UNIVERSITY OF TECHNOLOGY
IN THE EUROPEAN CAPITAL OF CULTURE
CHEMNITZ

Neurocomputing

Linear regression

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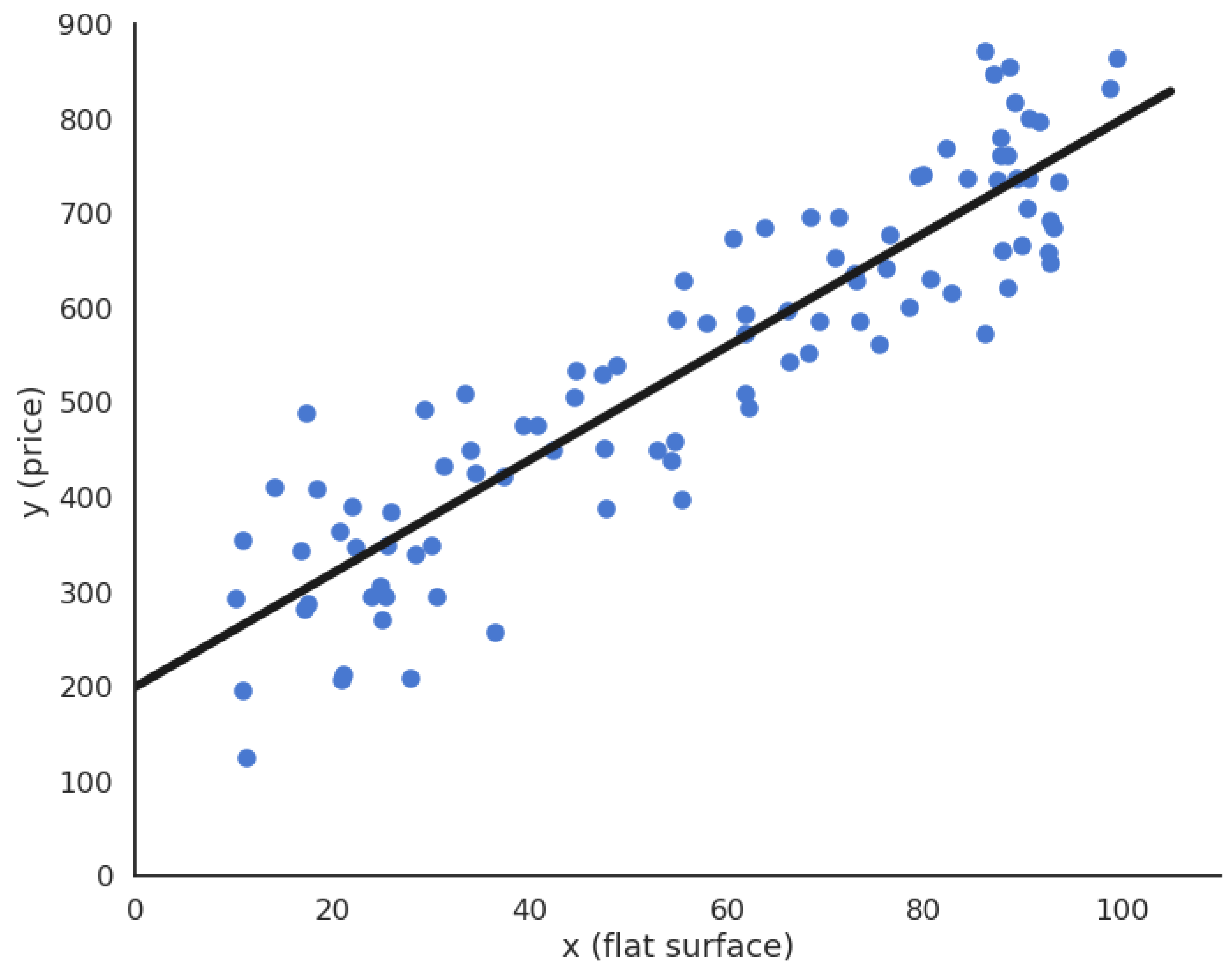
1 - Linear regression

Linear regression

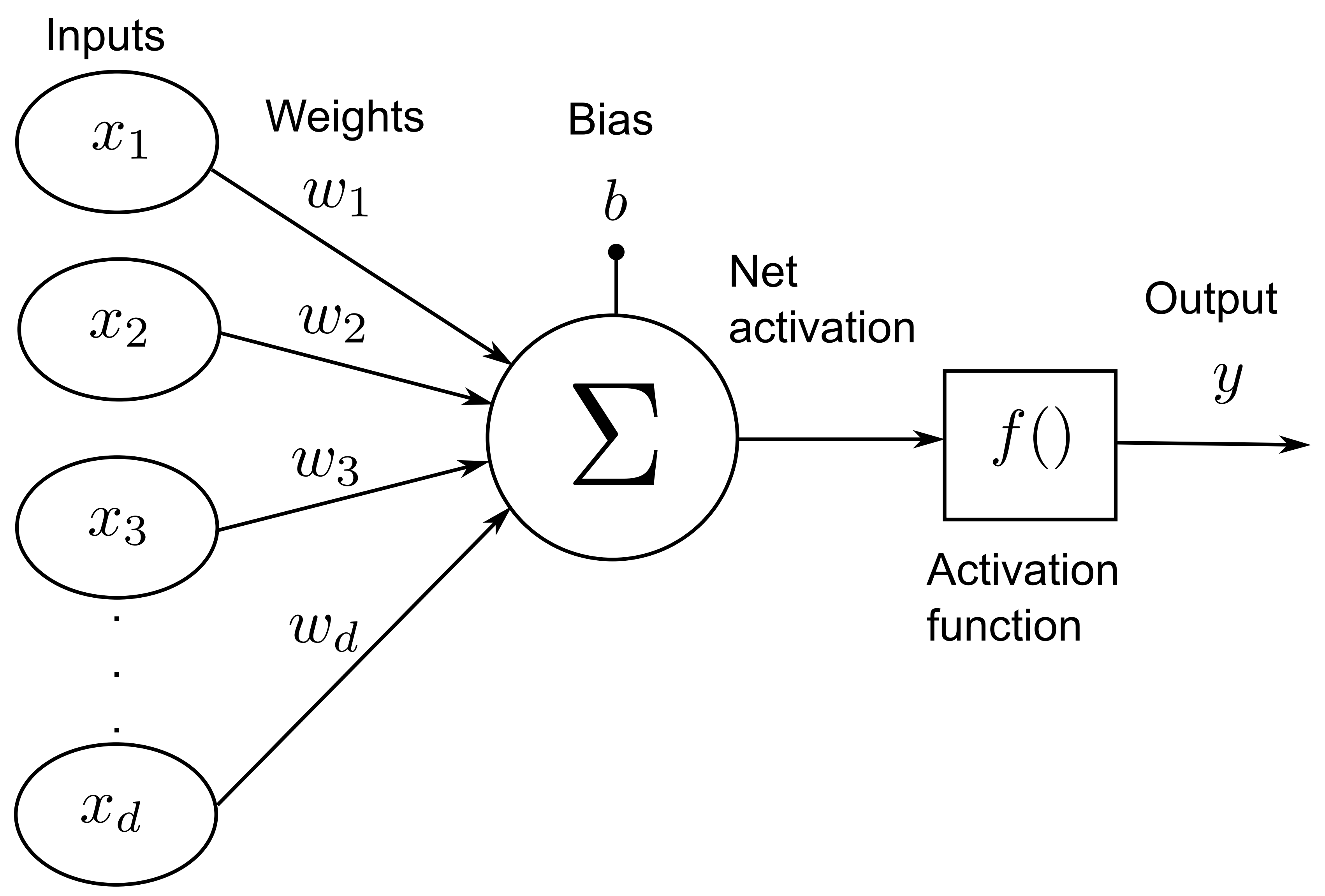


- We have a training set of N examples $\mathcal{D} = (x_i, t_i)_{i=1..N}$.
- In **linear regression**, we want to learn a linear model (hypothesis) y that is linearly dependent on the input x:

$$y = f_{w,b}(x) = w \, x + b$$

- The **free parameters** of the model are
  - the slope w,
  - the intercept b.
- The data $\mathcal{D} = (x_i, t_i)_{i=1..N}$ is given (fixed).

Linear regression



- Mathematical model:

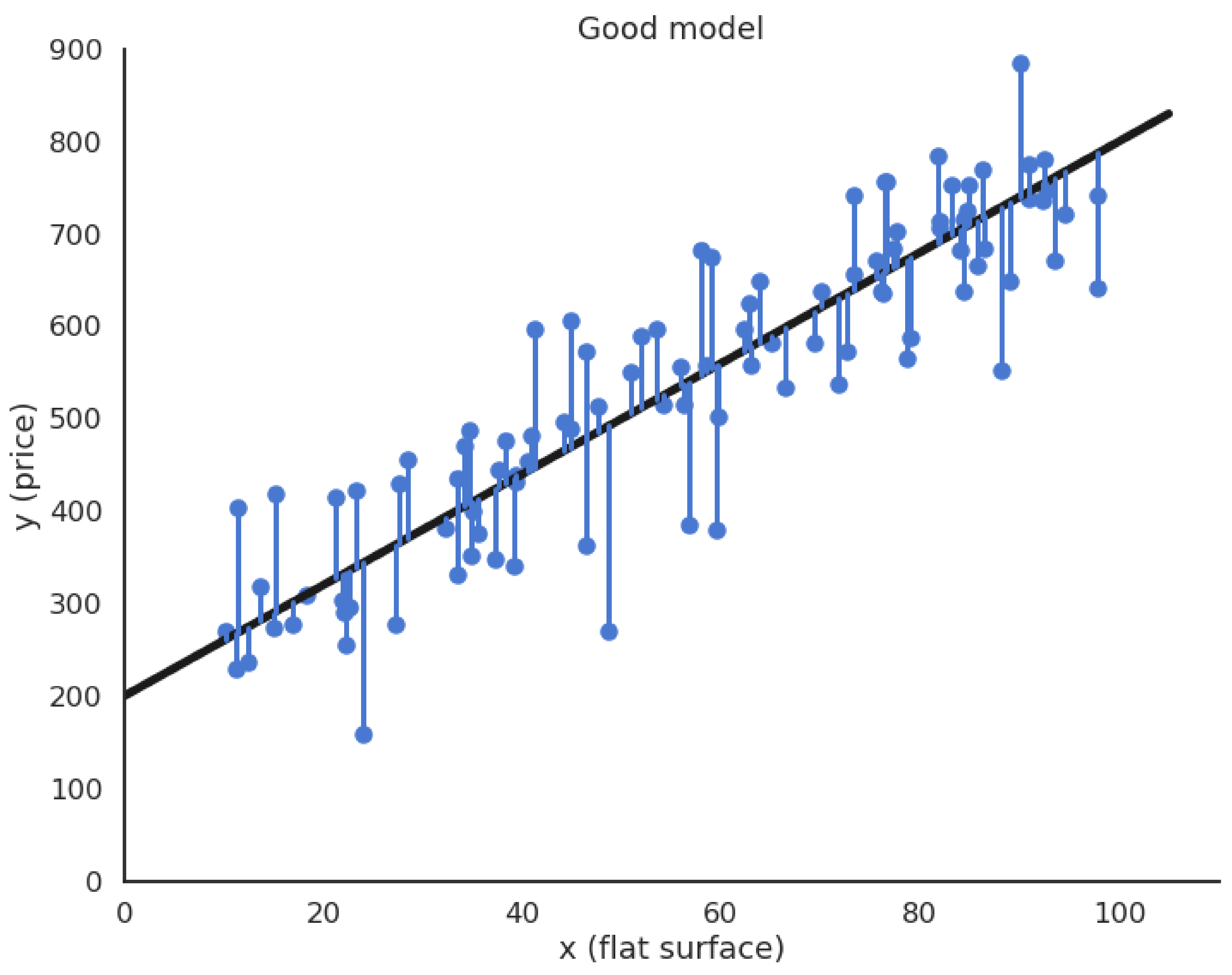
$$y = f_{w,b}(x) = w\,x + b$$

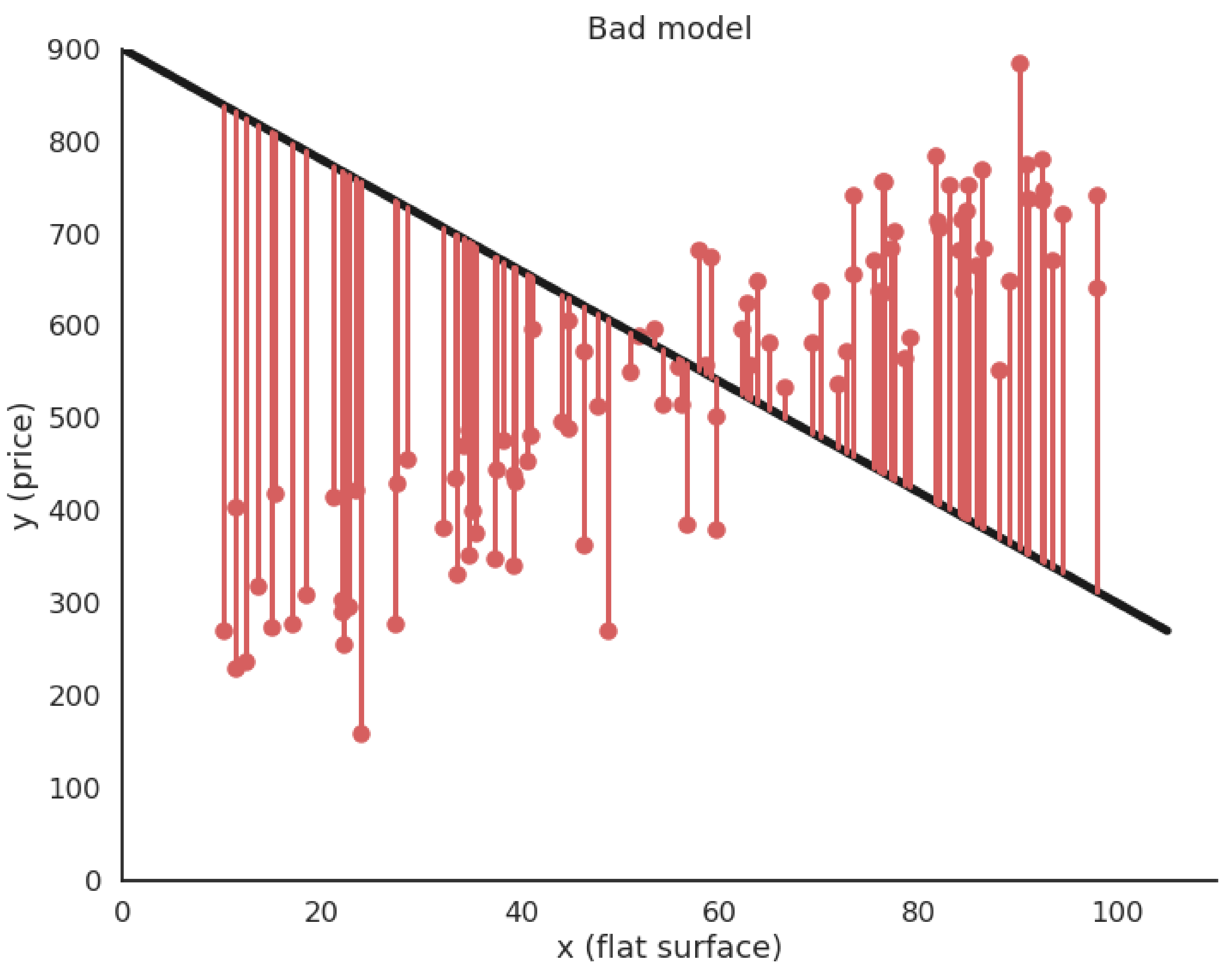
- This corresponds to a single artificial neuron y with:
  - one input x,
  - one weight w,
  - one bias b,
  - a **linear** activation function.
- We will see that this generalizes to multiple inputs and outputs.

Linear regression

- The goal of the linear regression (or least mean squares - LMS) is to minimize the **mean square error** (mse) between the targets and the predictions.
- It is defined as the mathematical expectation of the quadratic error over the training data:

$$\mathcal{L}(w, b) = \mathbb{E}_{x_i, t_i \in \mathcal{D}} [(t_i - y_i)^2]$$

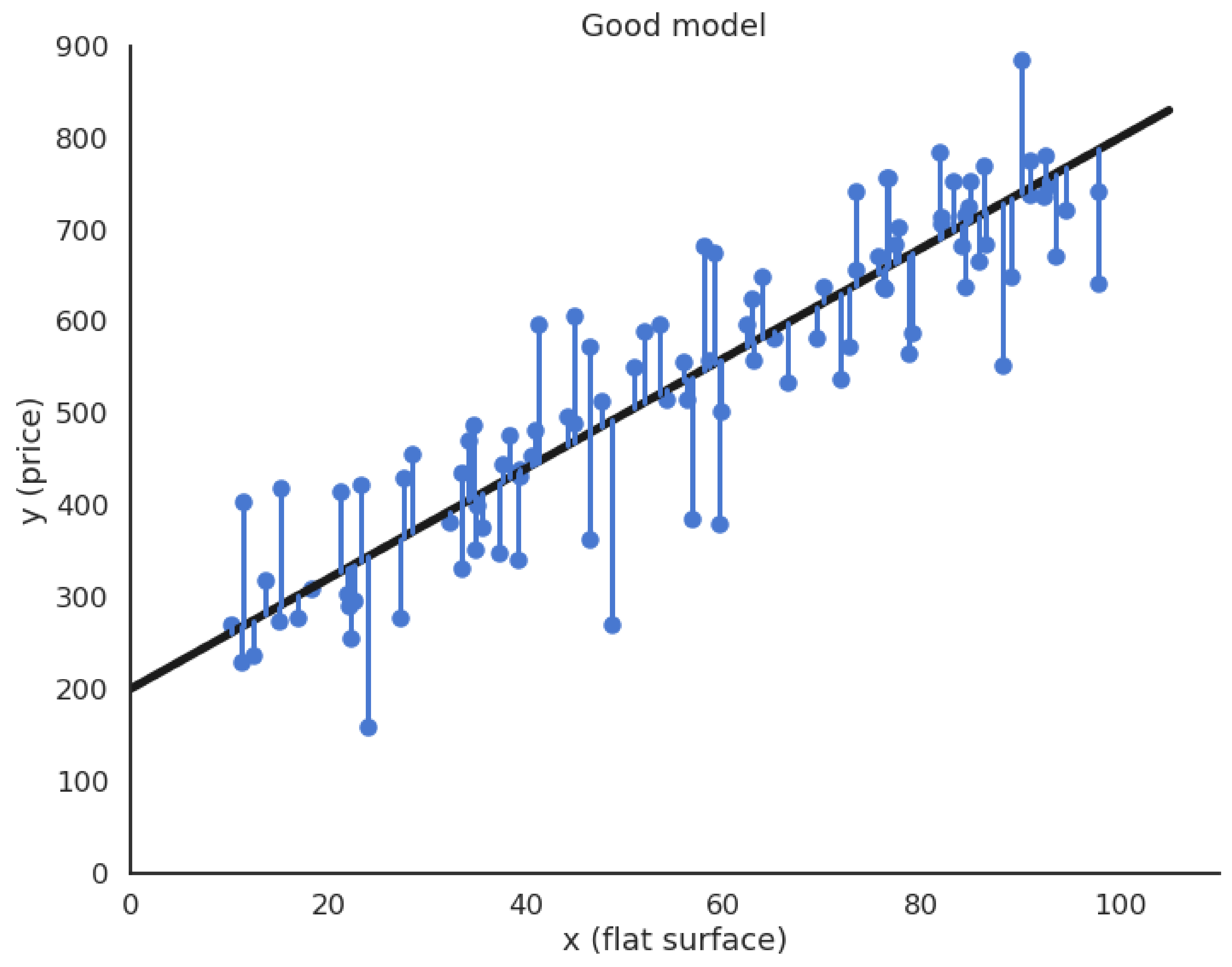


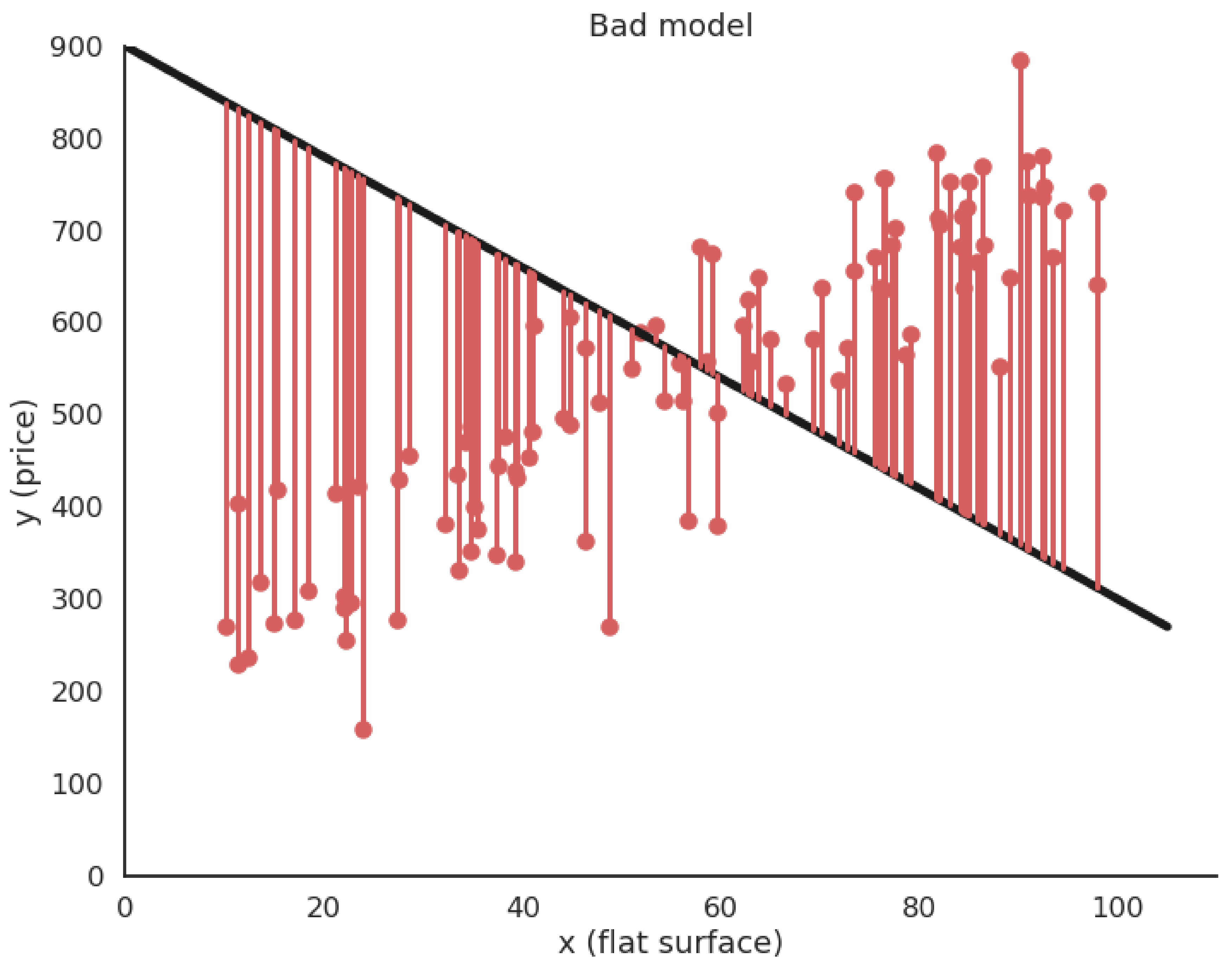


Linear regression

- As the training set is finite and the samples i.i.d (independent and identically distributed), we can simply replace the expectation by a sampling average:

