting and overfitting

Our goal is to ensure that our model does not underfit or overfit.
Instead, we want to find the "just right" model!

**How can we avoid underfitting and overfitting?**

Whether under- or overfit, the trained model will perform poorly when we try to estimate labels for new, unlabeled examples that were not seen during training
— therefore, **we want to avoid these phenomena**.

# How to deal with **underfitting**?

**Underfitting:** The complexity of our model is too low to accurately approximate the labels from the input. The task is too difficult.

**Solution:** A more complex model is needed to reduce estimation error.

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**Example:** We can try to use linear regression for complex tasks, such as estimating the age of celebrities from photographs. However, the model is **severely underfitted**, as linear regression can only produce age estimates from a linear combination of pixel brightness, which is not a good approach for age estimation. A more complex model, such as a convolutional neural network, may be more suitable for the task.

# How to deal with **overfitting**?

**Overfitting:** The model is complex enough to accurately learn the specifics of individual elements of the training set, losing its ability to generalize.
**The overfitted model performs poorly on the test set.**

**How to deal with it?**

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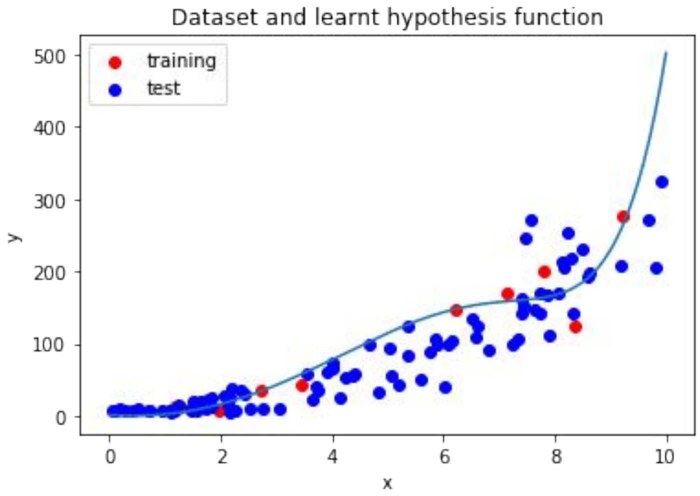
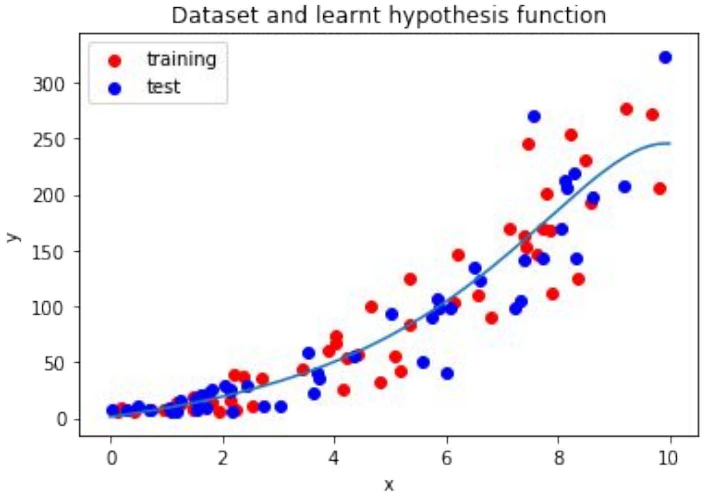
**Obtain more training data!**

$$h_\theta(x) = \theta_0 + \theta_1 x + \cdots + \theta_9 x^9$$




$|X_{train}| = 10$

J_train ≈ 250
J_test ≈ 800

$|X_{train}| = 50$

J_train ≈ 400
J_test ≈ 400

# How to deal with **overfitting**?

**Obtain more training data!**

**Problem:** Typically, we have no access to enough labeled training data to prevent overfitting in a deep neural network with hundreds of millions of parameters.

**We need alternative methods...**

# How to deal with **overfitting**?

**Overfitting:** The model is complex enough to accurately learn the specifics of individual elements of the training set, losing its ability to generalize.
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**Solutions:**

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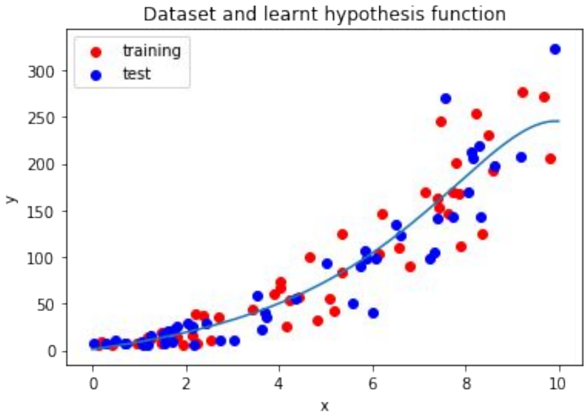
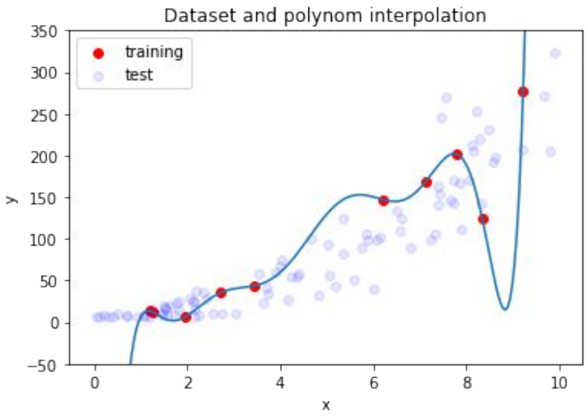
- Obtain more training data!
- Regularization methods (e.g., L2 regularization)

# How to deal with **overfitting**?

**Observation:** When fitting higher-degree polynomials, the **coefficients** (the **θ** parameters) typically **increase** as the fit becomes more and more accurate.




**θ** = [1., 7.46, 0.82, 0.06, 0.005, 0.0004, 0., 0., 0., 0., 0.]

**θ** = [[-2229., 7234., -9545., 6756., -2843., 743., -121., 12.05, -0.66, 0.015]

# How to deal with **overfitting**?

**Observation:** When fitting higher-degree polynomials, the **coefficients** (the **θ** parameters) typically **increase** as the fit becomes more and more accurate.