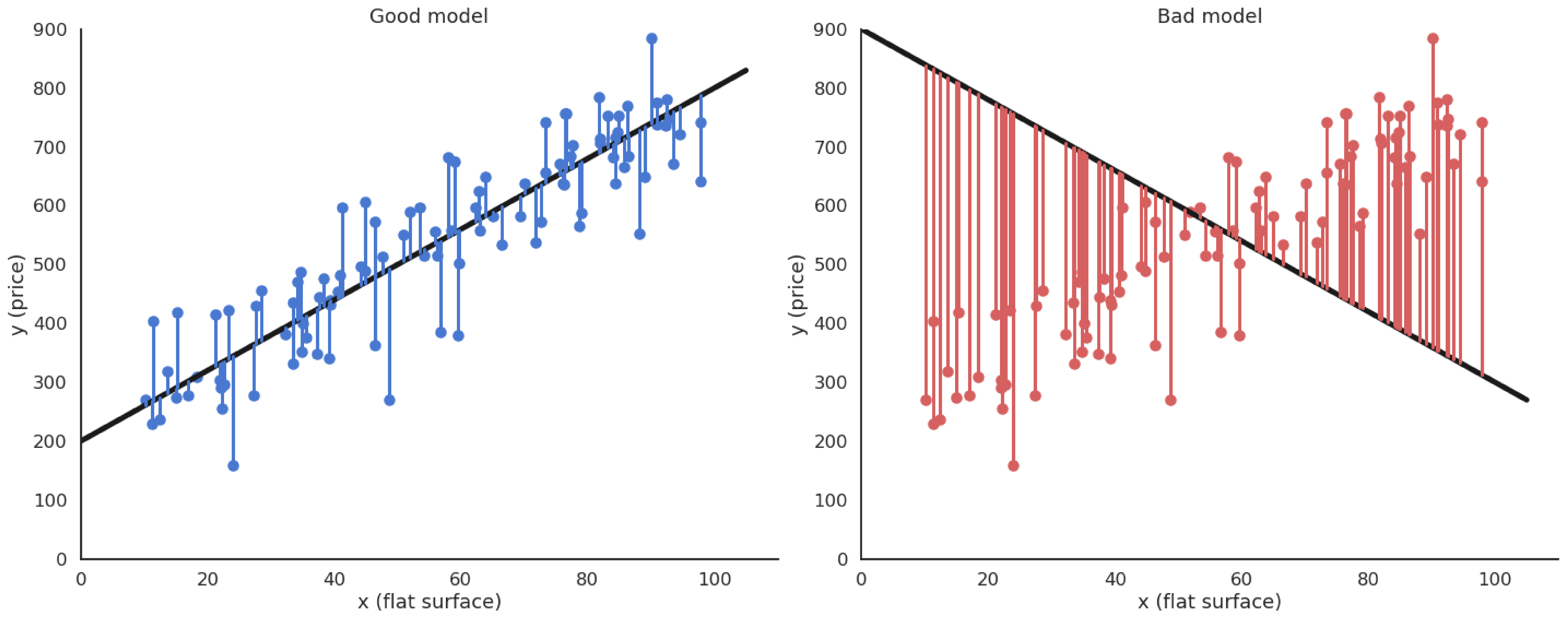
$$\mathcal{L}(w, b) = \frac{1}{N} \sum_{i=1}^{N} (t_i - y_i)^2$$





Linear regression

- The minimum of the mse is achieved when the **prediction** $y_i = f_{w,b}(x_i)$ is equal to the **ground truth** t_i for all training examples.
- In other words, we want to minimize the **residual error** of the model on the data.
- It is not always possible to obtain the global minimum (0) but the closer, the better.



Gradient descent for linear regression

- We search for w and b which minimize the mean square error:

$$\mathcal{L}(w, b) = \frac{1}{N} \sum_{i=1}^{N} (t_i - y_i)^2$$

- We will apply *gradient descent* to iteratively modify estimates of w and b:

$$\Delta w = -\eta \, \frac{\partial \mathcal{L}(w, b)}{\partial w}$$

$$\Delta b = -\eta \, \frac{\partial \mathcal{L}(w, b)}{\partial b}$$

Gradient descent for linear regression

- Let's search for the partial derivative (gradient) of the quadratic error with respect to w:

$$\frac{\partial \mathcal{L}(w, b)}{\partial w} = \frac{\partial}{\partial w} [\frac{1}{N} \sum_{i=1}^{N} (t_i - y_i)^2]$$

- Partial derivatives are linear, so the derivative of a sum is the sum of the derivatives:

$$\frac{\partial \mathcal{L}(w, b)}{\partial w} = \frac{1}{N} \sum_{i=1}^{N} \frac{\partial}{\partial w} (t_i - y_i)^2$$

- This means we can compute a gradient for each training example instead of for the whole training set (see later the distinction batch/online):

$$\frac{\partial \mathcal{L}(w, b)}{\partial w} = \frac{1}{N} \sum_{i=1}^{N} \frac{\partial}{\partial w} l_i(w, b) \qquad \text{with} \qquad l_i(w, b) = (t_i - y_i)^2$$

Gradient descent for linear regression

- The individual loss $l_i(w, b) = (t_i - y_i)^2$ is the composition of two functions:
    - a square error function $g_i(y_i) = (t_i - y_i)^2$.
    - the prediction $y_i = f_{w,b}(x_i) = w \, x_i + b$.
- The **chain rule** tells us how to derive such composite functions:

$$\frac{d f(g(x))}{dx} = \frac{d f(g(x))}{d g(x)} \times \frac{d g(x)}{dx} = \frac{d f(y)}{dy} \times \frac{d g(x)}{dx}$$

- The first derivative considers $g(x)$ to be a single variable.
- Applied to our problem, this gives:

$$\frac{\partial}{\partial w} l_i(w, b) = \frac{\partial g_i(y_i)}{\partial y_i} \times \frac{\partial y_i}{\partial w}$$

Gradient descent for linear regression

- The square error function $g_i(y) = (t_i - y)^2$ is easy to differentiate w.r.t y:

$$\frac{\partial g_i(y_i)}{\partial y_i} = -2\,(t_i - y_i)$$

- The prediction $y_i = w\,x_i + b$ also w.r.t w and b:

$$\frac{\partial y_i}{\partial w} = x_i$$

$$\frac{\partial y_i}{\partial b} = 1$$

- The partial derivative of the individual loss is:

$$\frac{\partial l_i(w, b)}{\partial w} = -2\,(t_i - y_i)\,x_i$$

$$\frac{\partial l_i(w, b)}{\partial b} = -2\,(t_i - y_i)$$

Gradient descent for linear regression

- This give us:

$$\frac{\partial \mathcal{L}(w, b)}{\partial w} = - \frac{2}{N} \sum_{i=1}^{N} (t_i - y_i) \, x_i$$

$$\frac{\partial \mathcal{L}(w, b)}{\partial b} = - \frac{2}{N} \sum_{i=1}^{N} (t_i - y_i)$$

- Gradient descent is then defined by the learning rules (absorbing the 2 in η):

$$\Delta w = \eta \, \frac{1}{N} \sum_{i=1}^{N} (t_i - y_i) \, x_i$$

$$\Delta b = \eta \, \frac{1}{N} \sum_{i=1}^{N} (t_i - y_i)$$

Least Mean Squares (LMS) - Ordinary Least Squares (OLS)

- LMS is a **batch** algorithm: the parameter changes are computed over the whole dataset.

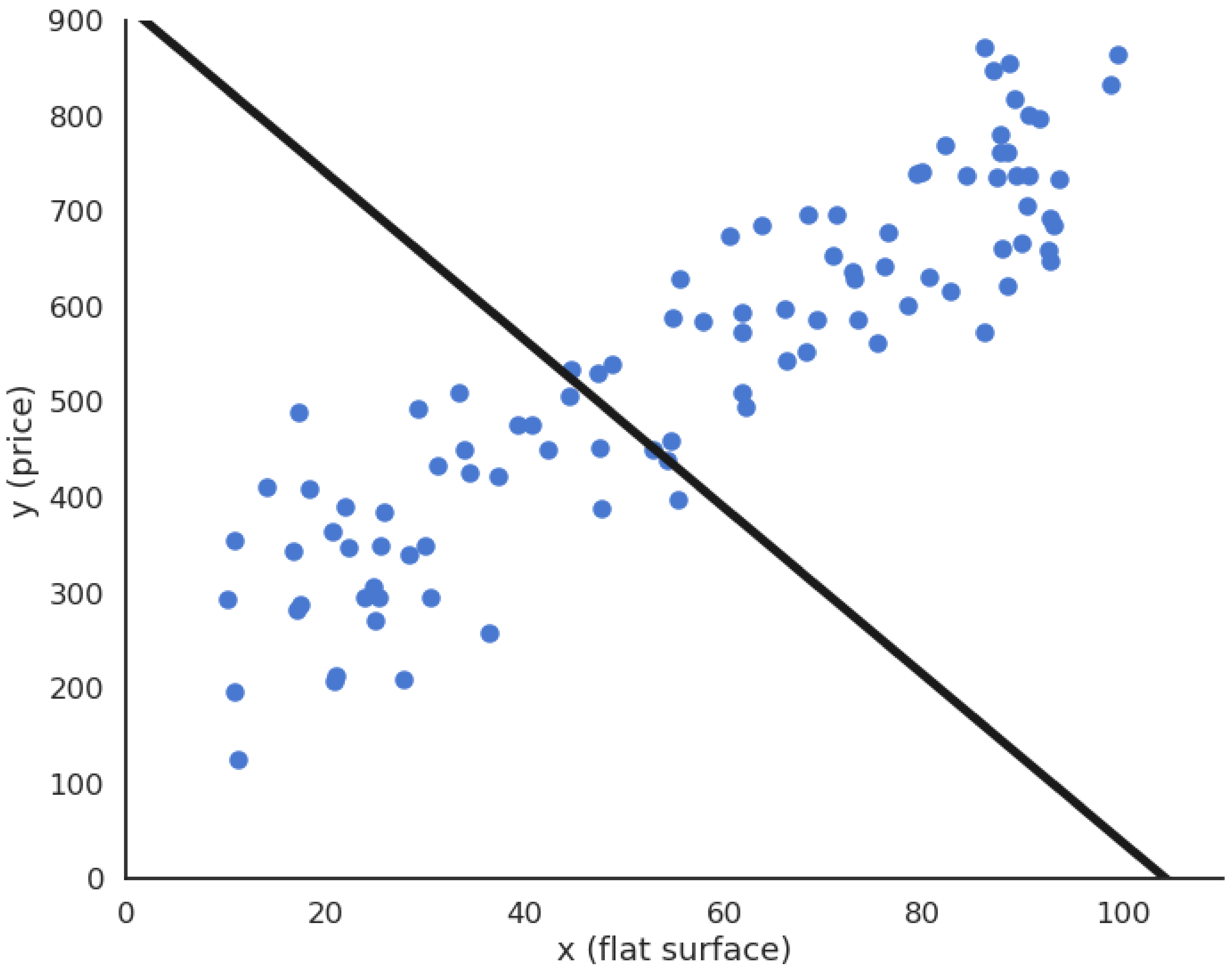
$$\begin{cases} \Delta w = \eta \, \frac{1}{N} \sum_{i=1}^{N} (t_i - y_i) \, x_i \\ \\ \Delta b = \eta \, \frac{1}{N} \sum_{i=1}^{N} (t_i - y_i) \end{cases}$$

- The parameter changes have to be applied multiple times (**epochs**) in order for the parameters to converge.
- One can stop when the parameters do not change much, or after a fixed number of epochs.

Least Mean Squares algorithm

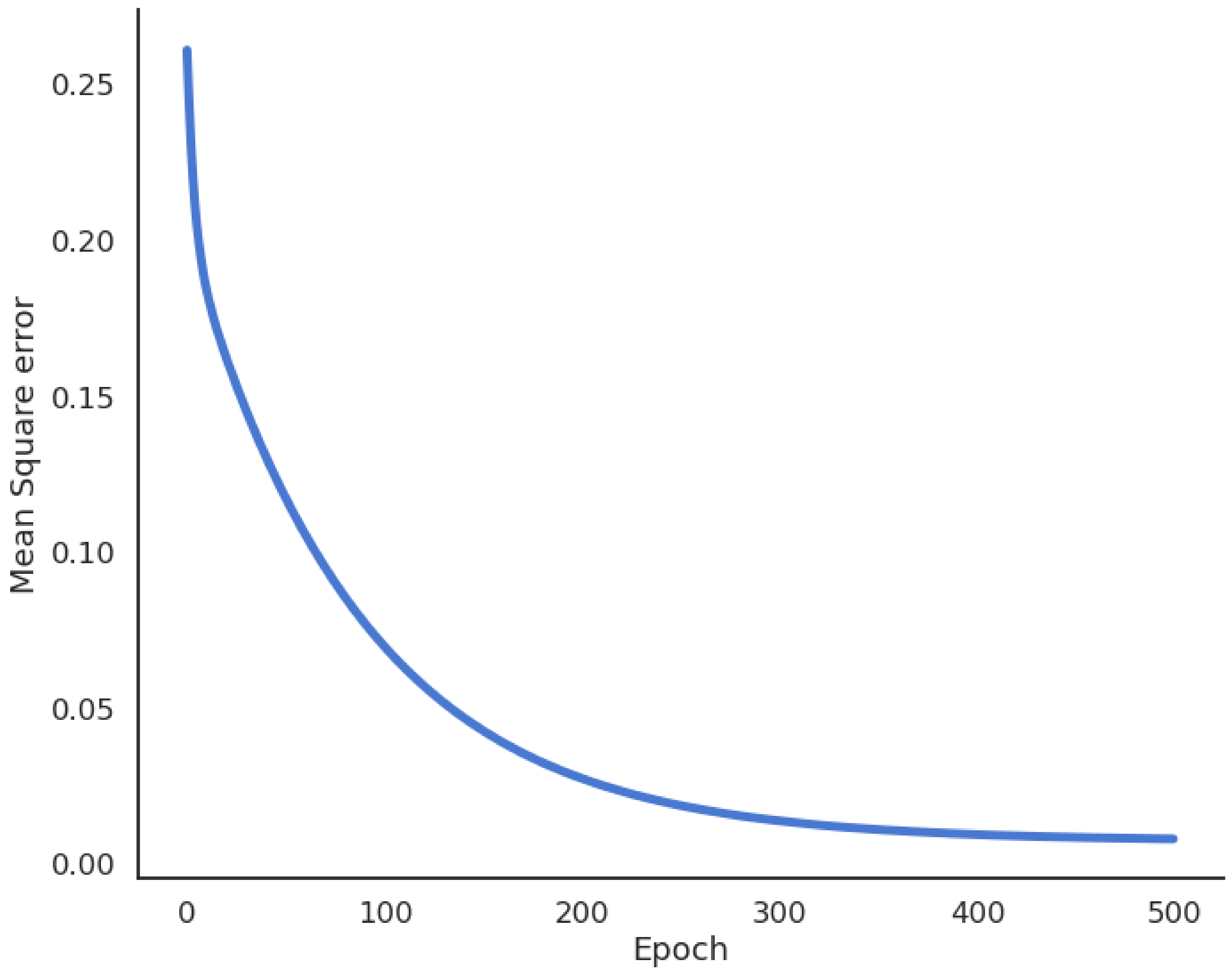
```
- $w = 0 \quad ; \quad b = 0$
- for M epochs:
    - $dw = 0 \quad ; \quad db = 0$
    - for each sample $(x_i, t_i)$:
        - $y_i = w \, x_i + b$
        - $dw = dw + (t_i - y_i) \, x_i$
        - $db = db + (t_i - y_i)$
    - $\Delta w = \eta \, \frac{1}{N} dw$
    - $\Delta b = \eta \, \frac{1}{N} db$
```

Least mean squares in action



Least mean squares

- During learning, the **mean square error** (mse) decreases with the number of epochs but does not reach zero because of the noise in the data.



Delta learning rule: Online version of LMS

- LMS is very slow, because it changes the weights only after the whole training set has been evaluated.

$$\begin{cases} \Delta w = \eta \, \frac{1}{N} \sum_{i=1}^{N} (t_i - y_i) \, x_i \\ \\ \Delta b = \eta \, \frac{1}{N} \sum_{i=1}^{N} (t_i - y_i) \end{cases}$$

Online version of LMS : delta learning rule

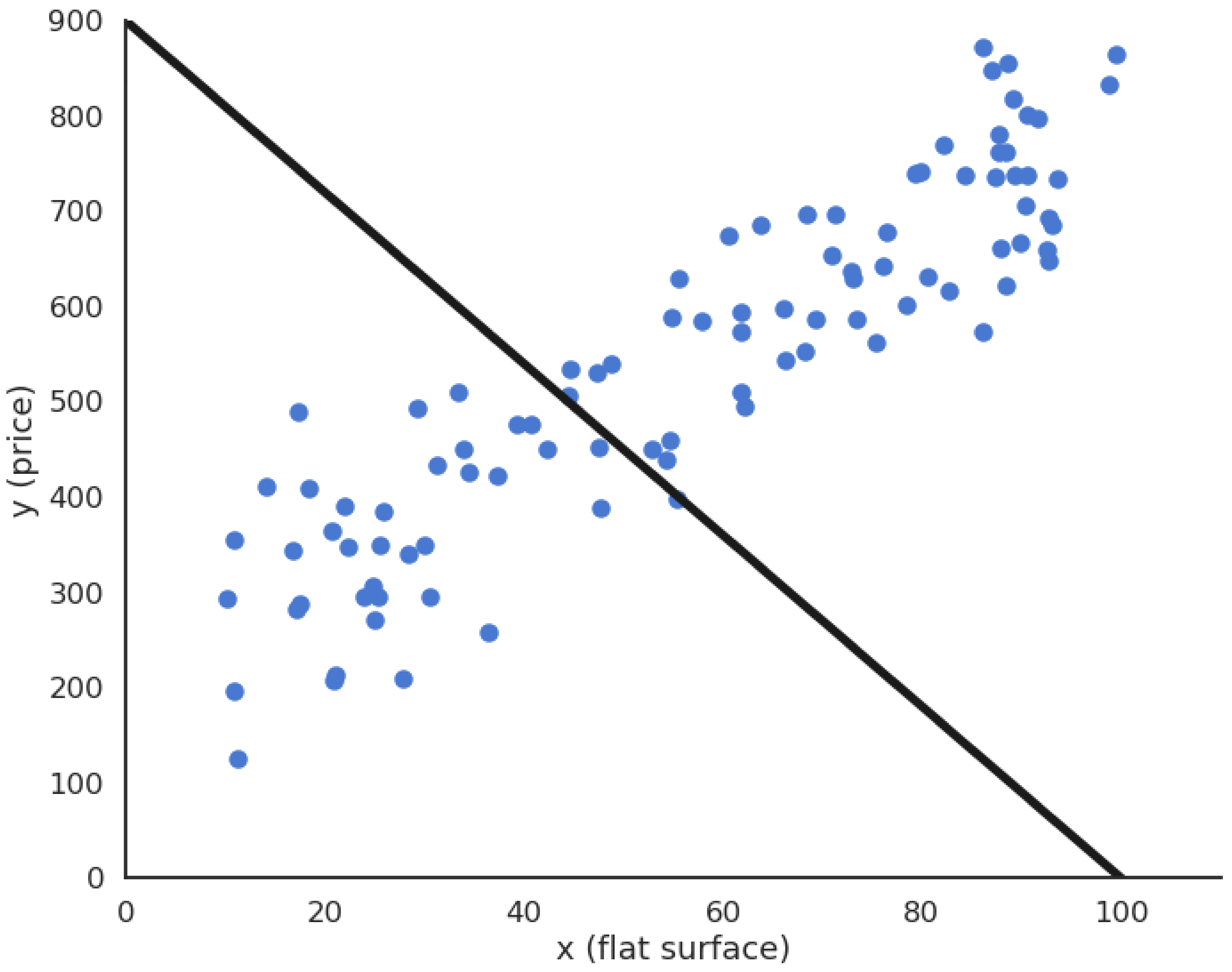
- $w = 0 \quad ; \quad b = 0$
- **for** M epochs:
    - **for** each sample (x_i, t_i):
        - $y_i = w \, x_i + b$
        - $\Delta w = \eta \, (t_i - y_i) \, x_i$
        - $\Delta b = \eta \, (t_i - y_i)$

- It is also possible to update the weights immediately after each example using the **delta learning rule**:

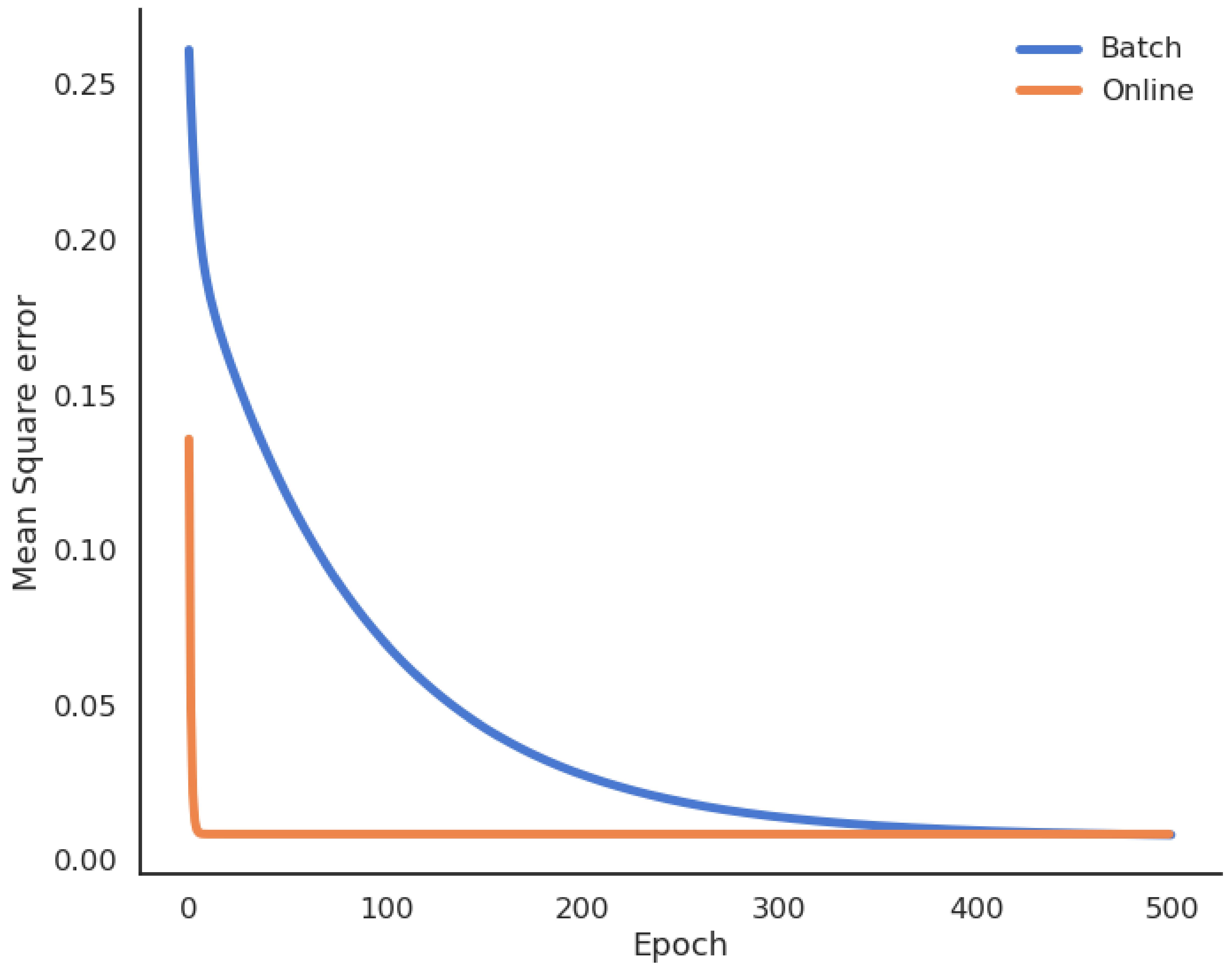
$$\begin{cases} \Delta w = \eta \, (t_i - y_i) \, x_i \\ \\ \Delta b = \eta \, (t_i - y_i) \end{cases}$$

- The batch version is more stable, but the online version is faster: the weights have already learned something when arriving at the end of the first epoch.

Delta learning rule in action (same learning rate!)



Delta learning rule



2 - Multiple linear regression

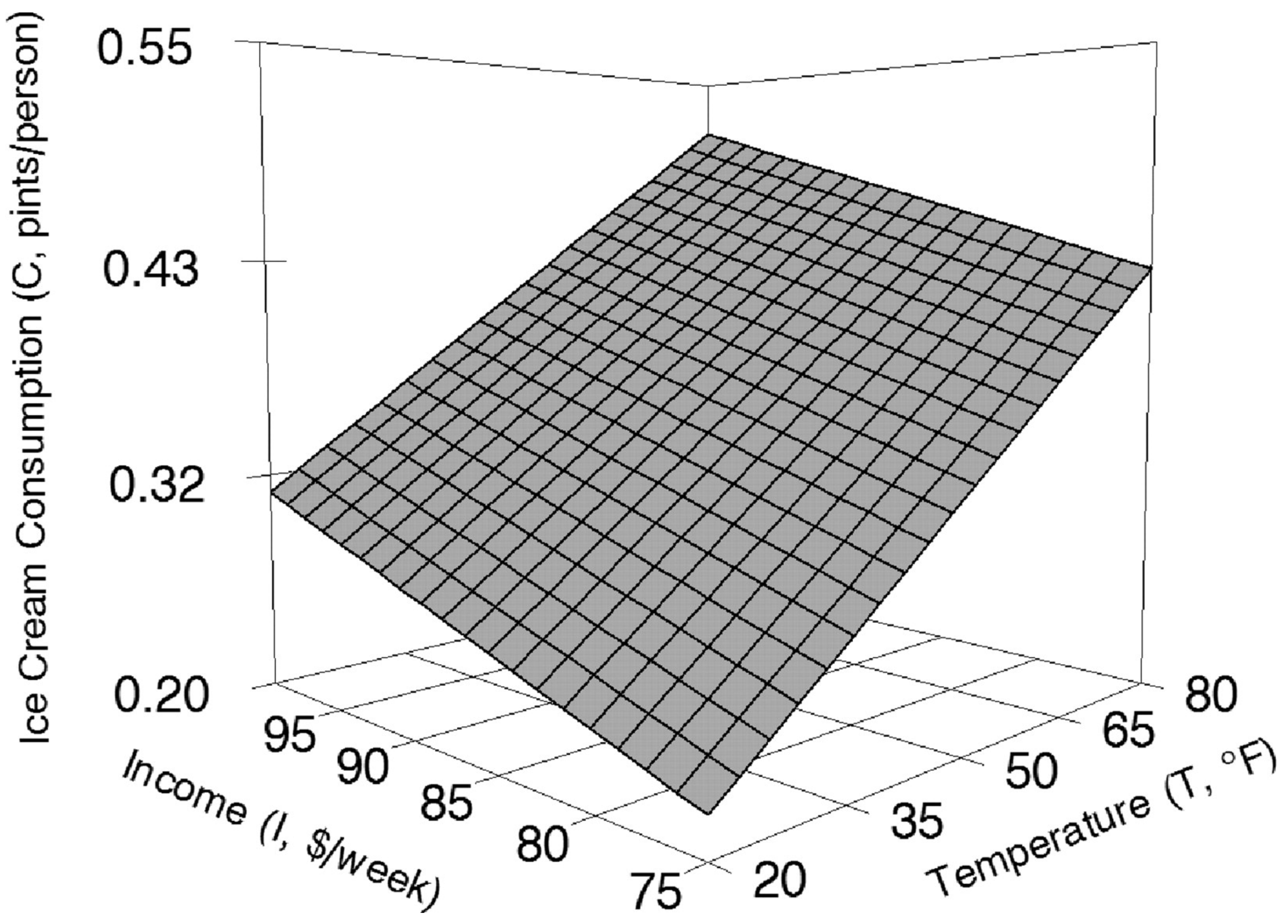
Multiple linear regression

- The key idea of linear regression (one input x, one output y) can be generalized to multiple inputs and outputs.

- **Multiple Linear Regression** (MLR) predicts several output variables based on several explanatory variables or **features**:

$$
\begin{cases}
y_1 = w_1 \, x_1 + w_2 \, x_2 + b_1 \\
\\
y_2 = w_3 \, x_1 + w_4 \, x_2 + b_2
\end{cases}
$$

- All we have is some samples: we want to know the best model for the data.

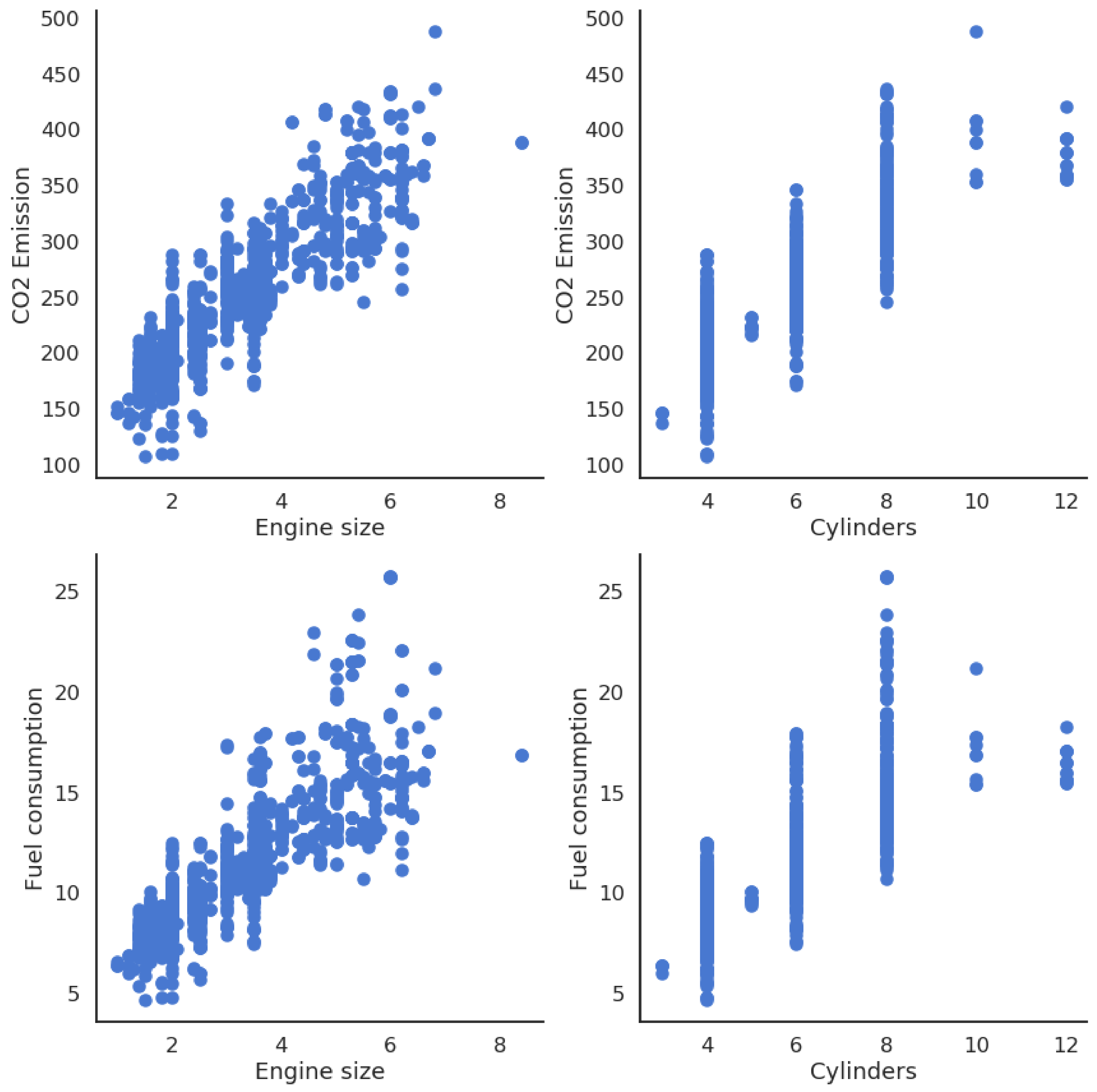


MLR example: fuel consumption and CO2 emissions

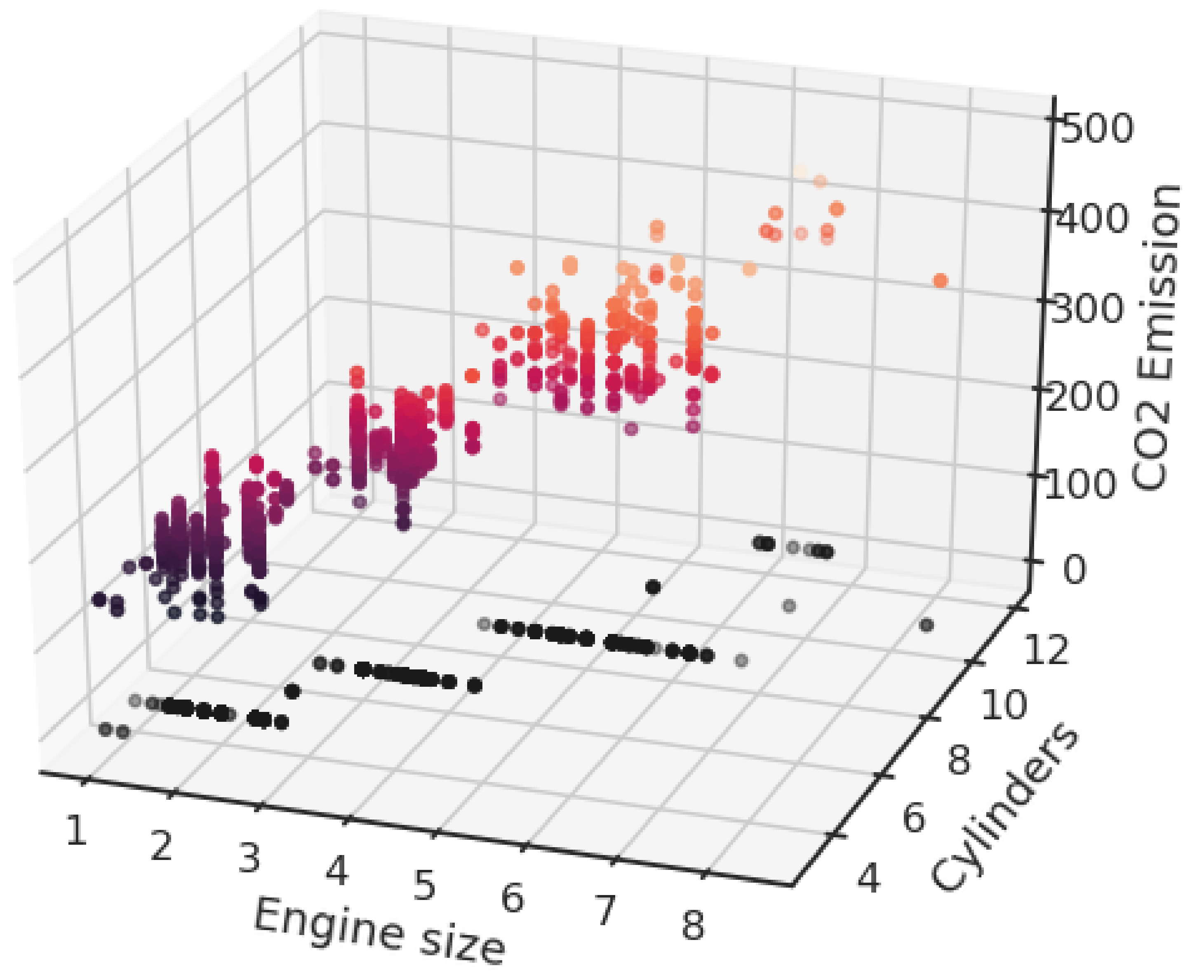
- Let’s suppose you have 13971 measurements in some Excel file, linking engine size, number of cylinders, fuel consumption and CO2 emissions of various cars.
- You want to predict fuel consumption and CO2 emissions when you know the engine size and the number of cylinders.

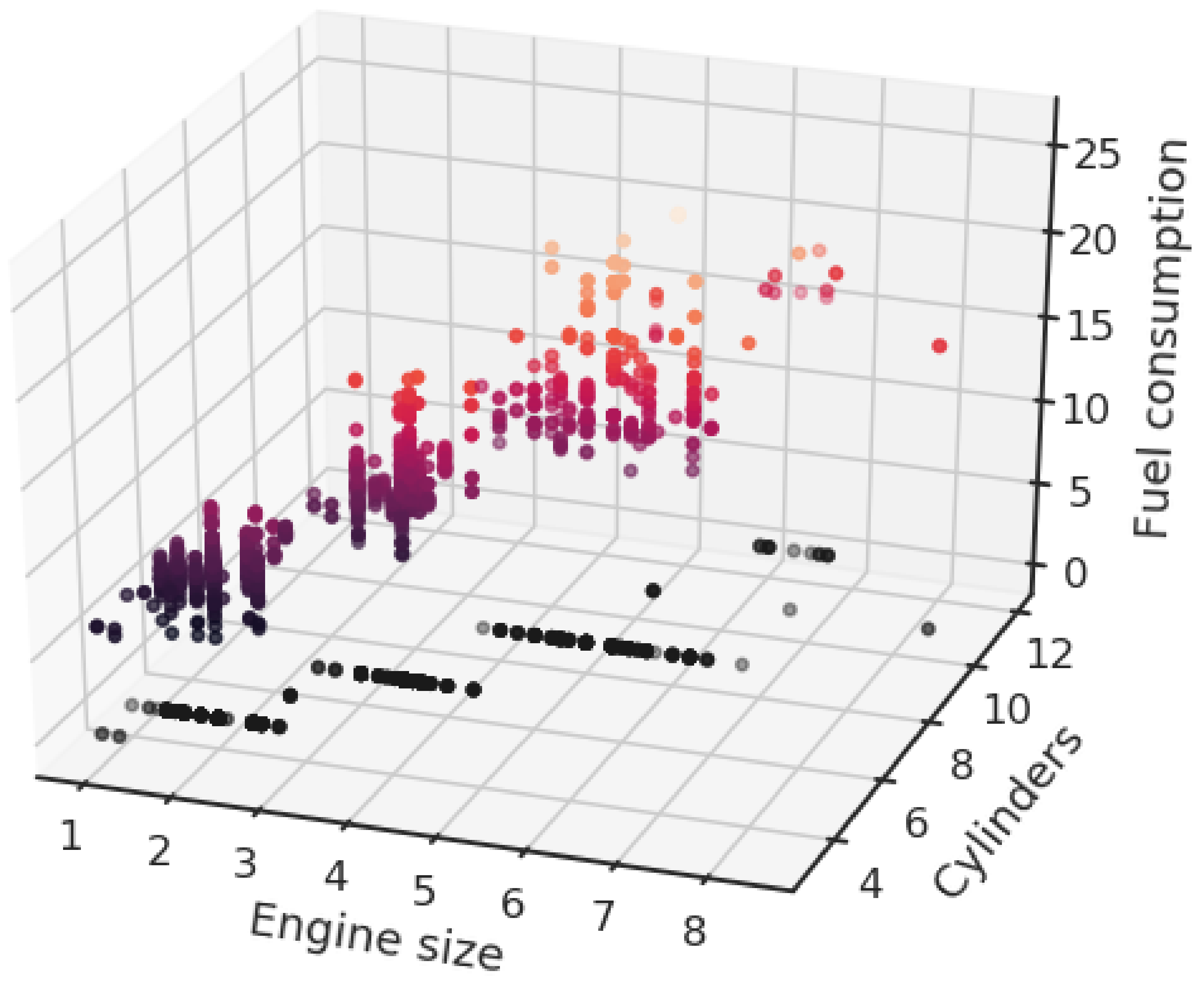
Engine size	Cylinders	Fuel consumption	CO2 emissions
2	4	8.5	196
2.4	4	9.6	221
1.5	4	5.9	136
3.5	6	11	255
3.5	6	11	244
3.5	6	10	230
3.5	6	10	232
3.7	6	11	255
3.7	6	12	267
…	…	…	…