**Penalizing large coefficients** (parameters) **can help!**

**How?**

# How to deal with **overfitting**?

**Observation:** When fitting higher-degree polynomials, the **coefficients** (the **θ** parameters) typically **increase** as the fit becomes more and more accurate.

**Let's include a penalty in the loss function:**

**Pl.:** $$h_\theta(x) = \theta_0 + \theta_1 x + \cdots + \theta_9 x^9$$

$$J(\theta) = \frac{1}{2m}\sum_{j=1}^{m}(h(x)^{(j)} - y^{(j)})^2 + \boxed{\lambda \sum_{i=1}^{n} \theta_i^2}$$

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**MSE loss:** Penalizing the label estimation error

$$J(\theta) = \frac{1}{2m} \sum_{j=1}^{m} (h(x)^{(j)} - y^{(j)})^2 + \lambda \sum_{i=1}^{n} \theta_i^2$$

**L2-regularization term:** Penalizing large parameters

**When λ = 0:** The original model without regularization

**When λ is too high:** It is easier to minimize the loss by learning all zero parameters instead of solving the task…

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The **bias** parameter ($\theta_0$) **is not penalized.**

# How to deal with **overfitting**?

**L2 regularization:**

$$h_\theta(x) = \theta_0 + \theta_1 x + \cdots + \theta_9 x^9$$

$$|X_{train}| = 10$$

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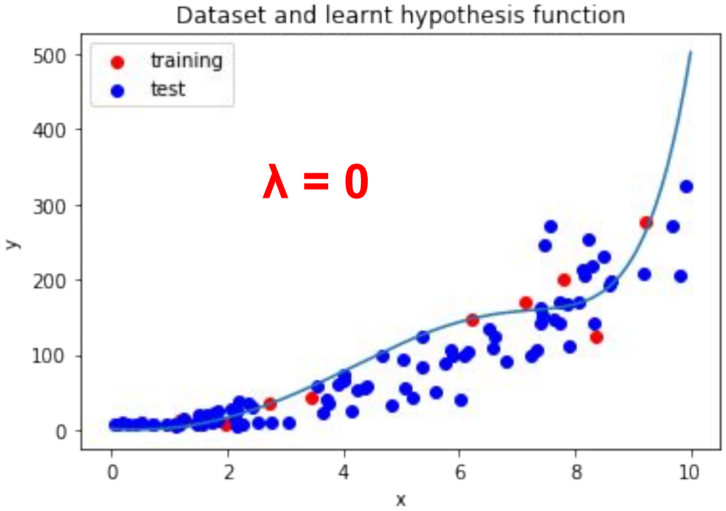


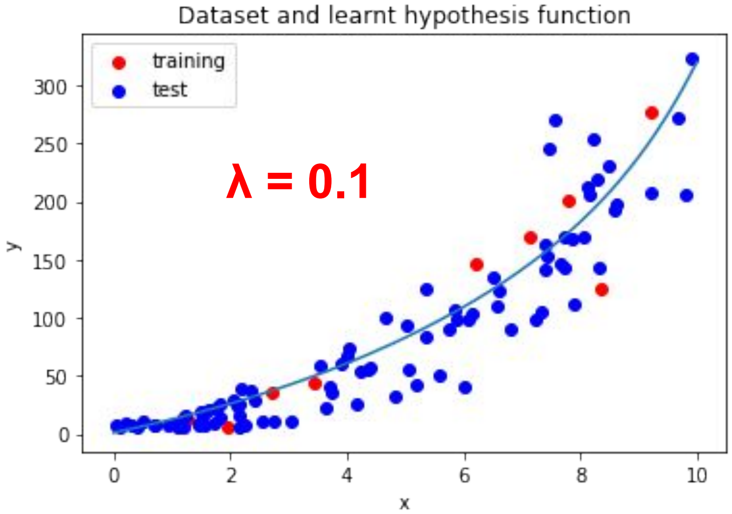

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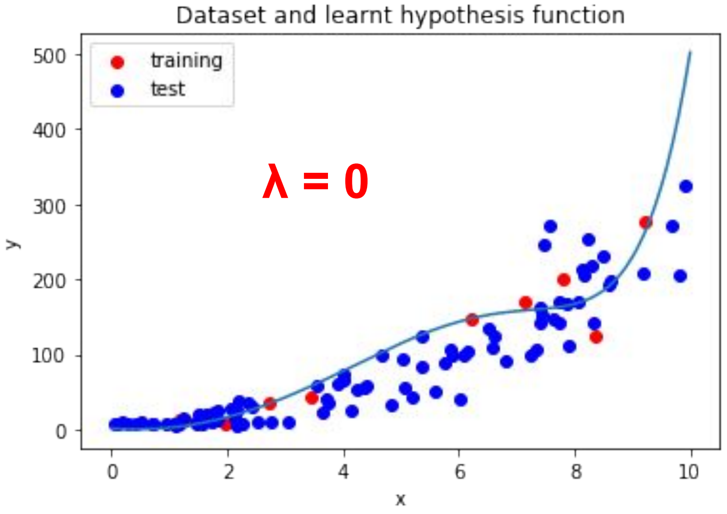
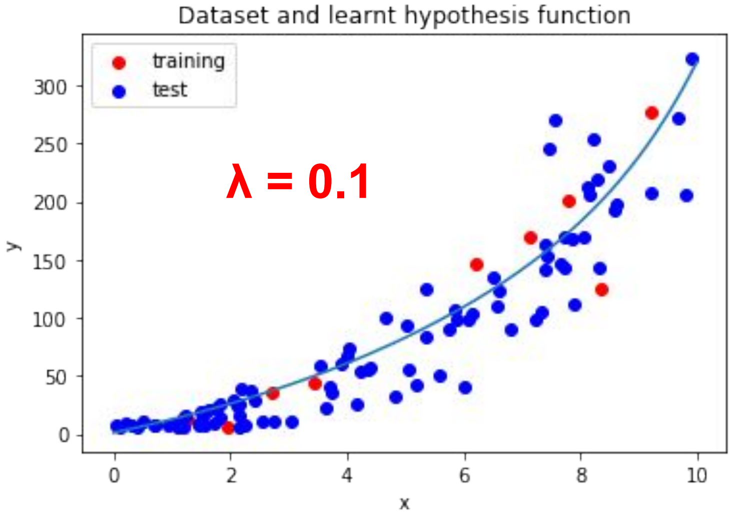
**Can also help when training data is scarce.**



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**L2 regularization:**

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**L2 regularization is not only effective for polynomial regression.**

Experience shows that, in general, weights (parameters) also increase in the case of neural networks when overfitting occurs.