MLR example: fuel consumption and CO2 emissions



MLR example: fuel consumption and CO2 emissions



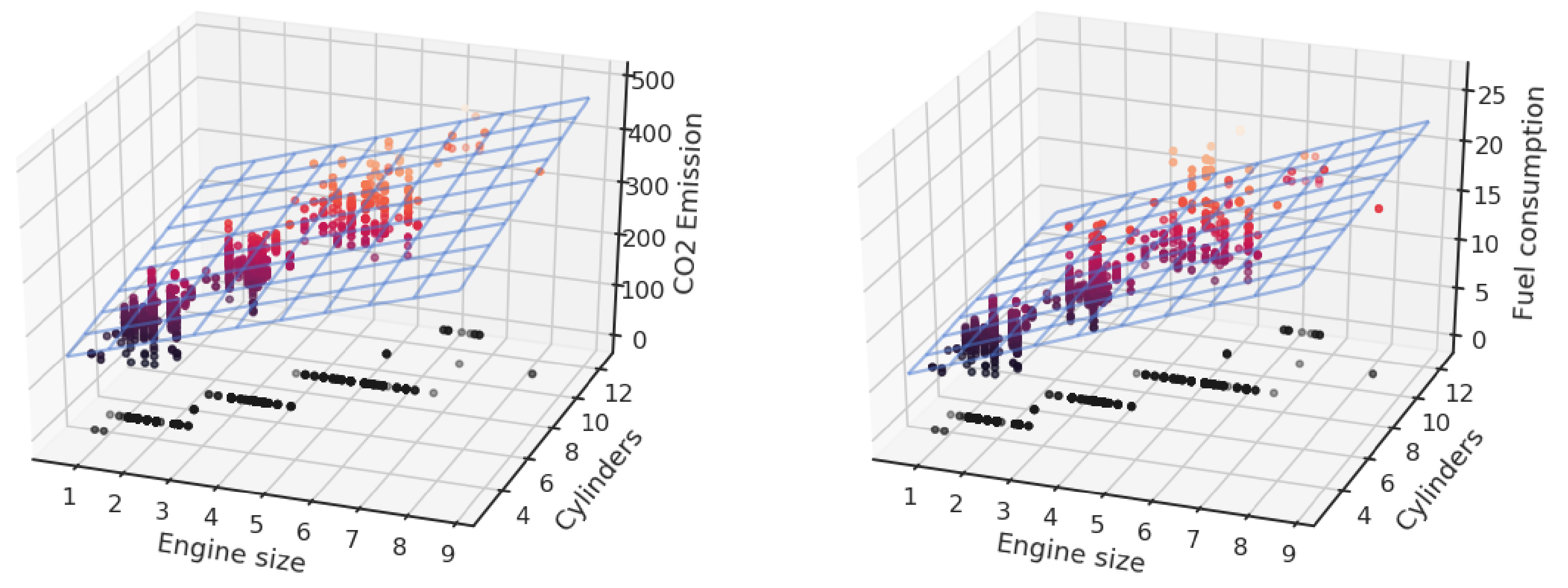


MLR example: fuel consumption and CO2 emissions

- Noting the variables x_1, x_2, y_1, y_2, we can define our MLR problem:

$$\begin{cases} y_1 = w_1\, x_1 + w_2\, x_2 + b_1 \\ y_2 = w_3\, x_1 + w_4\, x_2 + b_2 \end{cases}$$

and use the least mean squares method to obtain the value of the parameters.



- Note: using the Python library `scikit-learn` (https://scikit-learn.org), this is done in two lines of code:

```
from sklearn.linear_model import LinearRegression
reg = LinearRegression().fit(X, y)
```

Multiple linear regression

- The system of equations:

$$\begin{cases} y_1 = w_1 \, x_1 + w_2 \, x_2 + b_1 \\ \\ y_2 = w_3 \, x_1 + w_4 \, x_2 + b_2 \end{cases}$$

can be put in a matrix-vector form:

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} w_1 & w_2 \\ w_3 & w_4 \end{bmatrix} \times \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$$

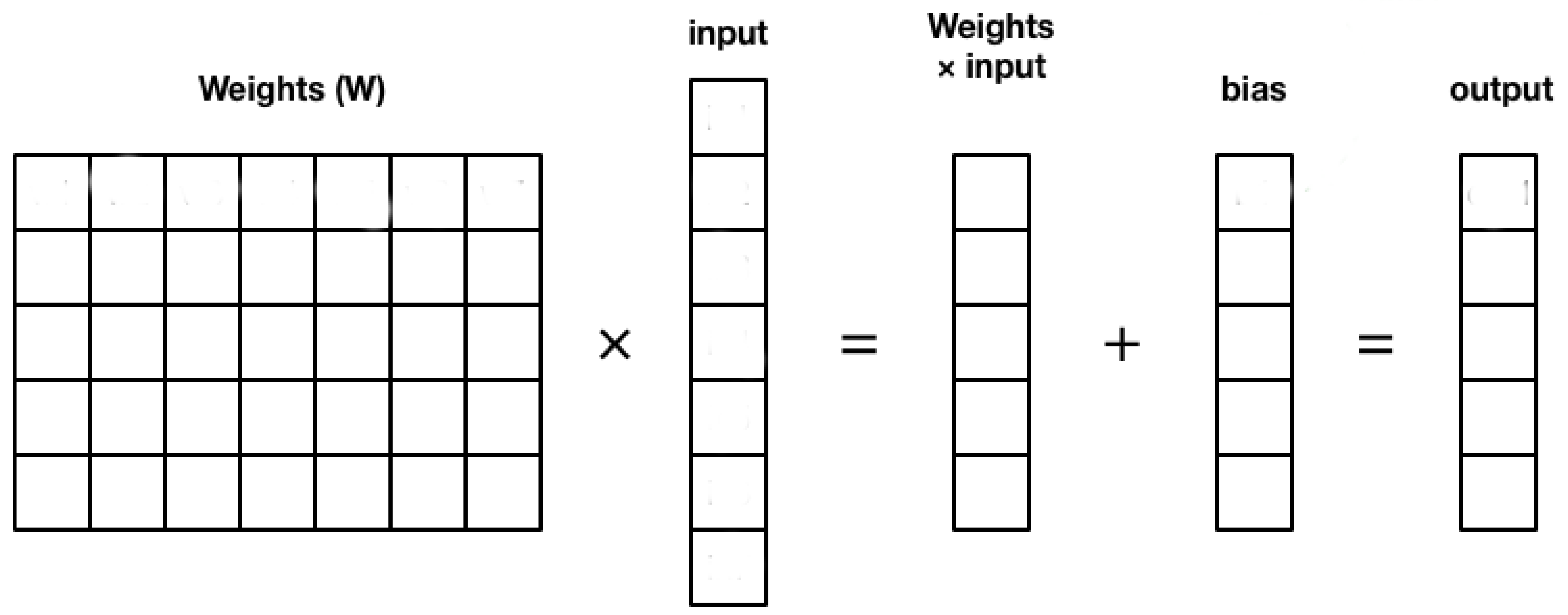
- We simply create the corresponding vectors and matrices:

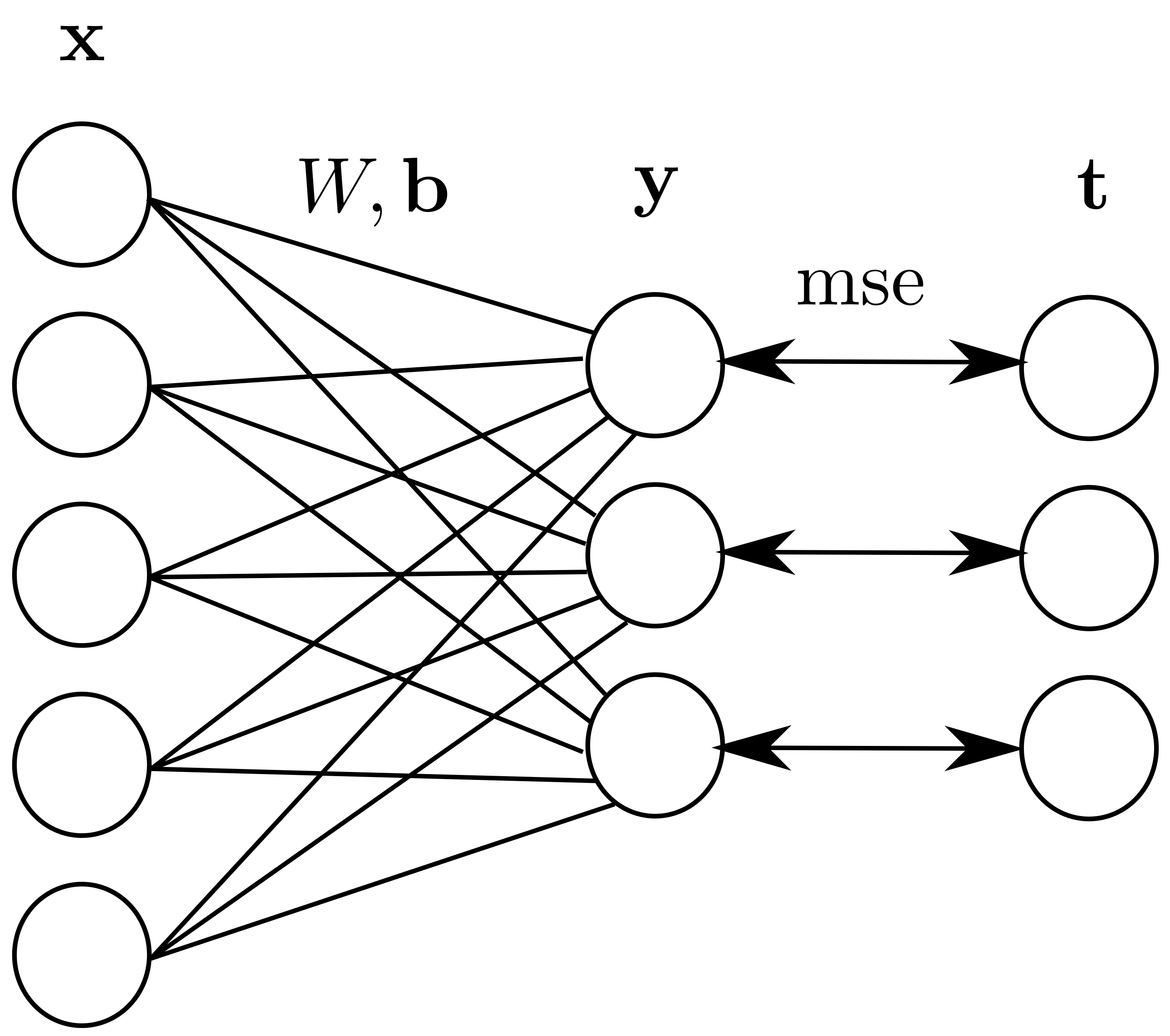
$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \qquad \mathbf{t} = \begin{bmatrix} t_1 \\ t_2 \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \qquad W = \begin{bmatrix} w_1 & w_2 \\ w_3 & w_4 \end{bmatrix}$$

- $\mathbf{x}$ is the input vector, $\mathbf{y}$ is the output vector, $\mathbf{t}$ is the target vector.
- W is called the **weight matrix** and $\mathbf{b}$ the **bias vector**.

$$\mathbf{y} = f_{W,\mathbf{b}}(\mathbf{x}) = W \times \mathbf{x} + \mathbf{b}$$

Multiple linear regression





- The model is now defined by:

$$\mathbf{y} = f_{W, \mathbf{b}}(\mathbf{x}) = W \times \mathbf{x} + \mathbf{b}$$

- The problem is exactly the same as before, except that we use vectors and matrices instead of scalars: $\mathbf{x}$ and $\mathbf{y}$ can have any number of dimensions, the same procedure will apply.
- This corresponds to a **linear neural network** (or linear perceptron), with one **output neuron** per predicted value y_i using the linear activation function.

Multiple linear regression

- The mean square error still needs to be a scalar in order to be minimized. We can define it as the squared norm of the error **vector**:

$$\min_{W, \mathbf{b}} \mathcal{L}(W, \mathbf{b}) = \mathbb{E}_\mathcal{D}[||\mathbf{t} - \mathbf{y}||^2] = \mathbb{E}_\mathcal{D}[((t_1 - y_1)^2 + (t_2 - y_2)^2)]$$

- In order to apply gradient descent, one needs to calculate partial derivatives w.r.t the weight matrix W and the bias vector $\mathbf{b}$, i.e. **gradients**:

$$\begin{cases} \Delta W = - \eta \, \nabla_W \, \mathcal{L}(W, \mathbf{b}) \\ \\ \Delta \mathbf{b} = - \eta \, \nabla_\mathbf{b} \, \mathcal{L}(W, \mathbf{b}) \end{cases}$$

- Some more advanced linear algebra becomes important to know how to compute these gradients:

https://web.stanford.edu/class/cs224n/readings/gradient-notes.pdf

Multiple linear regression

- We search the minimum of the mse loss function:

$$\min_{W, \mathbf{b}} \mathcal{L}(W, \mathbf{b}) = \mathbb{E}_\mathcal{D} [||\mathbf{t} - \mathbf{y}||^2] \approx \frac{1}{N} \sum_{i=1}^N ||\mathbf{t}_i - \mathbf{y}_i||^2 = \frac{1}{N} \sum_{i=1}^N l_i(W, \mathbf{b})$$

- The individual loss function $l_i(W, \mathbf{b})$ is the squared $\mathcal{L}^2$-norm of the error vector, what can be expressed as a dot product or a vector multiplication:

$$l_i(W, \mathbf{b}) = ||\mathbf{t}_i - \mathbf{y}_i||^2 = \langle \mathbf{t}_i - \mathbf{y}_i \cdot \mathbf{t}_i - \mathbf{y}_i \rangle = (\mathbf{t}_i - \mathbf{y}_i)^T \times (\mathbf{t}_i - \mathbf{y}_i)$$

- Remember:

$$\mathbf{x}^T \times \mathbf{x} = \begin{bmatrix} x_1 & x_2 & \ldots & x_n \end{bmatrix} \times \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = x_1 \, x_1 + x_2 \, x_2 + \ldots + x_n \, x_n = \langle \mathbf{x} \cdot \mathbf{x} \rangle = ||\mathbf{x}||^2_2$$

Multiple linear regression

- The chain rule tells us in principle that:

$$\nabla_{W} \, l_i(W, \mathbf{b}) = \nabla_{\mathbf{y}_i} \, l_i(W, \mathbf{b}) \times \nabla_{W} \, \mathbf{y}_i$$

- The gradient w.r.t the output vector $\mathbf{y}_i$ is quite easy to obtain, as it a quadratic function of $\mathbf{t}_i - \mathbf{y}_i$:

$$\nabla_{\mathbf{y}_i} \, l_i(W, \mathbf{b}) = \nabla_{\mathbf{y}_i} \, (\mathbf{t}_i - \mathbf{y}_i)^T \times (\mathbf{t}_i - \mathbf{y}_i)$$

- The proof relies on product differentiation $(f \times g)' = f' \, g + f \, g'$:

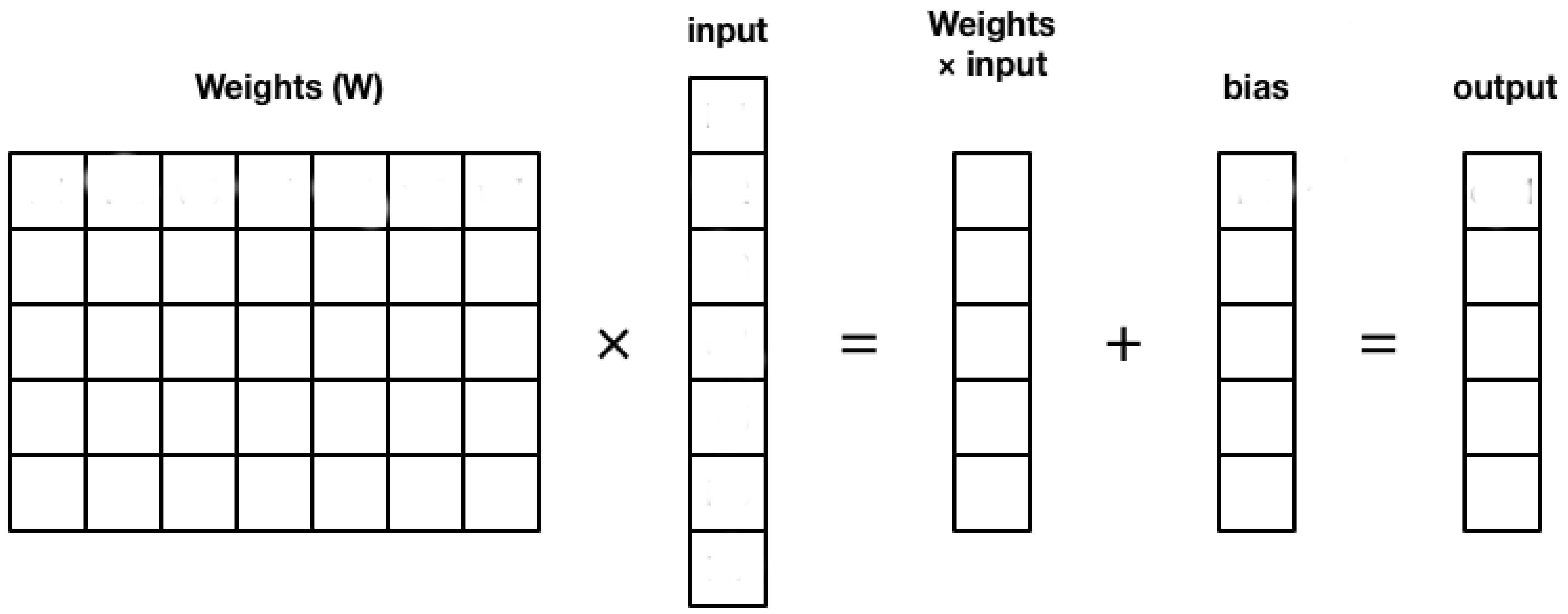
$$\nabla_{\mathbf{y}_i} \, (\mathbf{t}_i - \mathbf{y}_i)^T \times (\mathbf{t}_i - \mathbf{y}_i) = (\nabla_{\mathbf{y}_i} \, (\mathbf{t}_i - \mathbf{y}_i)) \times (\mathbf{t}_i - \mathbf{y}_i) + (\mathbf{t}_i - \mathbf{y}_i) \times \nabla_{\mathbf{y}_i} \, (\mathbf{t}_i - \mathbf{y}_i)$$

$$= -(\mathbf{t}_i - \mathbf{y}_i) - (\mathbf{t}_i - \mathbf{y}_i)$$

$$= -2 \, (\mathbf{t}_i - \mathbf{y}_i)$$

Note: We use the properties $\nabla_{\mathbf{x}} \, \mathbf{x}^T \times \mathbf{z} = \mathbf{z}$ and $\nabla_{\mathbf{z}} \, \mathbf{x}^T \times \mathbf{z} = \mathbf{x}$ to get rid of the transpose.