**L2 regularization is just one example.** There are many types of regularization methods that reduce overfitting by applying some kind of constraint during learning.

# How to deal with **overfitting**?

**Overfitting:** The model is complex enough to accurately learn the specifics of individual elements of the training set, losing its ability to generalize.
**The overfitted model performs poorly on the test set.**

**Solutions:**

- Use a simpler model (e.g., fewer parameters)!
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- Regularization methods (e.g., L2 regularization)
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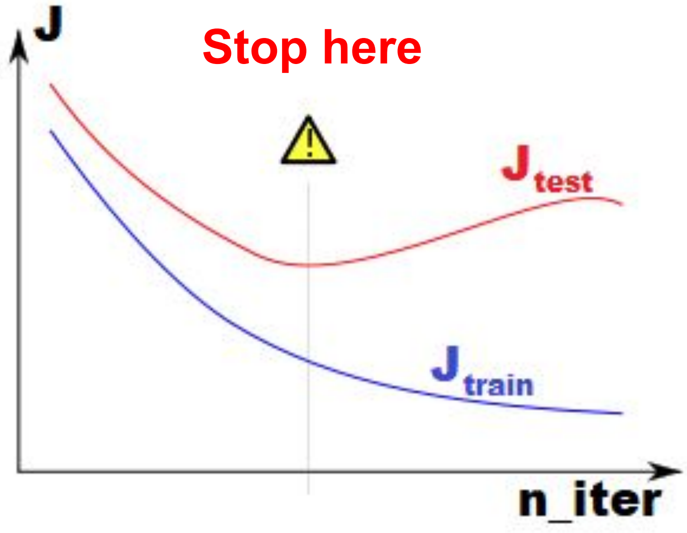
# How to deal with **overfitting**?

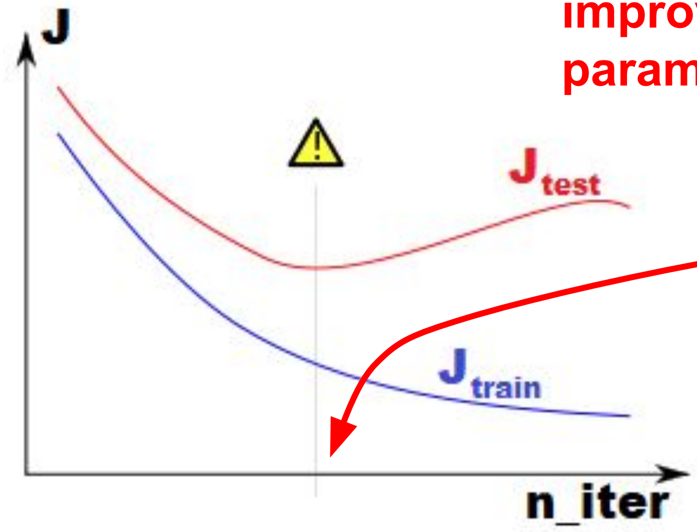
**Early stopping:** Overfitting often inevitably occurs after a certain number of iterations when training deep neural networks. **Early stopping** is generally an effective solution.



# How to deal with **overfitting**?

**Early stopping:** Overfitting often inevitably occurs after a certain number of iterations when training deep neural networks. **Early stopping** is generally an effective solution.

**Stop training if $J_{test}$ does not improve anymore and use the parameters from <u>this state</u>**



# How to deal with **overfitting**?

**Early stopping:**

**New loop condition:** Loop, while $J_{test}$ keeps reducing.

~~repeat until convergence~~ {

  for i ← 1 . . . n {

    $grad_i = \frac{\partial}{\partial \theta_i} J(\theta)$

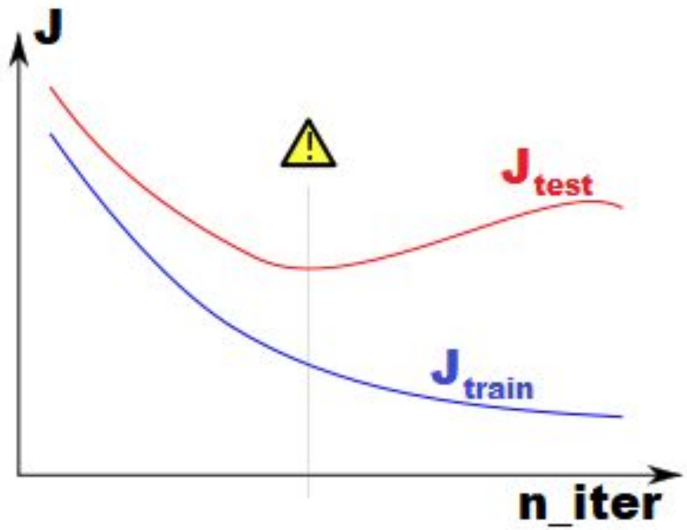
  }

  for i ← 1 . . . n {

    $\theta_i = \theta_i - \alpha \, grad_i$

  }

}



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$$\}$$

$\}$

(We should be **patient** for a while and not stop on the first sign of a plateauing test loss!)