Multiple linear regression



- The “problem” is when computing $\nabla_W \, \mathbf{y}_i = \nabla_W \, (W \times \mathbf{x}_i + \mathbf{b})$:
  - $\mathbf{y}_i$ is a vector and W a matrix.
  - $\nabla_W \, \mathbf{y}_i$ is then a Jacobian (matrix), not a gradient (vector).
- Intuitively, differentiating $W \times \mathbf{x}_i + \mathbf{b}$ w.r.t W should return $\mathbf{x}_i$, but it is a vector, not a matrix…
- The gradient (or Jacobian) of $l_i(W, \mathbf{b})$ w.r.t W should be a matrix of the same size as W so that we can apply gradient descent:

$$\Delta W = - \eta \, \nabla_W \, \mathcal{L}(W, \mathbf{b})$$

Multiple linear regression

- We already know that:

$$\nabla_W \, l_i(W, \mathbf{b}) = -2 \, (\mathbf{t}_i - \mathbf{y}_i) \times \nabla_W \, \mathbf{y}_i$$

- If $\mathbf{x}_i$ has n elements and $\mathbf{y}_i$ m elements, W is a $m \times n$ matrix.
- Remember the outer product between two vectors:

$$\mathbf{u} \times \mathbf{v}^\text{T} = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} \begin{bmatrix} v_1 & v_2 & v_3 \end{bmatrix} = \begin{bmatrix} u_1 v_1 & u_1 v_2 & u_1 v_3 \\ u_2 v_1 & u_2 v_2 & u_2 v_3 \\ u_3 v_1 & u_3 v_2 & u_3 v_3 \\ u_4 v_1 & u_4 v_2 & u_4 v_3 \end{bmatrix}.$$

- It is easy to see that the outer product between $(\mathbf{t}_i - \mathbf{y}_i)$ and $\mathbf{x}_i$ gives a $m \times n$ matrix:

$$\nabla_W \, l_i(W, \mathbf{b}) = -2 \, (\mathbf{t}_i - \mathbf{y}_i) \times \mathbf{x}_i^T$$

Example

- Let's prove it element per element:

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = W \times \mathbf{x} + \mathbf{b} = \begin{bmatrix} w_1 & w_2 \\ w_3 & w_4 \end{bmatrix} \times \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$$

$$l(W, \mathbf{b}) = (\mathbf{t} - \mathbf{y})^T \times (\mathbf{t} - \mathbf{y}) = \begin{bmatrix} t_1 - y_1 & t_2 - y_2 \end{bmatrix} \times \begin{bmatrix} t_1 - y_1 \\ t_2 - y_2 \end{bmatrix} = (t_1 - y_1)^2 + (t_2 - y_2)^2$$

- The Jacobian w.r.t W can be explicitly formed using partial derivatives:

$$\nabla_W \, l(W, \mathbf{b}) = \begin{bmatrix} \dfrac{\partial l(W, \mathbf{b})}{\partial w_1} & \dfrac{\partial l(W, \mathbf{b})}{\partial w_2} \\ \dfrac{\partial l(W, \mathbf{b})}{\partial w_3} & \dfrac{\partial l(W, \mathbf{b})}{\partial w_4} \end{bmatrix} = \begin{bmatrix} -2\,(t_1 - y_1)\,x_1 & -2\,(t_1 - y_1)\,x_2 \\ -2\,(t_2 - y_2)\,x_1 & -2\,(t_2 - y_2)\,x_2 \end{bmatrix}$$

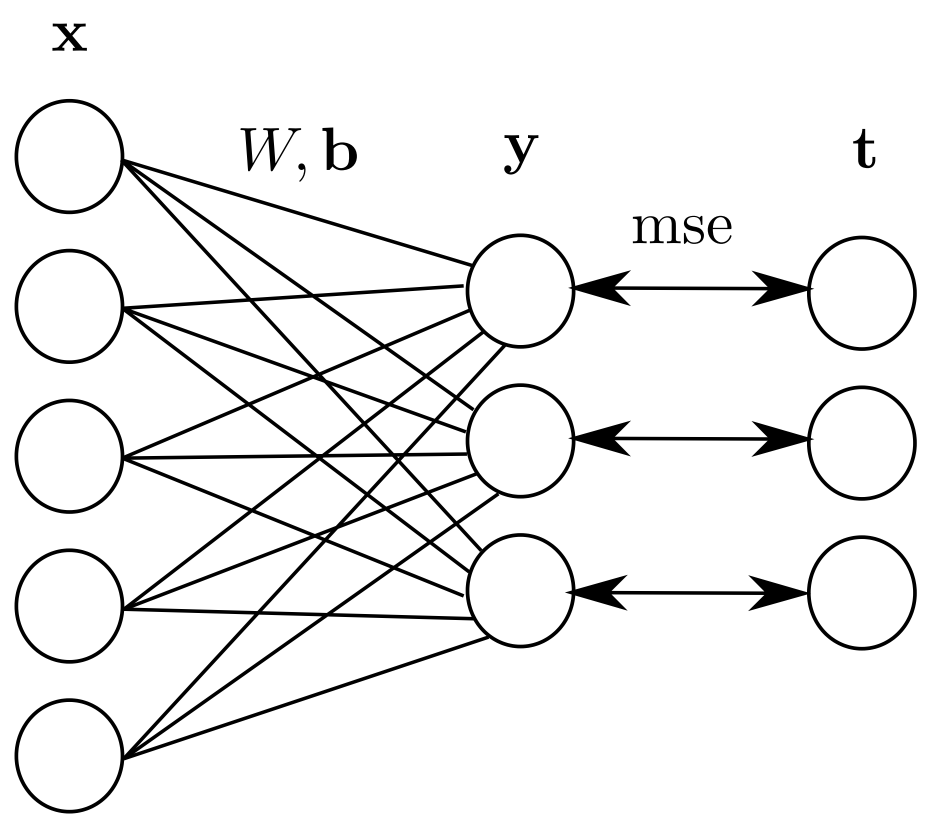
- We can rearrange this matrix as an outer product:

$$\nabla_W \, l(W, \mathbf{b}) = -2 \begin{bmatrix} t_1 - y_1 \\ t_2 - y_2 \end{bmatrix} \times \begin{bmatrix} x_1 & x_2 \end{bmatrix} = -2\,(\mathbf{t} - \mathbf{y}) \times \mathbf{x}^T$$

Multiple linear regression

- Batch version (**least mean squares**):

$$\begin{cases} \Delta W = \eta \, \frac{1}{N} \sum_{i=1}^N (\mathbf{t}_i - \mathbf{y}_i) \times \mathbf{x}_i^T \\ \\ \Delta \mathbf{b} = \eta \, \frac{1}{N} \sum_{i=1}^N (\mathbf{t}_i - \mathbf{y}_i) \\ \end{cases}$$



- Online version (**delta learning rule**):

$$\begin{cases} \Delta W = \eta \, (\mathbf{t}_i - \mathbf{y}_i) \times \mathbf{x}_i^T \\ \\ \Delta \mathbf{b} = \eta \, (\mathbf{t}_i - \mathbf{y}_i) \\ \end{cases}$$

- This is completely equivalent to having one learning rule per parameter:

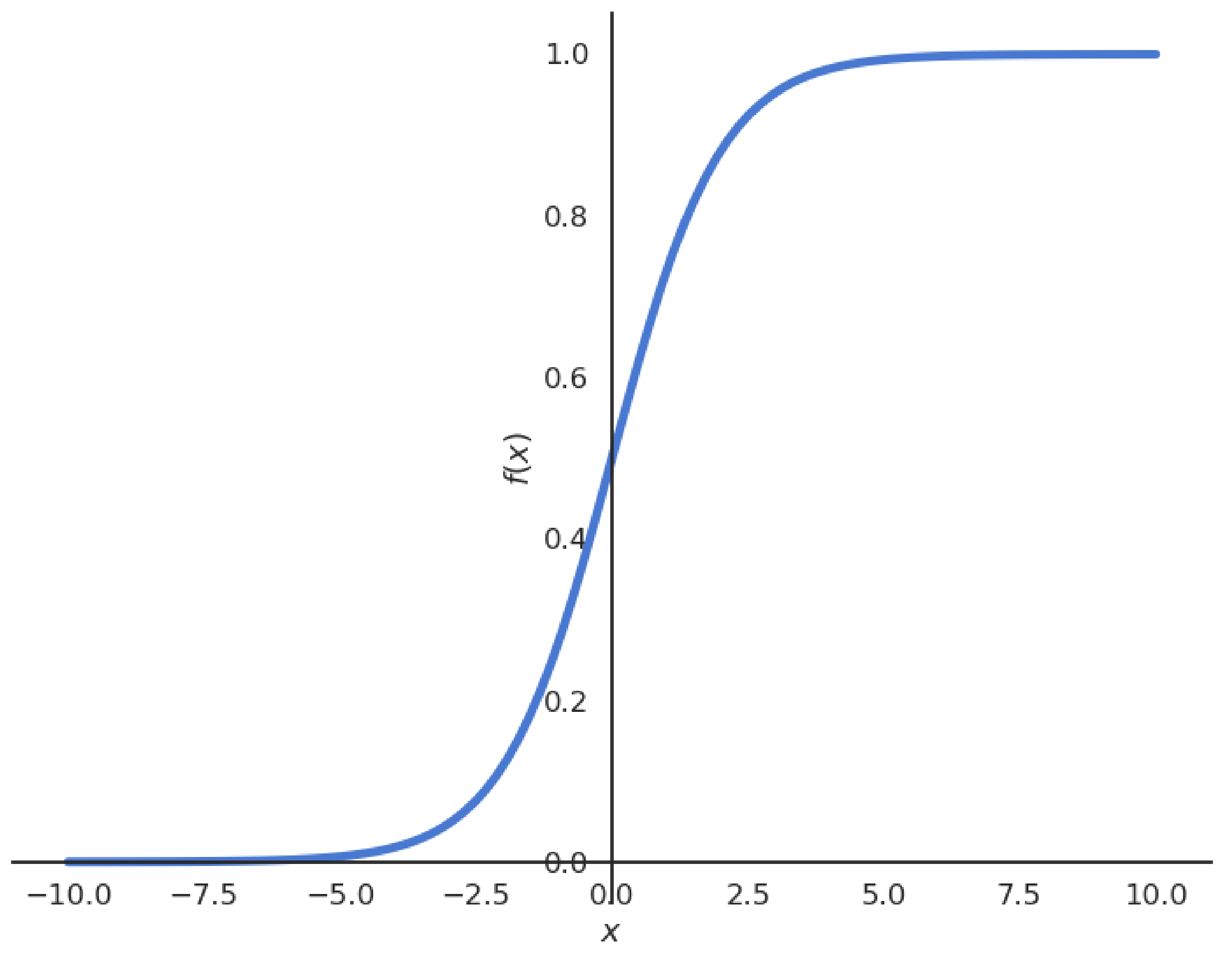
$$\begin{cases} \Delta w_1 = \eta \, (t_1 - y_1) \, x_1 \\ \Delta w_2 = \eta \, (t_1 - y_1) \, x_2 \\ \Delta w_3 = \eta \, (t_2 - y_2) \, x_1 \\ \Delta w_4 = \eta \, (t_2 - y_2) \, x_2 \\ \end{cases}$$

$$\begin{cases} \Delta b_1 = \eta \, (t_1 - y_1) \\ \Delta b_2 = \eta \, (t_2 - y_2) \\ \end{cases}$$

- The delta learning rule is always of the form: Δw = eta $\times$ error $\times$ input. Biases have an input of 1.

3 - Logistic regression

Logistic regression



- Let’s suppose we want to perform a regression, but where the outputs t_i are bounded between 0 and 1.
- We could use a logistic (or sigmoid) function instead of a linear function in order to transform the input into an output:

$$y = \sigma(w \, x + b) = \frac{1}{1 + \exp(-w \, x - b)}$$

- The logistic function

$$\sigma(x) = \frac{1}{1 + \exp(-x)}$$

has the nice property that

$$\sigma'(x) = \sigma(x) \, (1 - \sigma(x))$$

Logistic regression

- We can perform a logistic regression with the same online LMS method as in the linear case:

$$l_i(w, b) = (t_i - \sigma(w \, x_i + b))^2$$

- The partial derivative of the individual loss is easy to find using the chain rule:

$$\frac{\partial l_i(w, b)}{\partial w} = 2 \, (t_i - y_i) \, \frac{\partial}{\partial w} (t_i - \sigma(w \, x_i + b))$$

$$= -2 \, (t_i - y_i) \, \sigma'(w \, x_i + b) \, x_i$$

- The non-linear transfer function $\sigma(x)$ adds its derivative into the gradient:

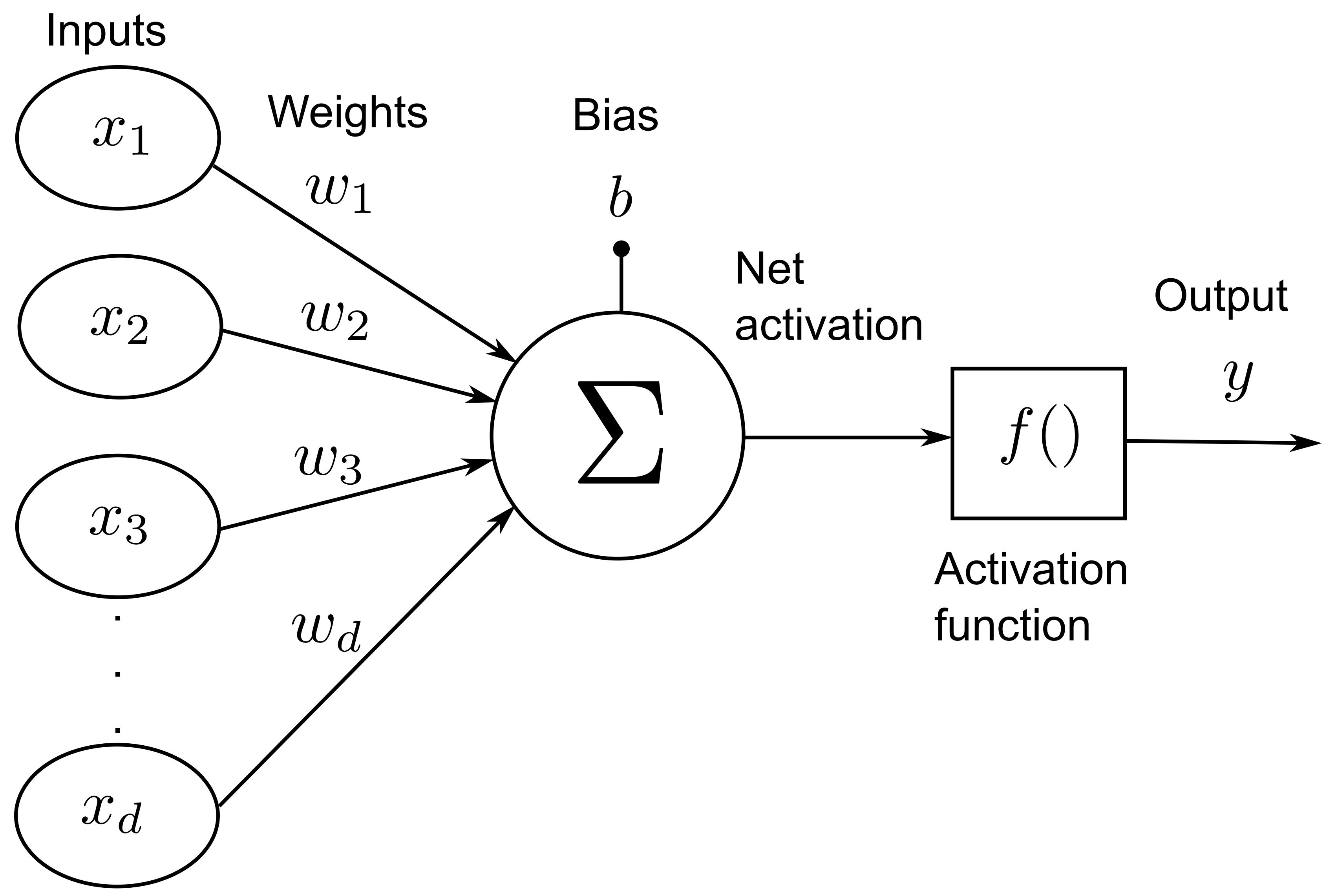
$$\Delta w = \eta \, (t_i - y_i) \, \sigma'(w \, x_i + b) \, x_i$$

- With the property $\sigma'(x) = \sigma(x) \, (1 - \sigma(x))$, it even becomes:

$$\Delta w = \eta \, (t_i - y_i) \, y_i \, (1 - y_i) \, x_i$$

so we do not even need to compute the derivative!

Logistic regression



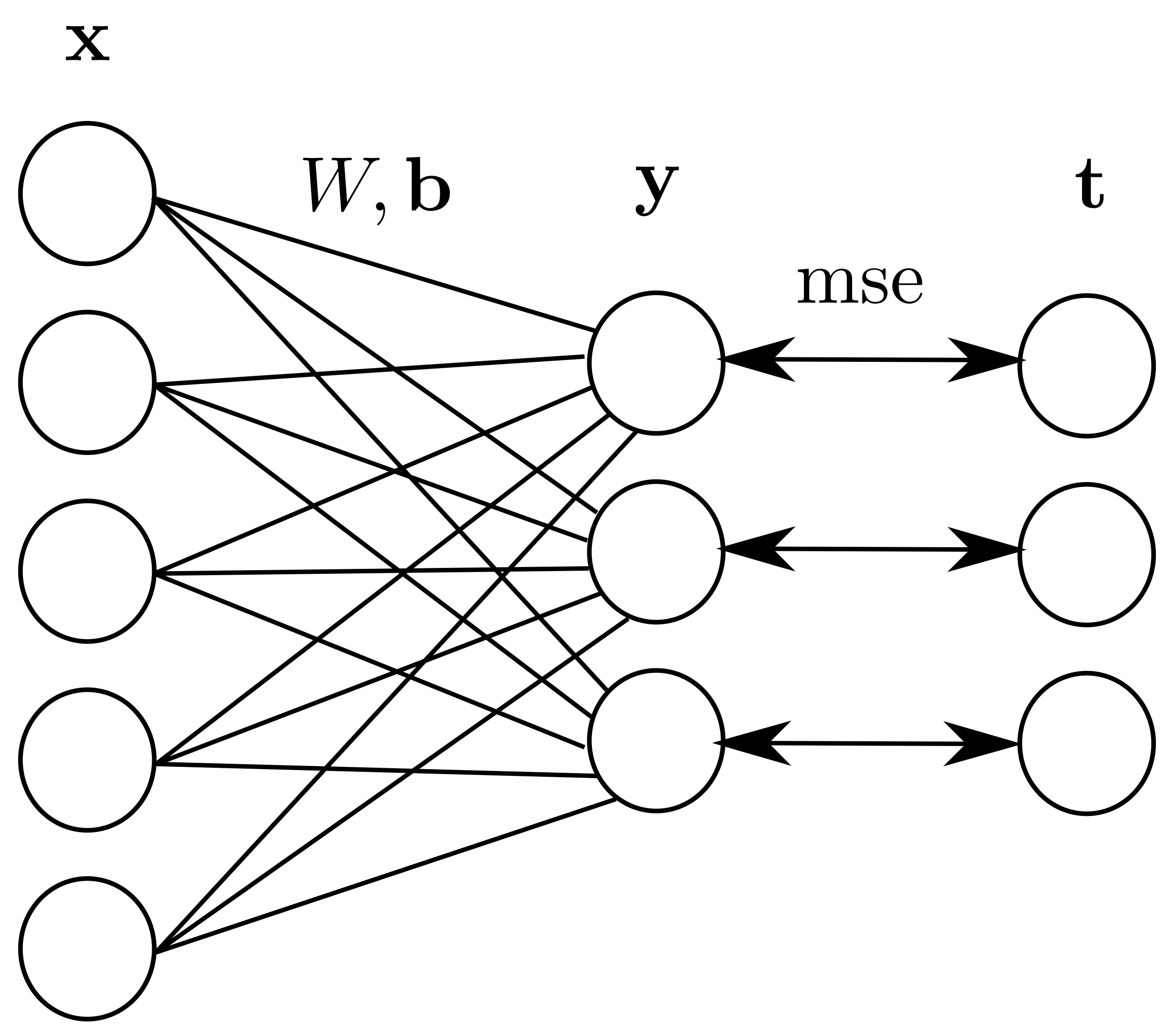
- Model:

$$y = \sigma(w\, x + b) = \frac{1}{1 + \exp(-w\, x - b)}$$

- The delta learning rule in case of logistic regression is:

$$\begin{cases} \Delta w = \eta \, (t_i - y_i) \, y_i \, (1 - y_i) \, x_i \\ \\ \Delta b = \eta \, (t_i - y_i) \, y_i \, (1 - y_i) \end{cases}$$

Generalized form of the delta learning rule



- Model:

$$\mathbf{y} = f(W \times \mathbf{x} + \mathbf{b})$$

- Loss function (mse):

$$\mathcal{L}(W, \mathbf{b}) = \mathbb{E}_{\mathbf{x}, \mathbf{t} \in \mathcal{D}}[||\mathbf{t} - \mathbf{y}||^2]$$