# How to deal with **overfitting**?

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~~repeat until convergence~~ {

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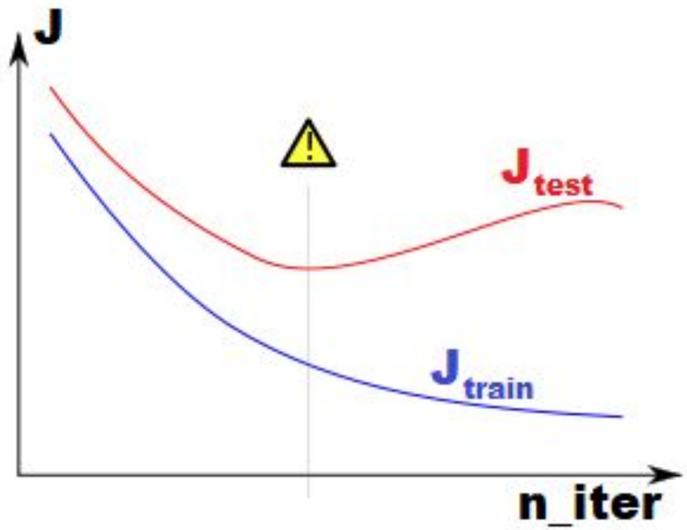
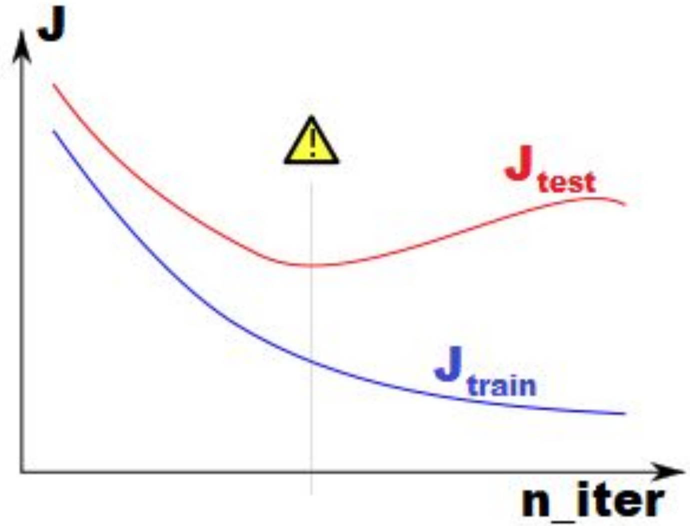



**Can we see the problem with this technique?**

# Early stopping

We stated that we should not train the model using the test set.

**What is actually happening?**

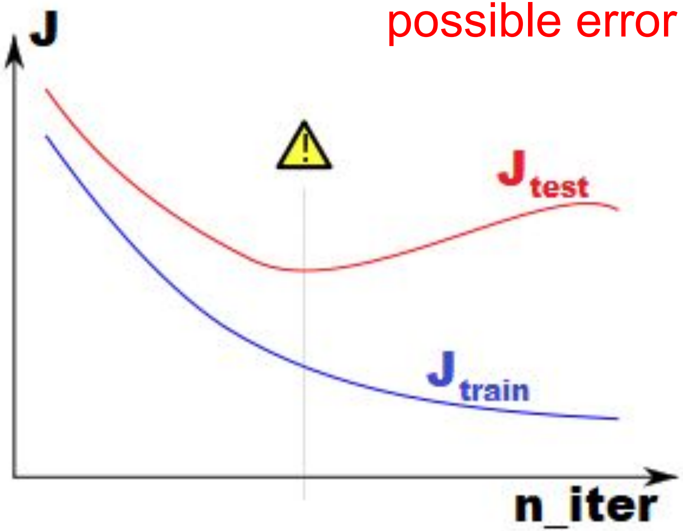


# Early stopping

We stated that we should not train the model using the test set.

**What is actually happening?**

**We adjust the model to the test set,** as we stop training when we have presumably achieved the smallest possible error on the test set.




**This is cheating…**

# Splitting the sample

**New approach:**

Training set, **validation set,** test set

For example, 50%, 25%, 25% of the sample

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**New approach:**

Training set, **validation set,** test set

For example, 50%, 25%, 25% of the sample

**In critical applications,** proportions can change, e.g., 20%, 10%, 70%.
We expect the test set to enable us to estimate the future performance of the trained model as accurately as possible, based on data that was unseen during training.

# Validation set, hyperparameters

**We will use the validation set to optimize the following parameters:**

- *Learning rate (alpha)*
- *Polynomial degree, or neural network architecture (layers, number of neurons, etc.)*
- *Number of iterations for the gradient method (early stopping)*
- *...*

**Such parameters are called hyperparameters.**

**We will use the validation set to find optimal hyperparameters.**

# Hyperparameters

**Finding the model with the lowest errors thus consists of two optimization tasks.**

Until now: $\theta^* = argmin_\theta \; J(\theta)$

From now: $\psi^*, \theta^* = argmin_\psi \; argmin_\theta \; J_\psi(\theta)$

**ψ*:** Optimal hyperparameters

**ψ:** hyperparameters

# Model training procedure

**The task:** $\psi^*, \theta^* = argmin_{\psi}\ argmin_{\theta}\ J_{\psi}(\theta)$

1) Select a new hyperparameter configuration **Ψ**.
2) Optimize the model parameters (**θ**) on the **training set** with gradient descent.
3) Evaluate the trained model on the **validation set**, then GOTO 1

**Finally:**

- **Ψ*** := The hyperparameter configuration with the best performance on the validation set.
- **θ*** := The trained model parameters with hyperparameters **Ψ***.
- Evaluate model with parameters **θ*** and hyperparameters **Ψ*** on the **test set.**

# Optimizing hyperparameters

**Gradient descent cannot generally be used for this purpose**
(It is not always possible to specify a differentiable loss function w.r.t. hyperparameters).

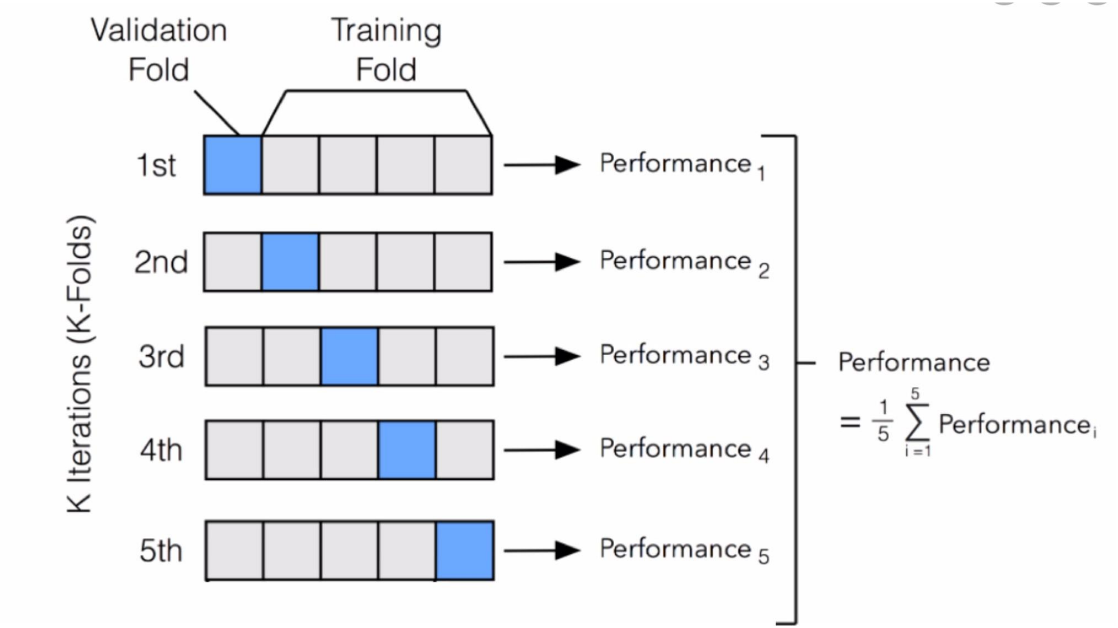
**Common techniques:**

- Manual trial and error
- Grid search
- Random search
- Bayesian optimization
- Evolutionary/genetic algorithms
- ...

Image source: https://medium.com/analytics-vidhya/

# Selecting the validation set

## Cross validation



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# Selecting the validation set

## Cross validation

A popular technique for evaluating hyperparameters. It is most useful **when we have little data available** for training/validation.

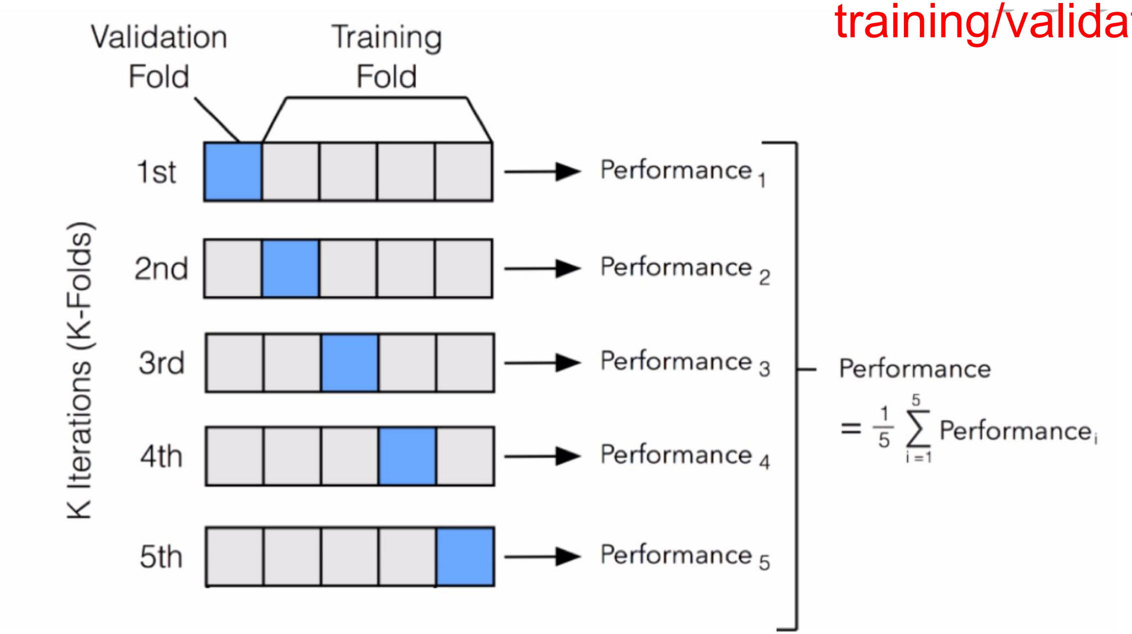
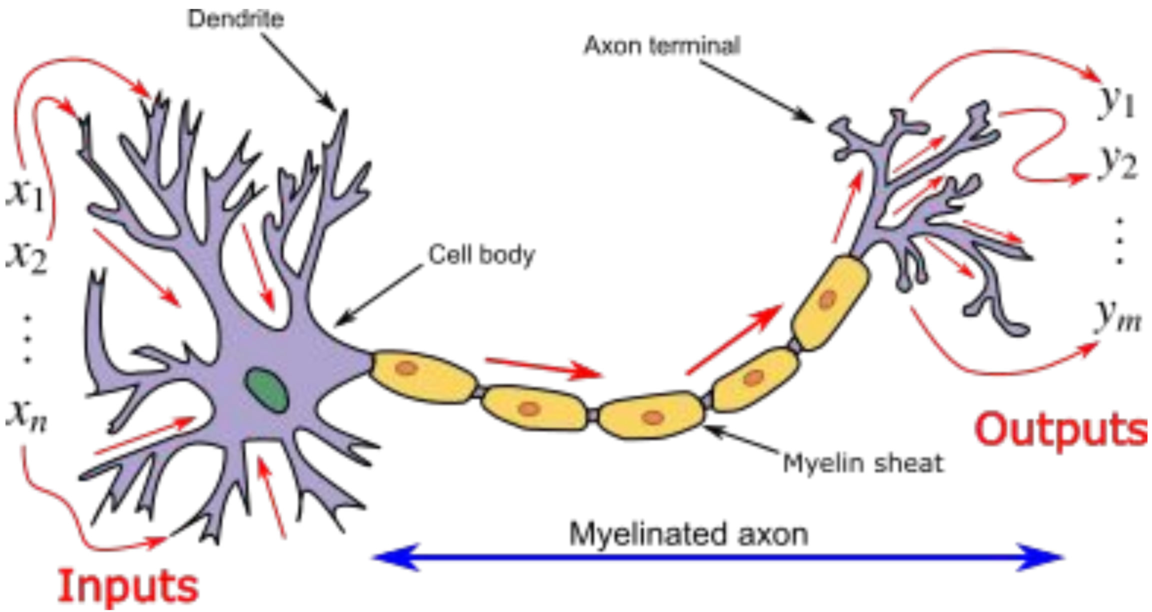