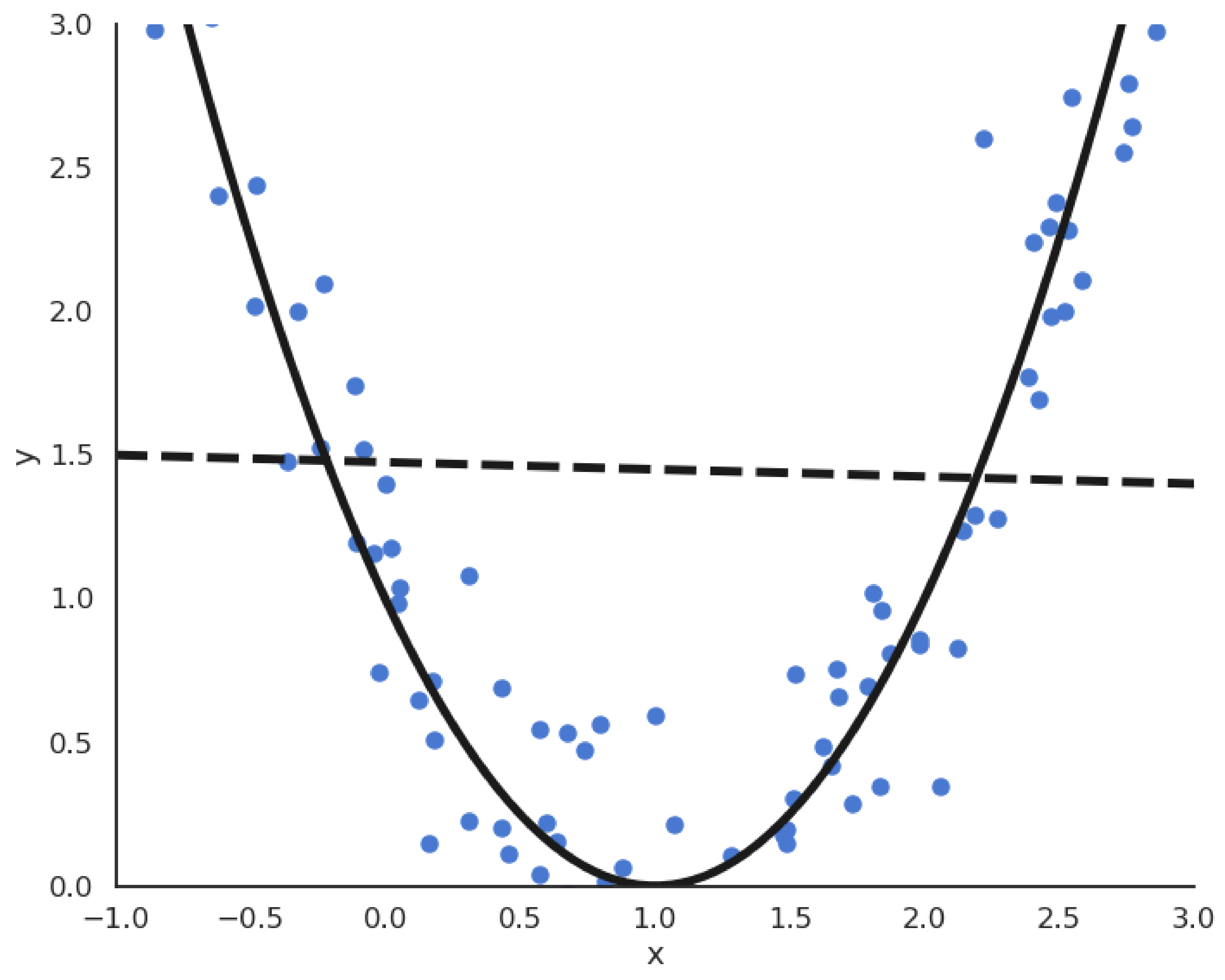
- Delta learning rule:

$$\begin{cases} \Delta W = \eta \, [(\mathbf{t} - \mathbf{y}) \odot f'(W \times \mathbf{x} + \mathbf{b})] \times \mathbf{x}^T \\ \\ \Delta \mathbf{b} = \eta \, (\mathbf{t} - \mathbf{y}) \odot f'(W \times \mathbf{x} + \mathbf{b}) \end{cases}$$

- $\odot$ denotes element-wise multiplication, i.e. $(\mathbf{t} - \mathbf{y}) \odot f'(W \times \mathbf{x} + \mathbf{b})$ is also a vector.
- In the linear case, $f'(x) = 1$.
- One can use any non-linear function, e.g hyperbolic tangent tanh(), ReLU, etc.
- Transfer functions are chosen for neural networks so that we can compute their derivative easily.

4 - Polynomial regression

Polynomial regression



- The functions underlying real data are rarely linear plus some noise around the ideal value.
- In the figure, the input/output function would be better modeled by a second-order polynomial (or higher):

$$y = f_{\mathbf{w},b}(x) = w_1 \, x + w_2 \, x^2 + b$$

Polynomial regression

- Model:

$$y = f_{\mathbf{w}, b}(x) = w_1 \, x + w_2 \, x^2 + b$$

- We can transform the input into a vector of coordinates:

$$\mathbf{x} = \begin{bmatrix} x \\ x^2 \end{bmatrix} \qquad \mathbf{w} = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}$$

- The problem becomes:

$$y = \langle \mathbf{w} . \mathbf{x} \rangle + b = \sum_j w_j \, x_j + b$$

- We can simply apply multiple linear regression (MLR) to find $\mathbf{w}$ and b:

$$\begin{cases} \Delta \mathbf{w} = \eta \, (t - y) \, \mathbf{x} \\ \\ \Delta b = \eta \, (t - y) \end{cases}$$

Polynomial regression

- This generalizes to polynomials of any order p:

$$y = f_{\mathbf{w}, b}(x) = w_1 \, x + w_2 \, x^2 + \ldots + w_p \, x^p + b$$

- We create a vector of powers of x (called **polynomial features**):

$$\mathbf{x} = \begin{bmatrix} x \\ x^2 \\ \ldots \\ x^p \end{bmatrix} \qquad \mathbf{w} = \begin{bmatrix} w_1 \\ w_2 \\ \ldots \\ w_p \end{bmatrix}$$

- And apply multiple linear regression (MLR) to find $\mathbf{w}$ and b:

$$\begin{cases} \Delta \mathbf{w} = \eta \, (t - y) \, \mathbf{x} \\ \\ \Delta b = \eta \, (t - y) \end{cases}$$

- Non-linear problem solved! The only unknown is which order for the polynomial matches best the data.
- One can perform regression with any kind of parameterized function using gradient descent.

5 - A bit of learning theory

What matters during training?

- Before going further, let's think about what we have been doing so far. We had a bunch of data samples $\mathcal{D} = (x_i, t_i)_{i=1..N}$ (the **training set**) and we decided to apply a (linear) model on it:

$$y_i = w \, x_i + b$$

- We then minimized the mean square error (mse) on that training set using gradient descent. At the end of learning, we can measure the **residual error** of the model on the data:

$$\epsilon_\mathcal{D} = \frac{1}{N} \, \sum_{i=1}^{N} (t_i - y_i)^2$$

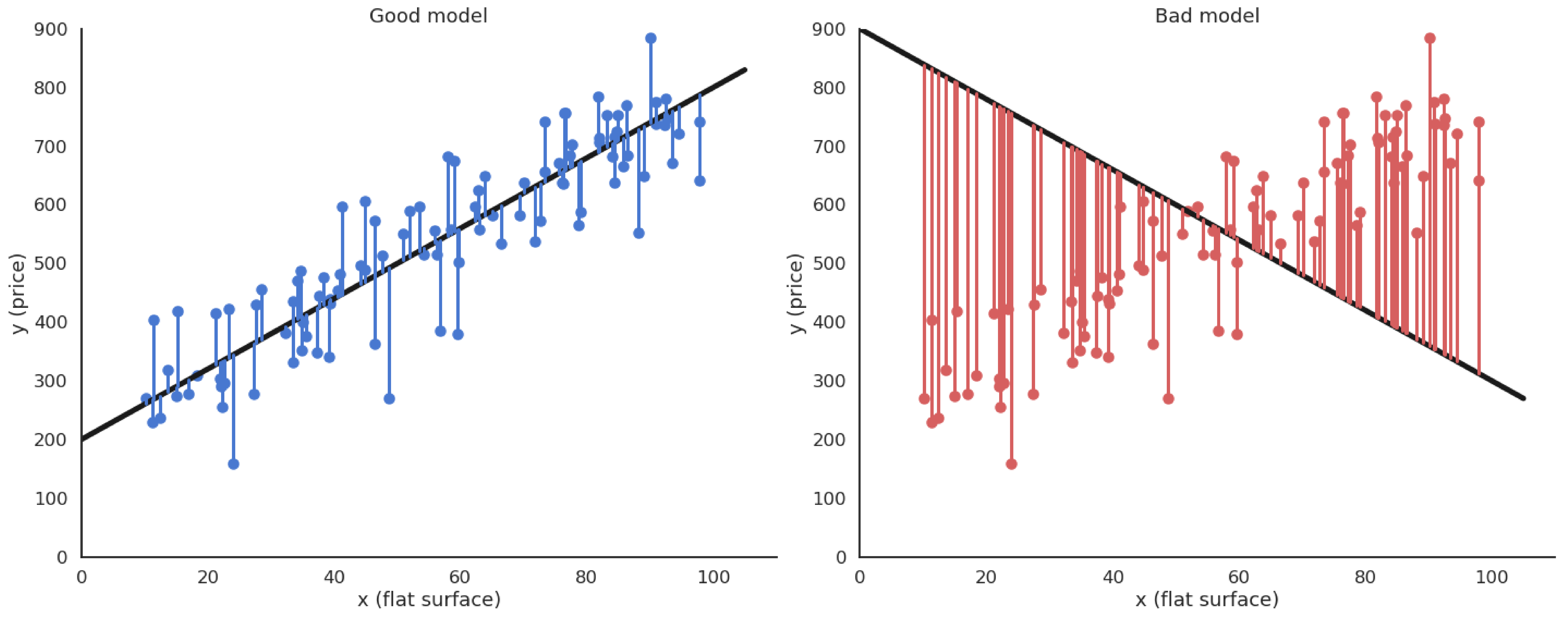
- We get a number, for example 0.04567. Is that good?

Regression error

- The **mean square error** mse is not very informative, as its value depends on how the outputs are scaled:

$$\epsilon_\mathcal{D} = \frac{1}{N} \sum_{i=1}^N (t_i - y_i)^2$$

- If you multiply both the data t and the prediction y by 10, the residual error will be 100 times higher, without any change to the quality of the model.

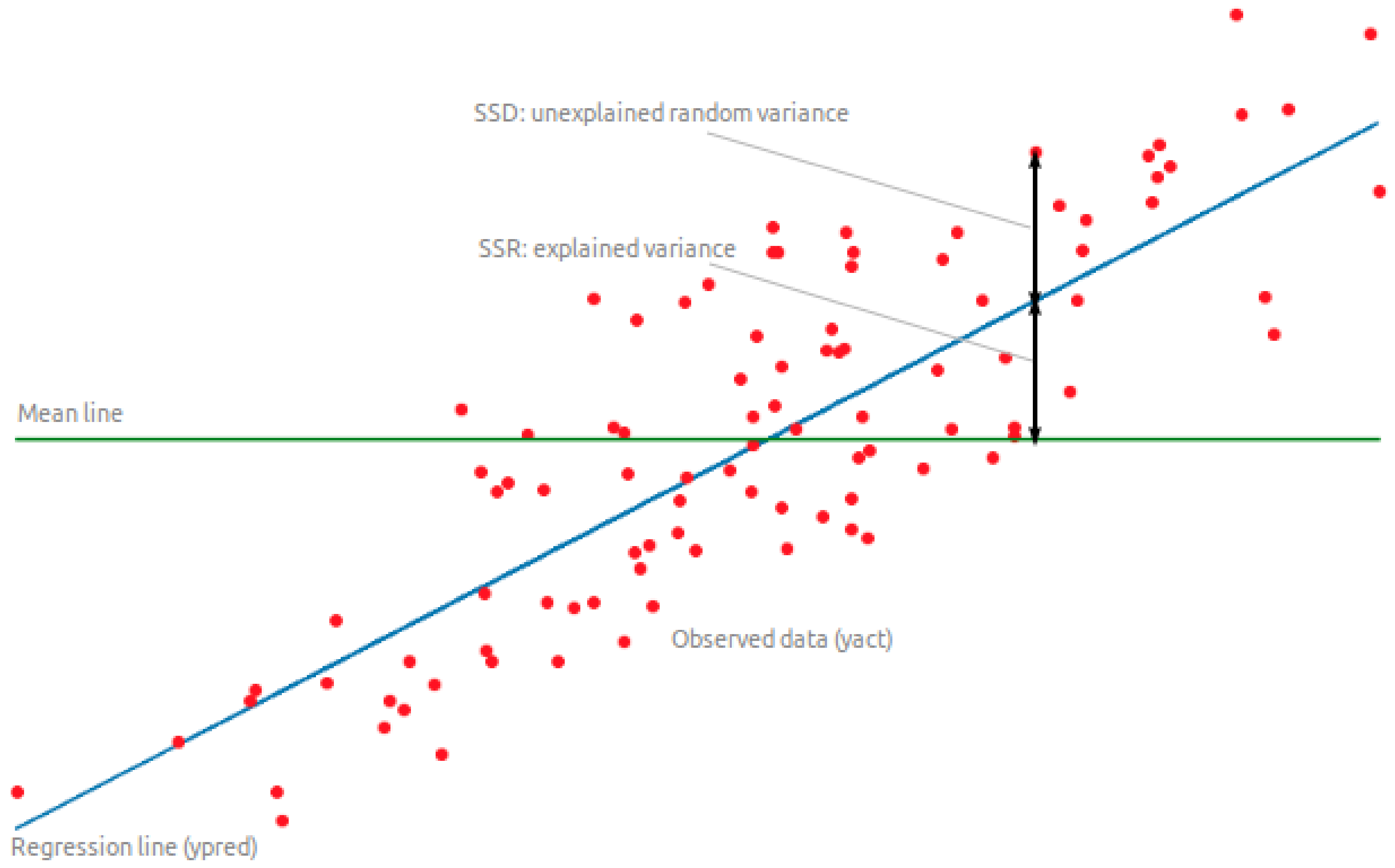


Coefficient of determination

- The **coefficient of determination** R^2 is a rescaled variant of the mse comparing the variance of the residuals to the variance of the data around its mean $\hat{t}$:

$$R^2 = 1 - \frac{\text{Var}(\text{residuals})}{\text{Var}(\text{data})} = 1 - \frac{\sum_{i=1}^N (t_i - y_i)^2}{\sum_{i=1}^N (t_i - \hat{t})^2}$$

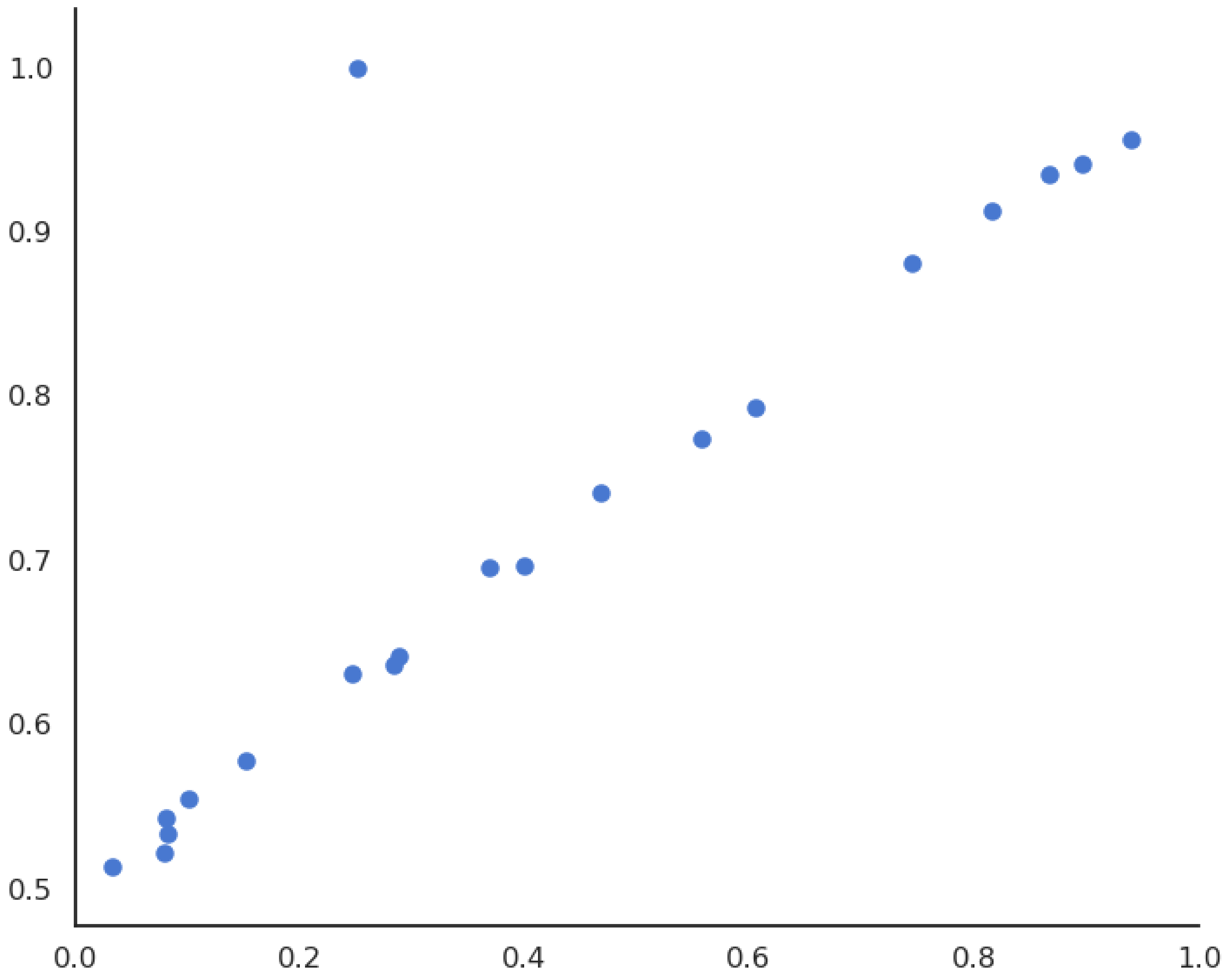
- R^2 should be as close from 1 as possible. For example, if $R^2 = 0.8$, we can say that the **model explains 80% of the variance of the data**.



Source: https://towardsdatascience.com/introduction-to-linear-regression-in-python-c12a072bedf0

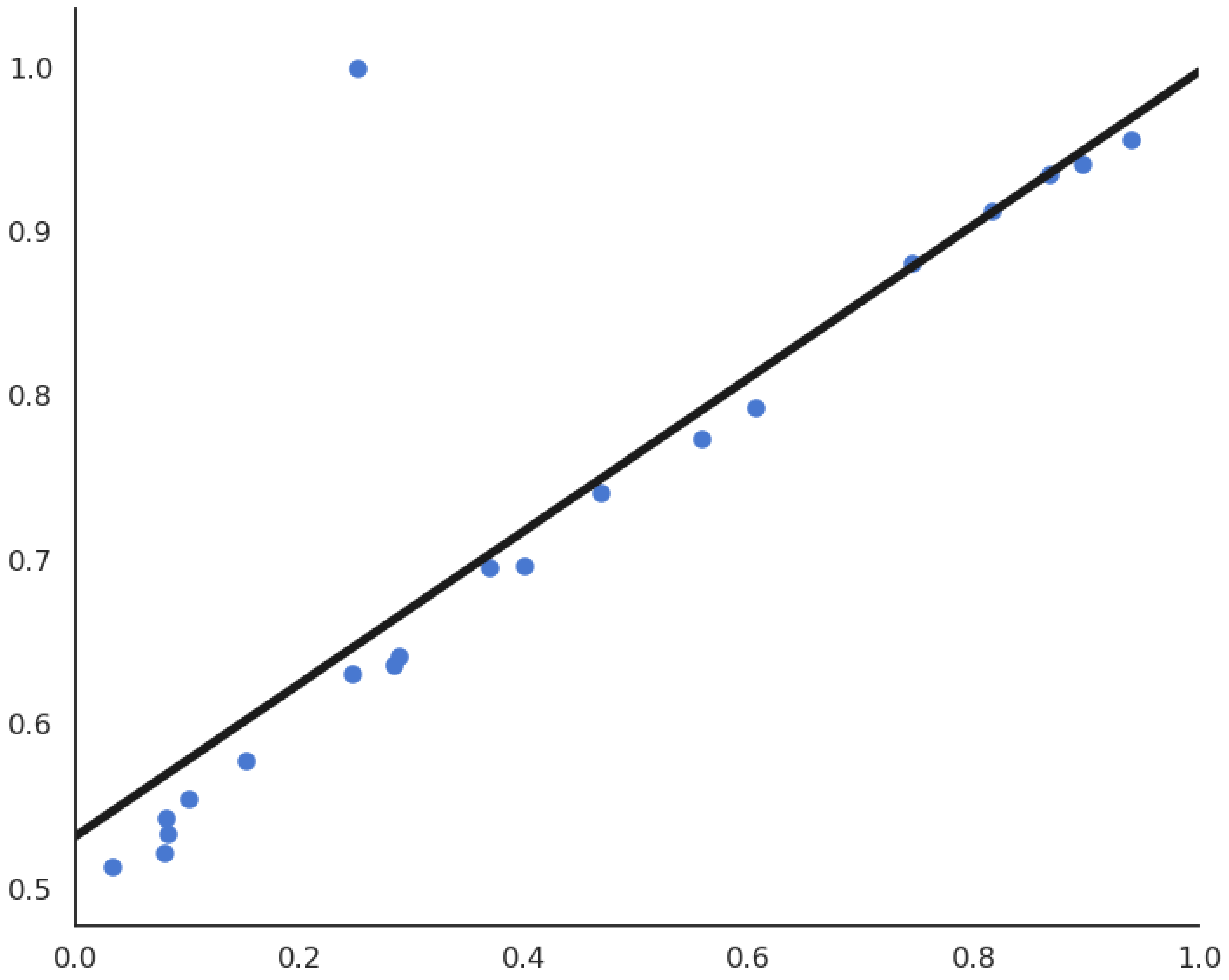
Sensibility to outliers

- Suppose we have a training set with one **outlier** (bad measurement, bad luck, etc).