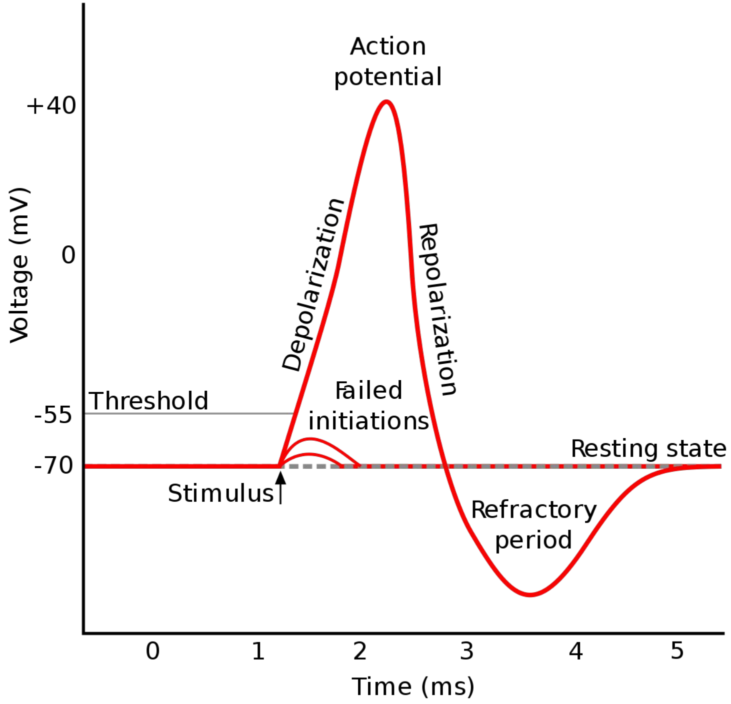
Image source: Egm4313.s12 at English Wikipedia

# The biological neuron model



# The functioning of biological neurons simplified

## The functioning of brain cells



# The functioning of biological neurons simplified

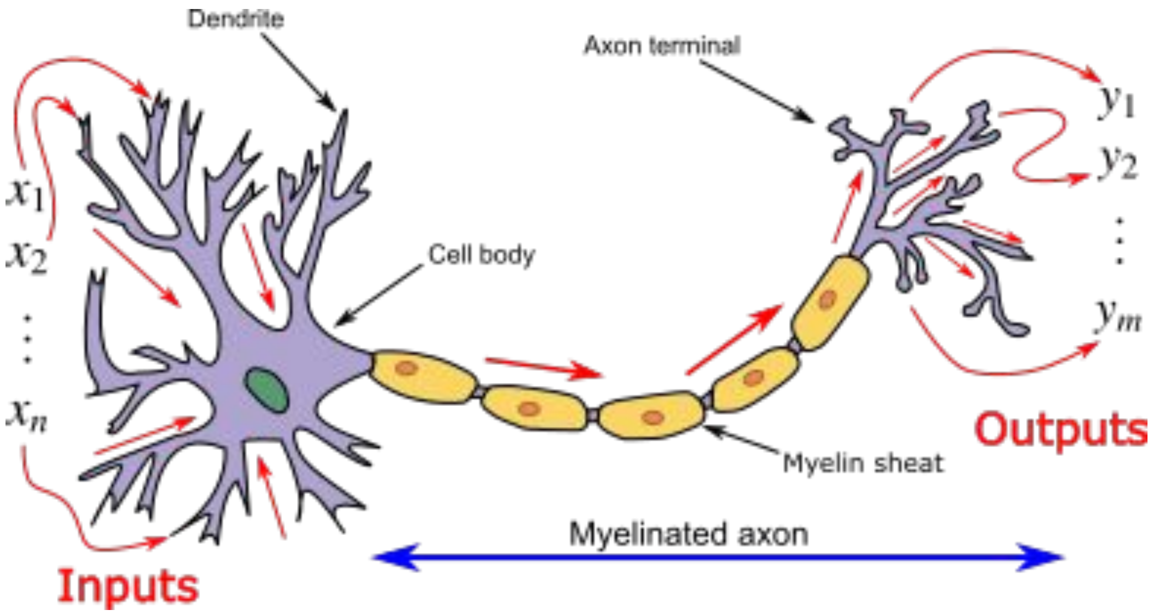
## The functioning of brain cells

- **Membrane potential:** The voltage difference between the inner and outer walls of the cell
- **In the absence of input**, the membrane potential **continuously decreases** to a resting level.
- The membrane potential **increases in response to input.**
- **Inputs** arriving at different branches (dendrites) are amplified or attenuated (can also be negative) with **different weights**.
- When the membrane potential **reaches a threshold** (specific to each neuron), the neuron **“fires”** and charge passes through the output.