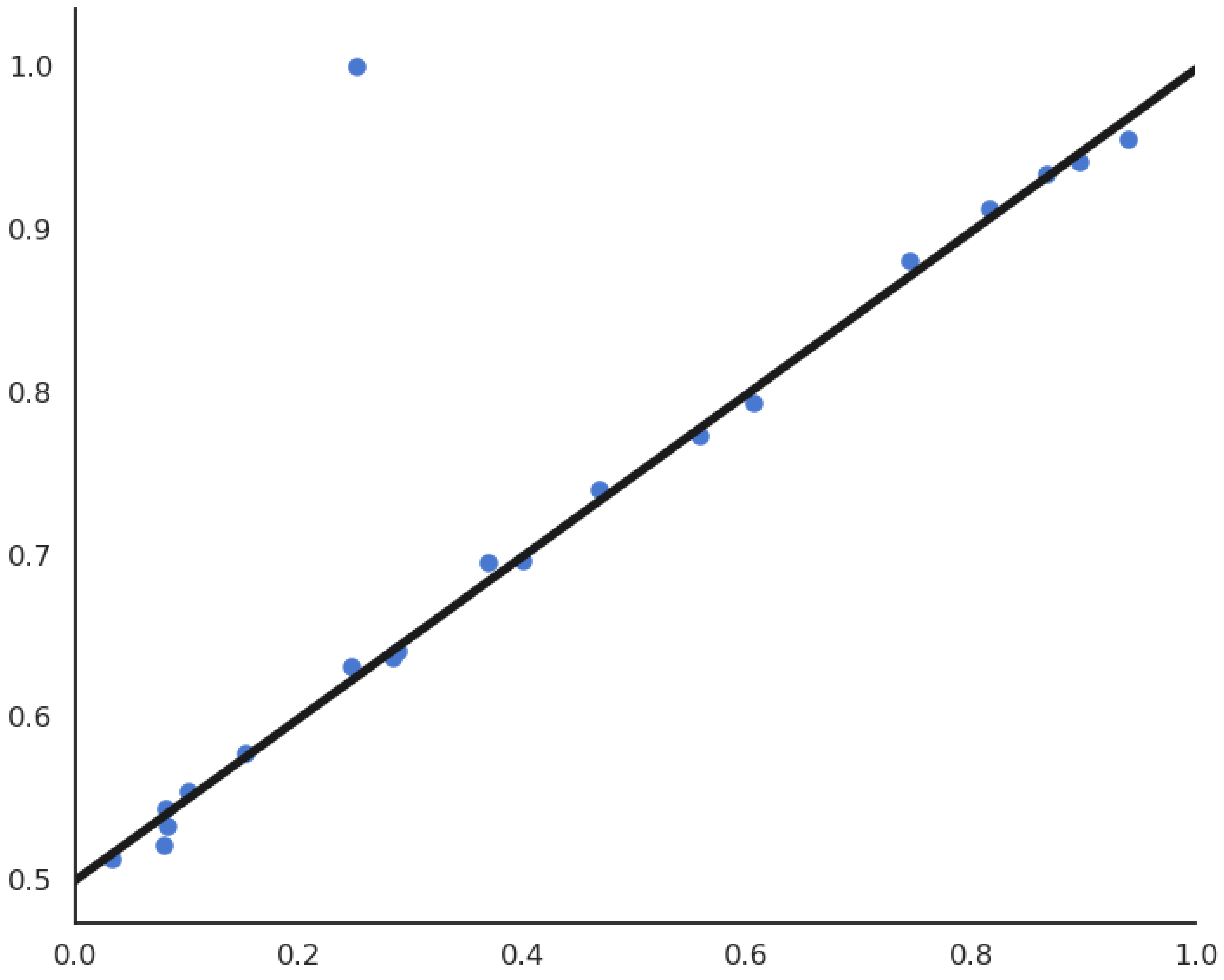
Sensibility to outliers

- LMS would find the minimum of the mse, but it is clearly a bad fit for most points.

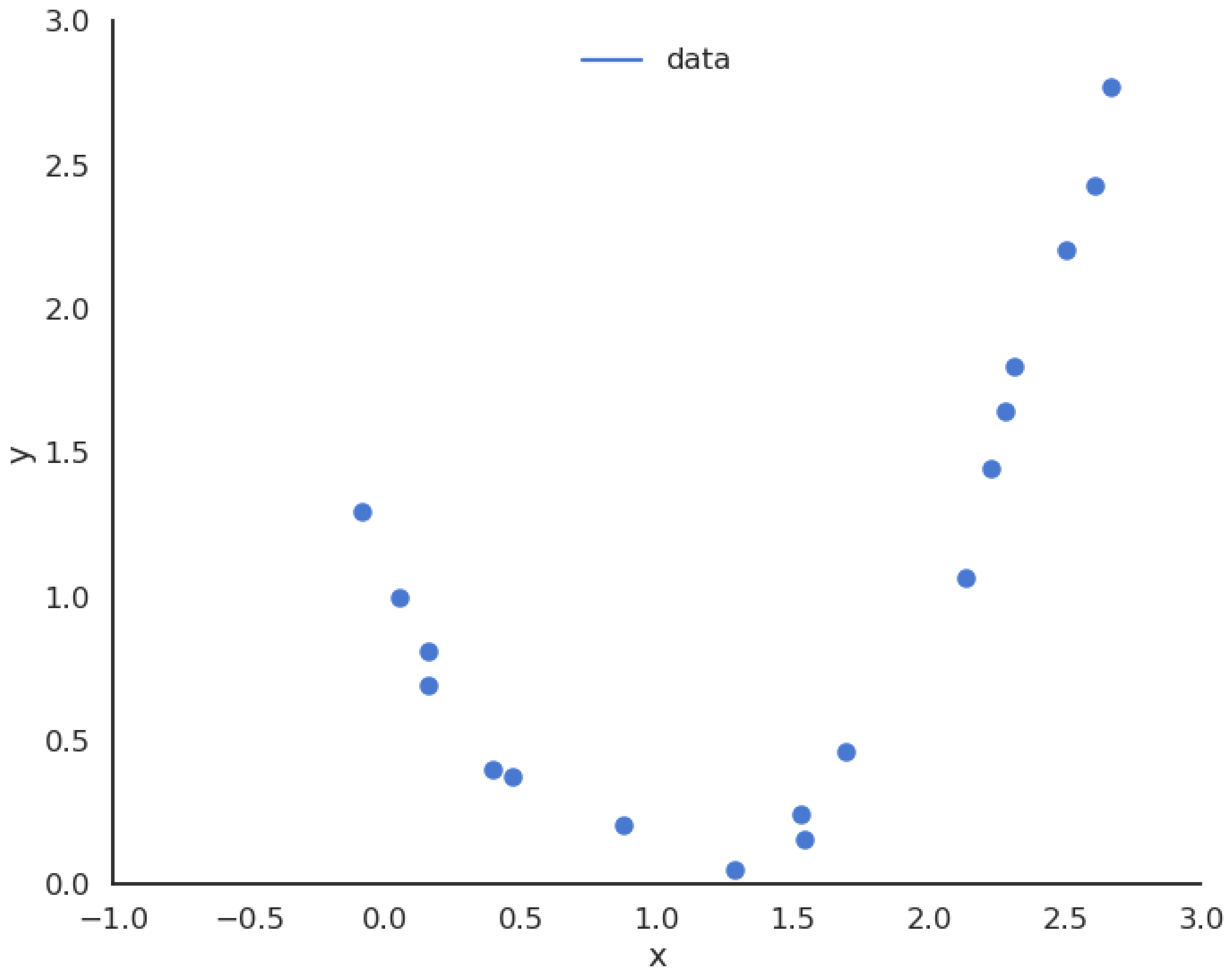


Sensibility to outliers

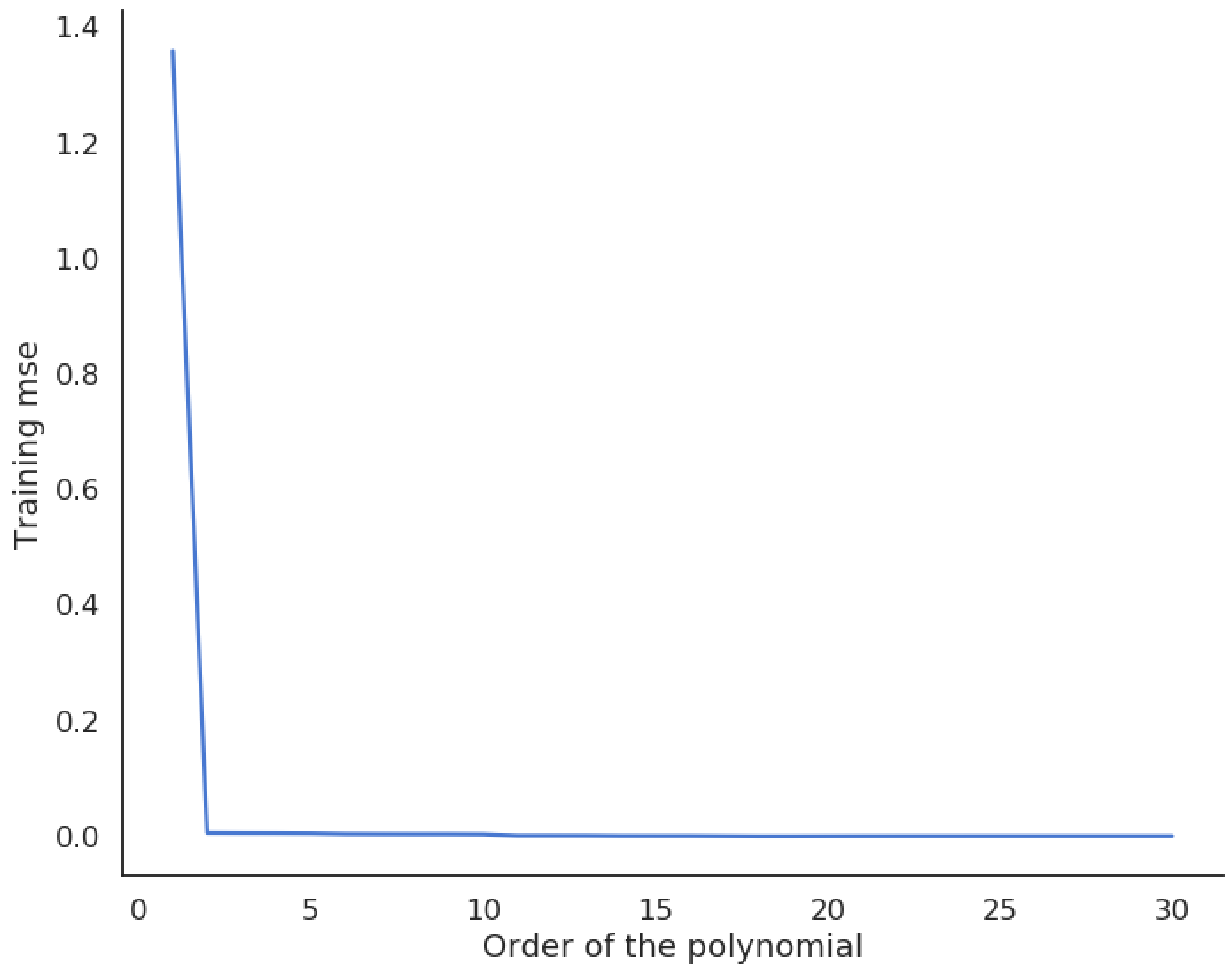
- This model feels much better, but its residual mse is higher…



Polynomial regression



Polynomial regression



- When only looking at the residual mse on the training data, one could think that the higher the order of the polynomial, the better.
- But it is obvious that the interpolation quickly becomes very bad when the order is too high.
- A **complex** model (with a lot of parameters) is useless for predicting new values.
- We actually do **not** care about the error on the training set.
- We care about **generalization**.

Cross-validation

- Let's suppose we dispose of m models $\mathcal{M} = \{M_1, ..., M_m\}$ that could be used to fit (or classify) some data $\mathcal{D} = \{x_i, t_i\}_{i=1}^N$.
- Such a class could be the ensemble of polynomes with different orders, different algorithms (NN, SVM) or the same algorithm with different values for the hyperparameters (learning rate, regularization parameters…).
- The naive and **wrong** method to find the best hypothesis would be:

Wrong method!

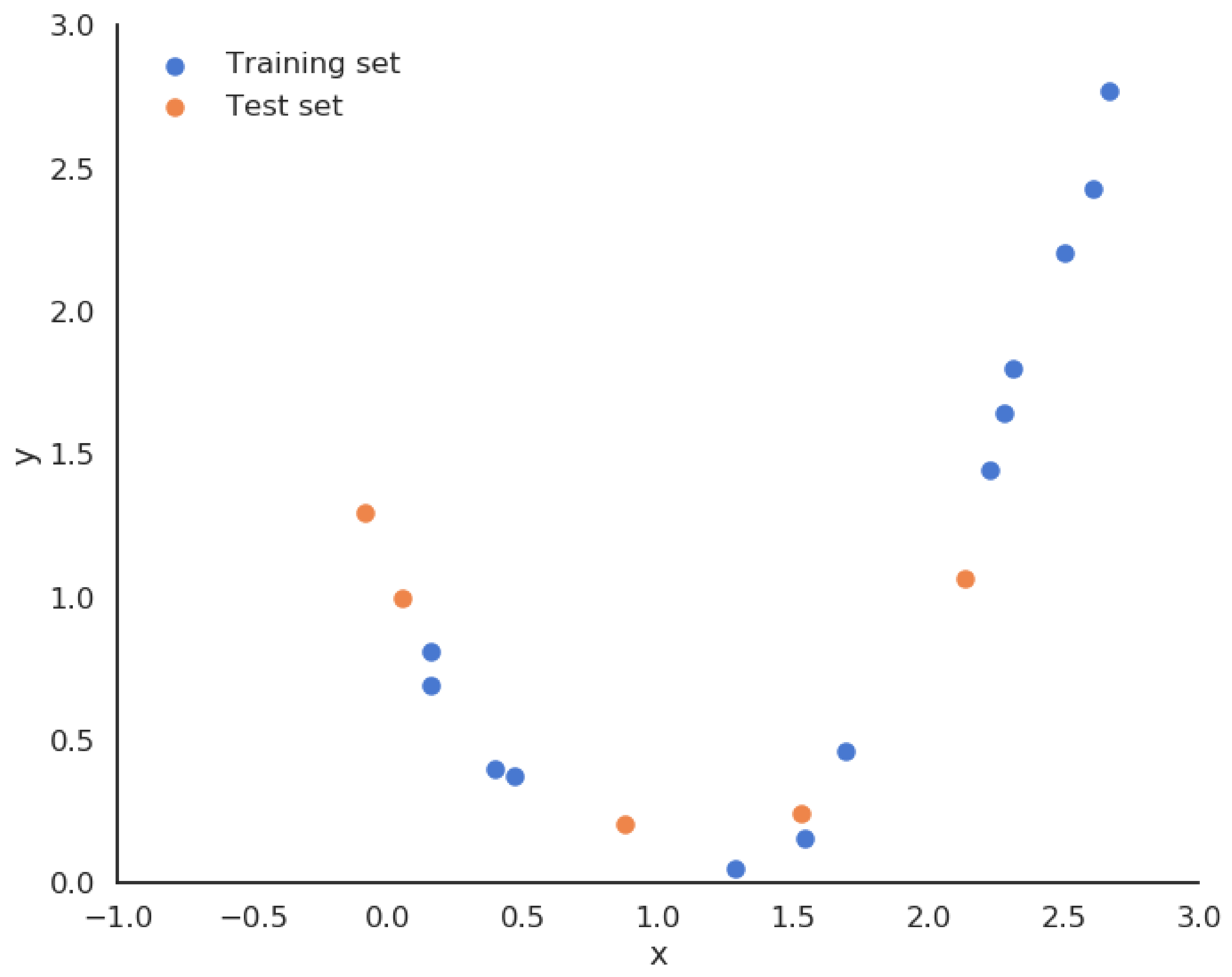
- For all models M_i:
  - Train M_i on $\mathcal{D}$ to obtain an hypothesis h_i.
  - Compute the training error $\epsilon_\mathcal{D}(h_i)$ of h_i on $\mathcal{D}$:

$$\epsilon_\mathcal{D}(h_i) = \mathbb{E}_{(\mathbf{x}, t) \in \mathcal{D}} [(h_i(\mathbf{x}) - t)^2]$$

- Select the hypothesis h_i^* with the minimal training error : $h_i^* = \text{argmin}_{h_i \in \mathcal{M}} \quad \epsilon_\mathcal{D}(h_i)$

- This method leads to **overfitting**, as only the training error is used.

Cross-validation: training and test sets



- The solution is randomly take some samples out of the training set to form the **test set**.
- Typical values are 20 or 30 % of the samples in the test set.
- Method:
    1. Train the model on the training set (70% of the data).
    2. Test the performance of the model on the test set (30% of the data).
- The test performance will better measure how well the model generalizes to new examples.

Simple hold-out cross-validation

Algorithm

- Split the training data $\mathcal{D}$ into $\mathcal{S}_{\text{train}}$ and $\mathcal{S}_{\text{test}}$.
- For all models M_i:
    - Train M_i on $\mathcal{S}_{\text{train}}$ to obtain an hypothesis h_i.
    - Compute the empirical error $\epsilon_{\text{test}}(h_i)$ of h_i on $\mathcal{S}_{\text{test}}$:

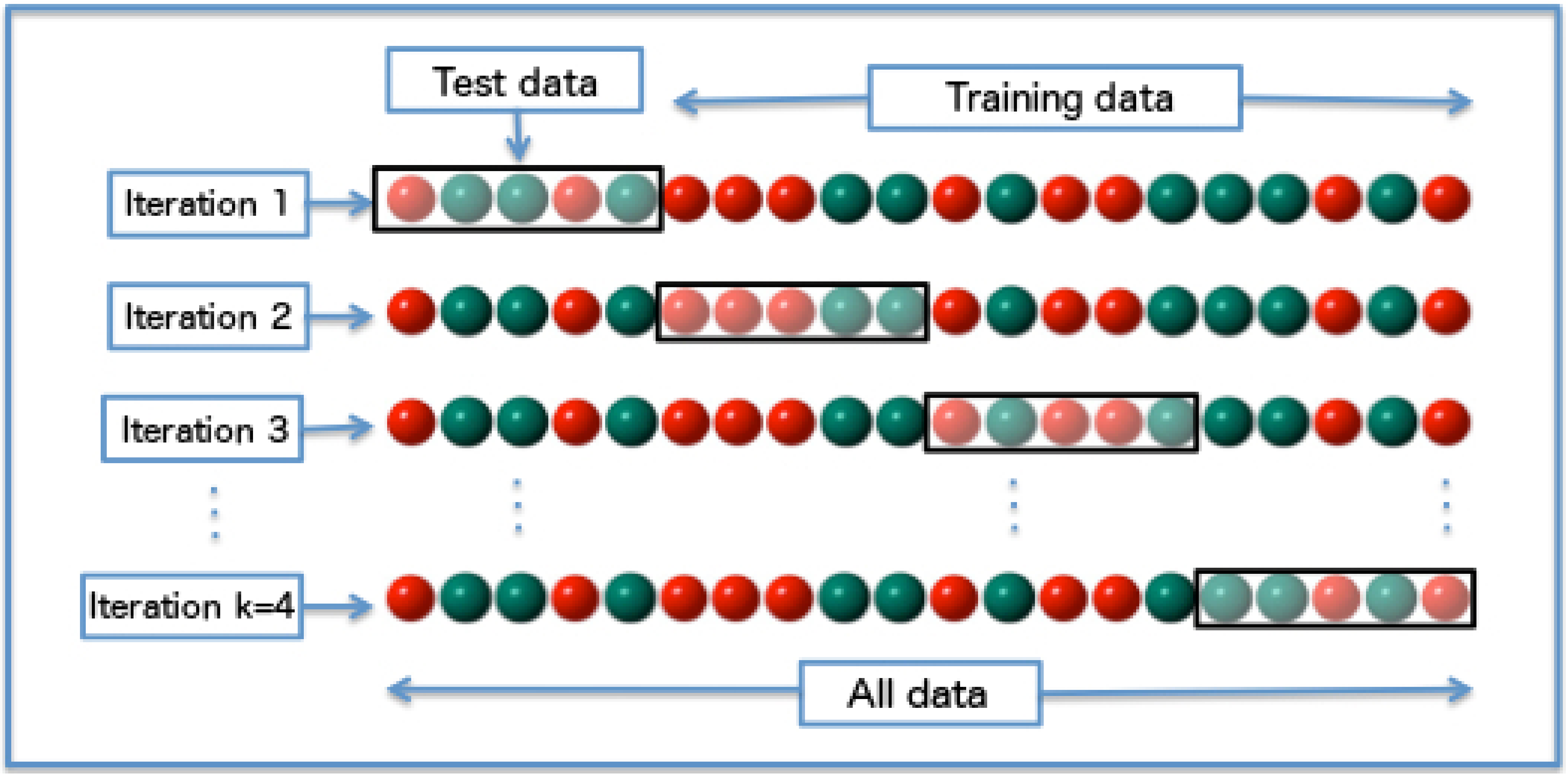
$$\epsilon_{\text{test}}(h_i) = \mathbb{E}_{(\mathbf{x}, t) \in \mathcal{S}_{\text{test}}} [(h_i(\mathbf{x}) - t)^2]$$