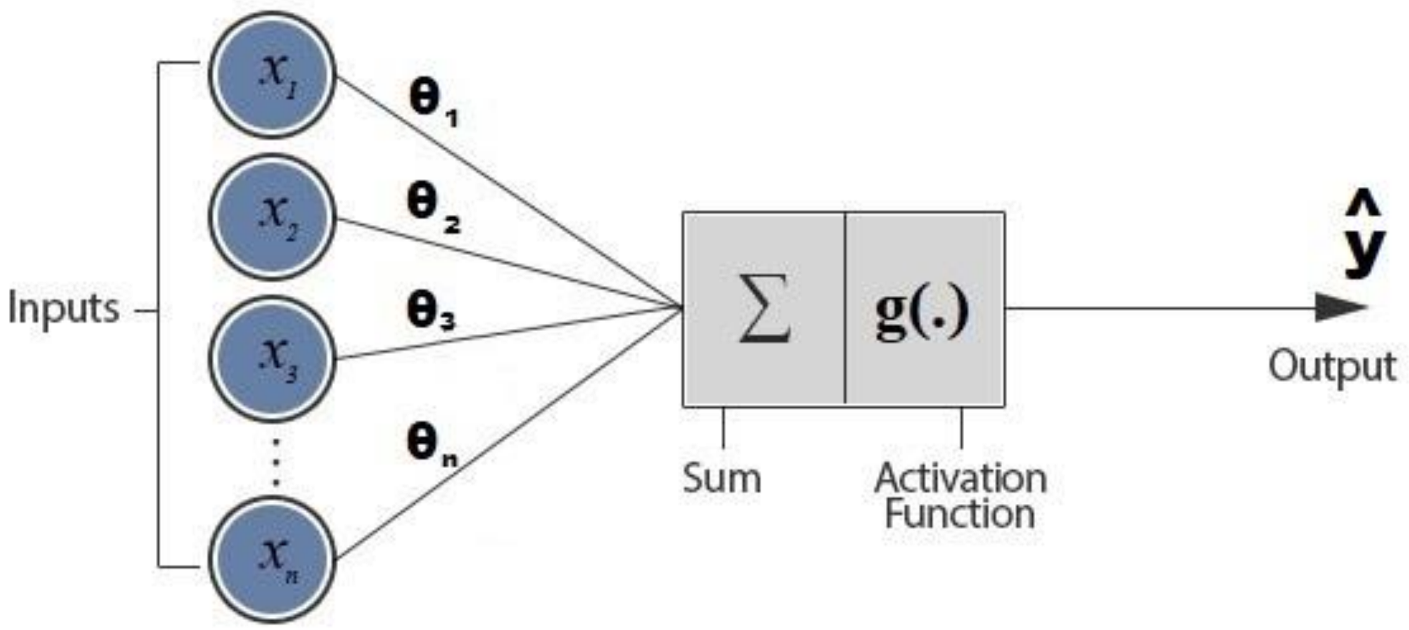
Image source: Egm4313.s12 at English Wikipedia

# The biological neuron model

**What does its functioning resemble?**



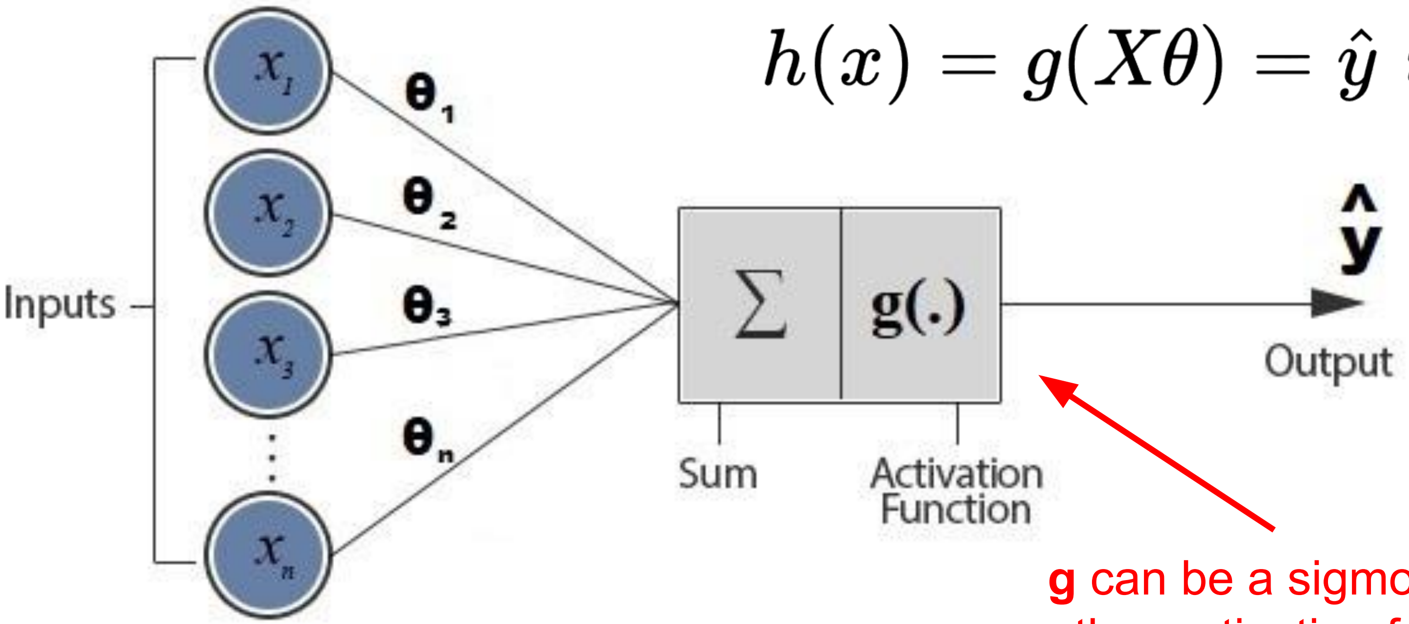
# The artificial neuron model (Rosenblatt, 1958)




The simplified, discretized model of a biological neuron. **What does it resemble?**

# The artificial neuron model (Rosenblatt, 1958)

$$h(x) = g(X\theta) = \hat{y} \approx y$$

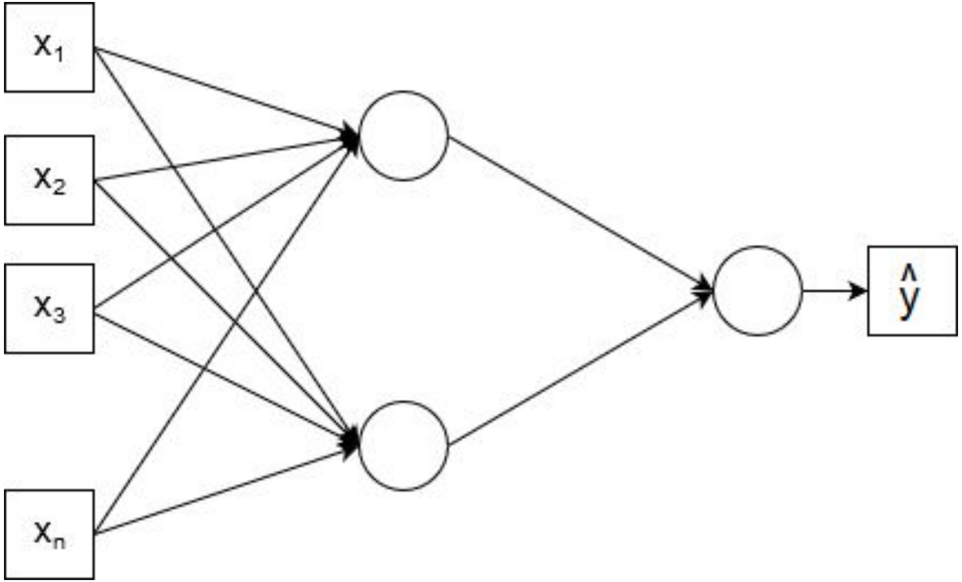



**g** can be a sigmoid or other activation functions

**An artificial neuron is a** (multivariate) **logistic regression if g is sigmoid!**

# Building blocks of neural networks

**Artificial neurons are the building blocks of one of the basic types of artificial neural networks** (the Multilayer Perceptron, MLP).



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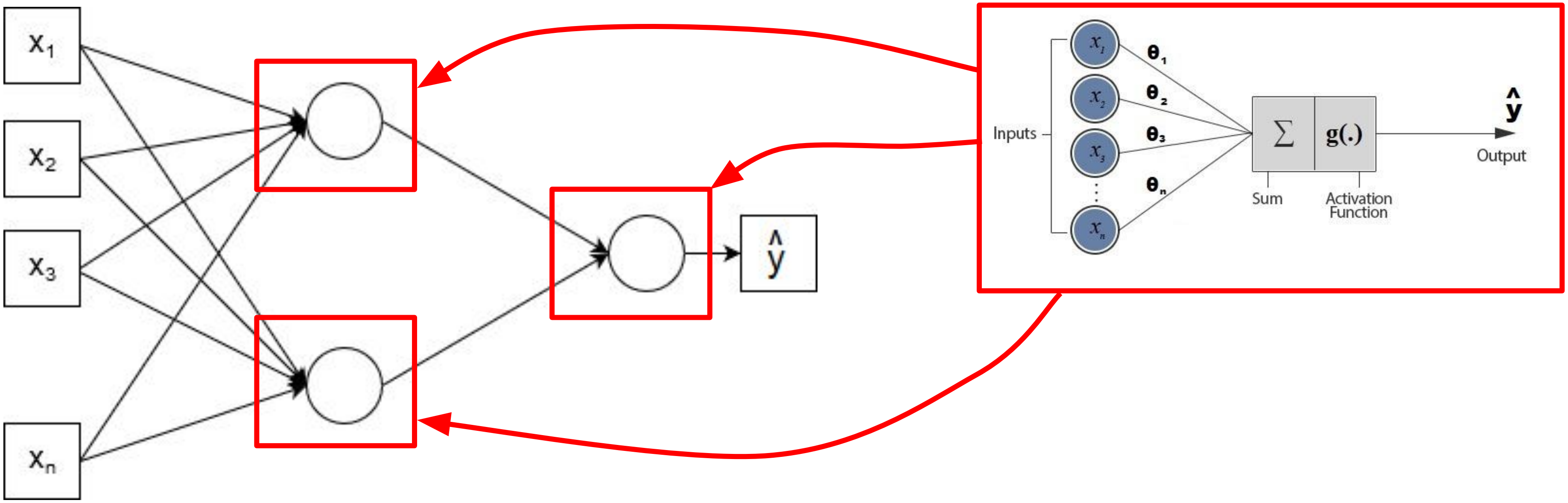
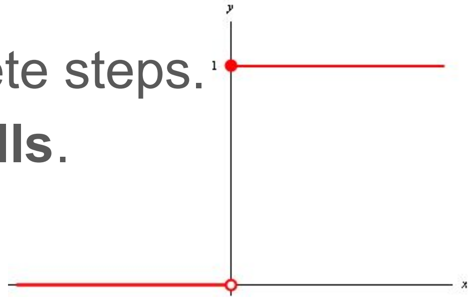


# The functioning of biological neurons simplified

**Differences from the artificial neuron model:**

- Continuous signal in the nerve cell instead of discrete steps.
  → **Sum in artificial neurons, integral in nerve cells**.



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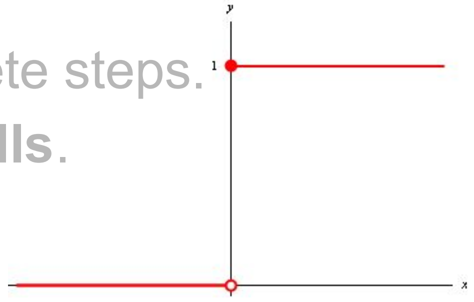
  → **In an artificial neuron, continuous, a differentiable nonlinearity is required.**




(and the derivative should not be zero everywhere…)

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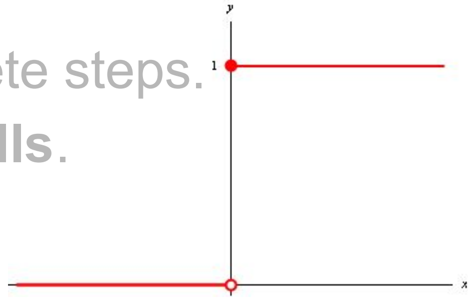


- The weight of a nerve cell is either always negative or always positive; the sign does not change (excitor vs. inhibitor)
  → **In an artificial neuron, the sign of the weight can change.**

# Summary

**May be included in tests / exam:**

- Identifying and handling of under- and overfitting, hyperparameters, validation set
- Artificial neural network model

**Will not be included in tests / exam:**

- Polynomial regression
- Polynomial interpolation
- The biological neuron model and differences from the artificial model