- Select the hypothesis h_i^* with the minimal empirical error : $h_i^* = \text{argmin}_{h_i \in \mathcal{M}} \quad \epsilon_{\text{test}}(h_i)$

- Disadvantages:
    - 20 or 30% of the data is wasted and not used for learning. It may be a problem when data is rare or expensive.
    - The test set must be representative of the difficulty of the training set (same distribution).

k-fold cross-validation

- **Idea:**
  - build several different training/test sets with the same data.
  - train and test each model repeatedly on each partition.
  - choose the hypothesis that works best on average.



k-fold cross-validation

Algorithm

- Randomly split the data $\mathcal{D}$ into k subsets of $\frac{N}{k}$ examples $\{\mathcal{S}_1, \ldots, \mathcal{S}_k\}$
- For all models M_i:
    - For all k subsets $\mathcal{S}_j$:
        - Train M_i on $\mathcal{D} - \mathcal{S}_j$ to obtain an hypothesis h_{ij}
        - Compute the empirical error $\epsilon_{\mathcal{S}_j}(h_{ij})$ of h_{ij} on $\mathcal{S}_j$
    - The empirical error of the model M_i on $\mathcal{D}$ is the average of empirical errors made on $(\mathcal{S}_j)_{j=1}^{k}$

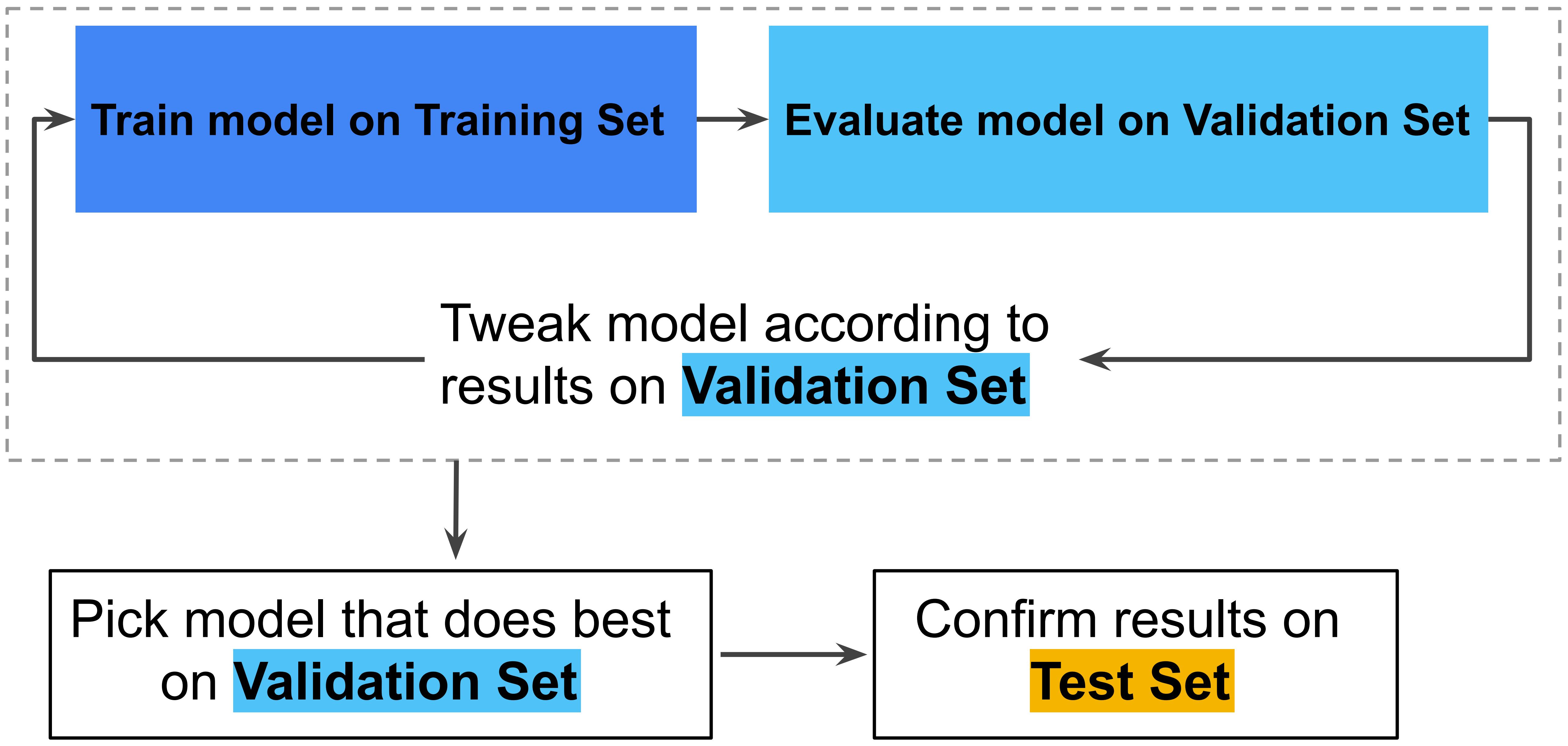
$$\epsilon_{\mathcal{D}}(M_i) = \frac{1}{k} \cdot \sum_{j=1}^{k} \epsilon_{\mathcal{S}_j}(h_{ij})$$

- Select the model M_i^* with the minimal empirical error on $\mathcal{D}$.

- In general $k = 10$. Extreme cases take $k = N$: **leave-one-out cross-validation**.
- k-fold cross-validation works well, but needs a lot of repeated learning.

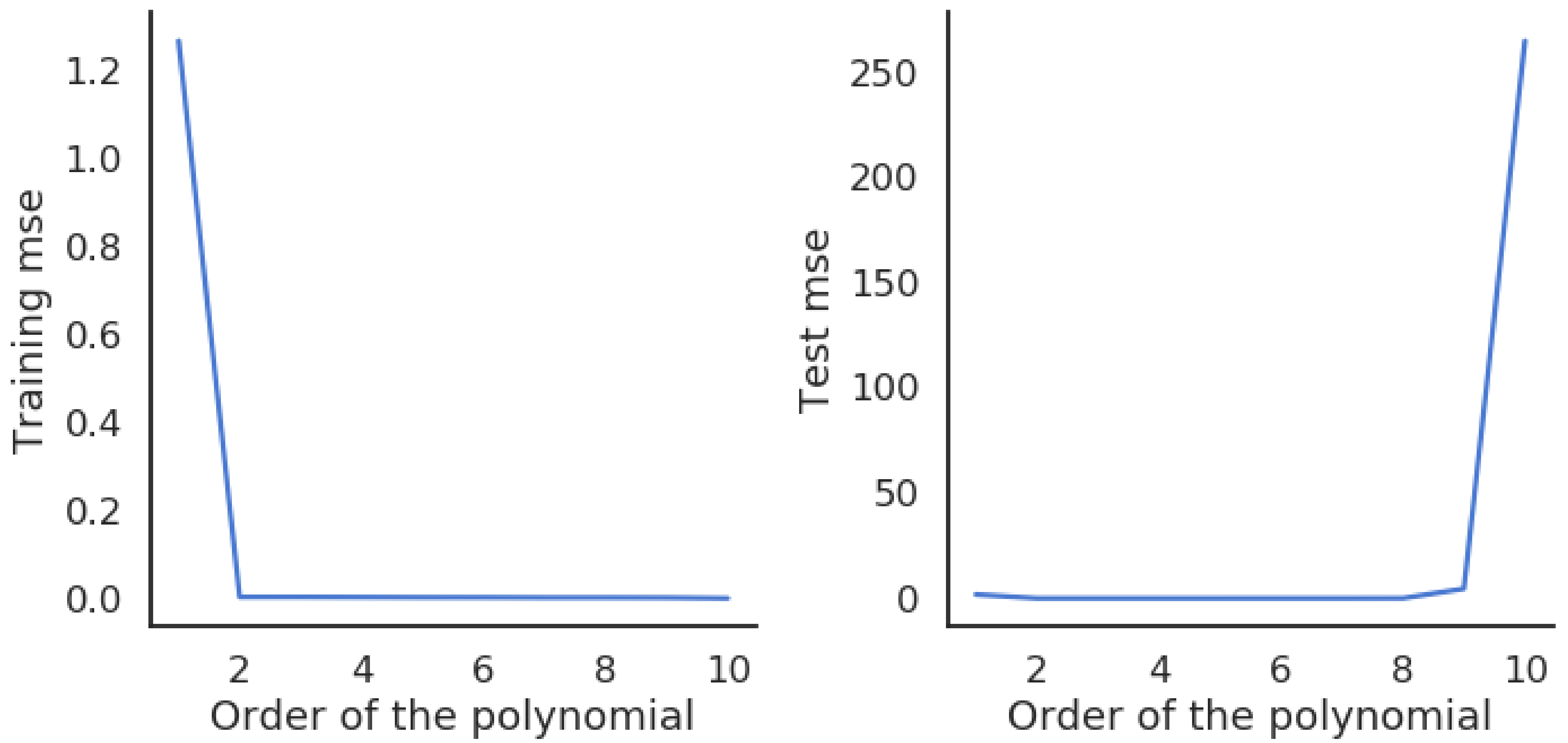
Validation data

- The bare minimum in ML is to have separate training and test sets. However, the test set should only be used once:
  - If you try many variations of the same algorithm on a single test set and keep the best one, you end up overfitting the test set: the model may not generalize well to novel data…
- A third **validation set** is typically used to track overfitting during training and perform model selection.
- The test set is ultimately used to report the final performance.


Train model on Training Set
Evaluate model on Validation Set
Tweak model according to results on Validation Set
Pick model that does best on Validation Set
Confirm results on Test Set

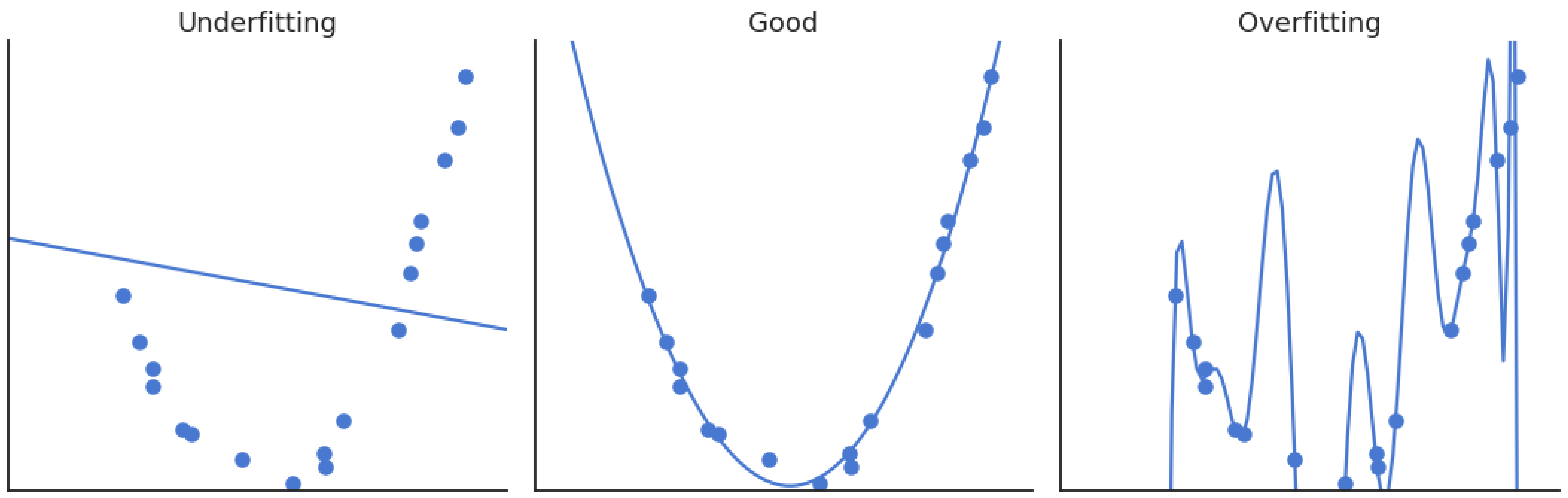
Source: https://developers.google.com/machine-learning/crash-course/validation/another-partition

Training and test errors



- While the training mse always decrease with more complex models, the validation/test mse increases after a while.
- This is called **overfitting**: learning by heart the data without caring about generalization.
- The two curves suggest that we should chose a polynomial order between 2 and 9.

Underfitting / Overfitting



- A model not complex enough for the data will **underfit**: its training error is high.
- A model too complex for the data will **overfit**: its test error is high.
- In between, there is the right complexity for the model: it learns the data correctly but does not overfit.

What does complexity mean?

- In polynomial regression, the complexity is related to the order of the polynomial, i.e. the number of coefficients to estimate:

$$y = f_{\mathbf{w},b}(x) = \sum_{k=1}^p w_k \, x^k + b$$

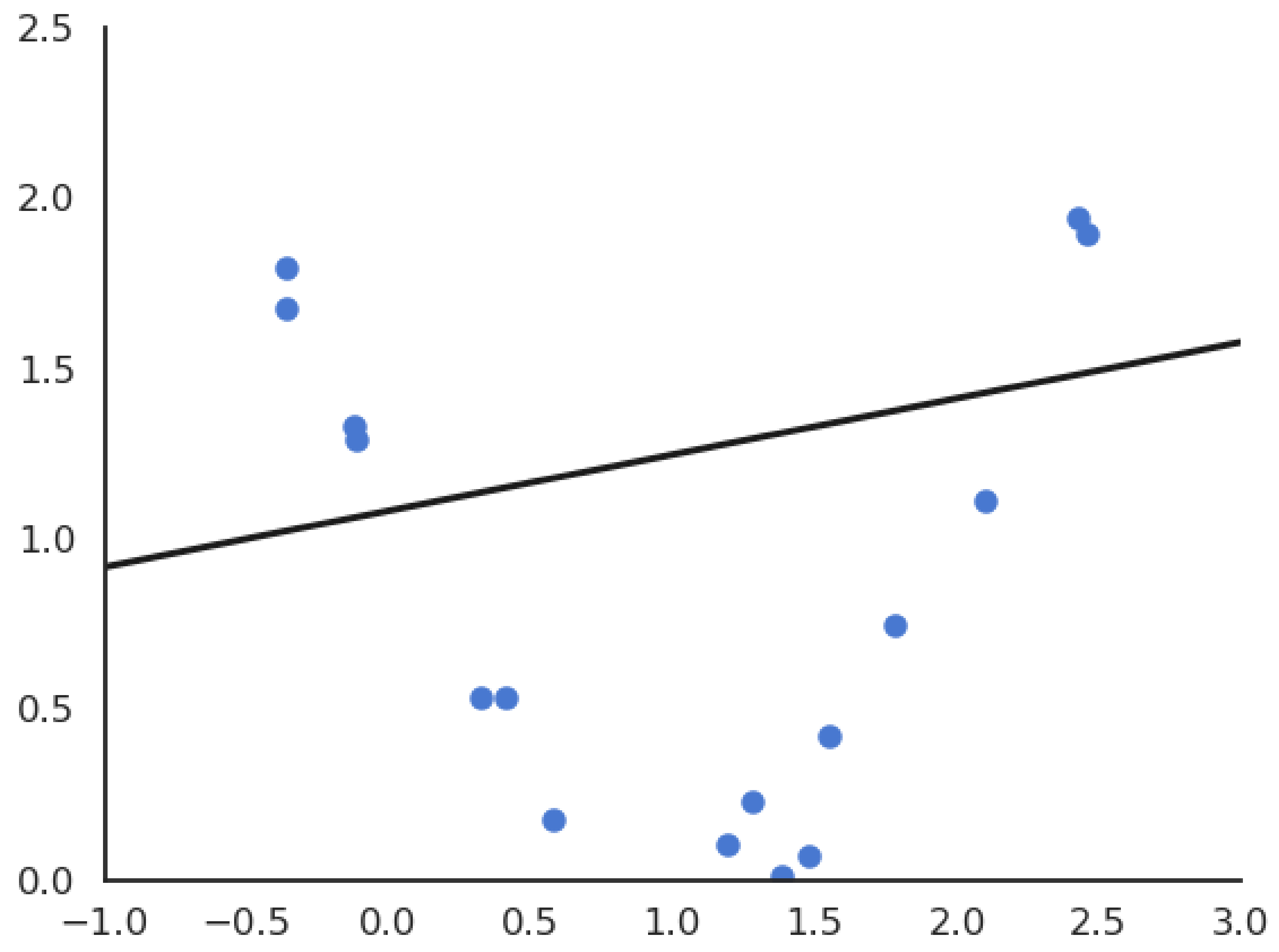
$$\mathbf{x} = \begin{bmatrix} x \\ x^2 \\ \ldots \\ x^p \end{bmatrix} \qquad \mathbf{w} = \begin{bmatrix} w_1 \\ w_2 \\ \ldots \\ w_p \end{bmatrix}$$

- A polynomial of order p has $p+1$ unknown parameters (**free parameters**): the p weights and the bias.
- Generally, the **complexity of a model** relates to its **number of free parameters**:
    - **The more free parameters, the more complex the model is, the more likely it will overfit.**

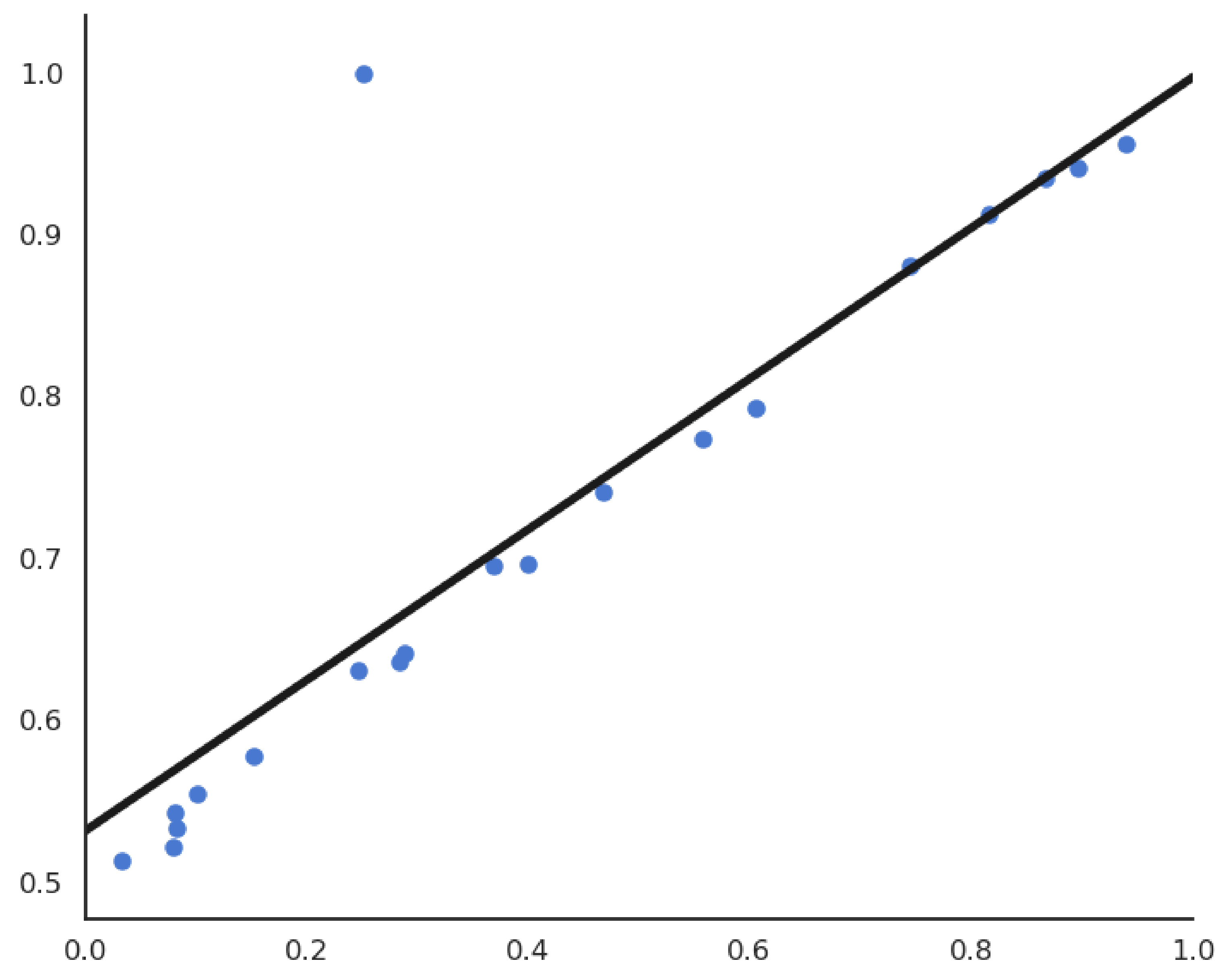
6 - Regularized regression

Linear regression can either underfit or overfit depending on the data

Underfitting

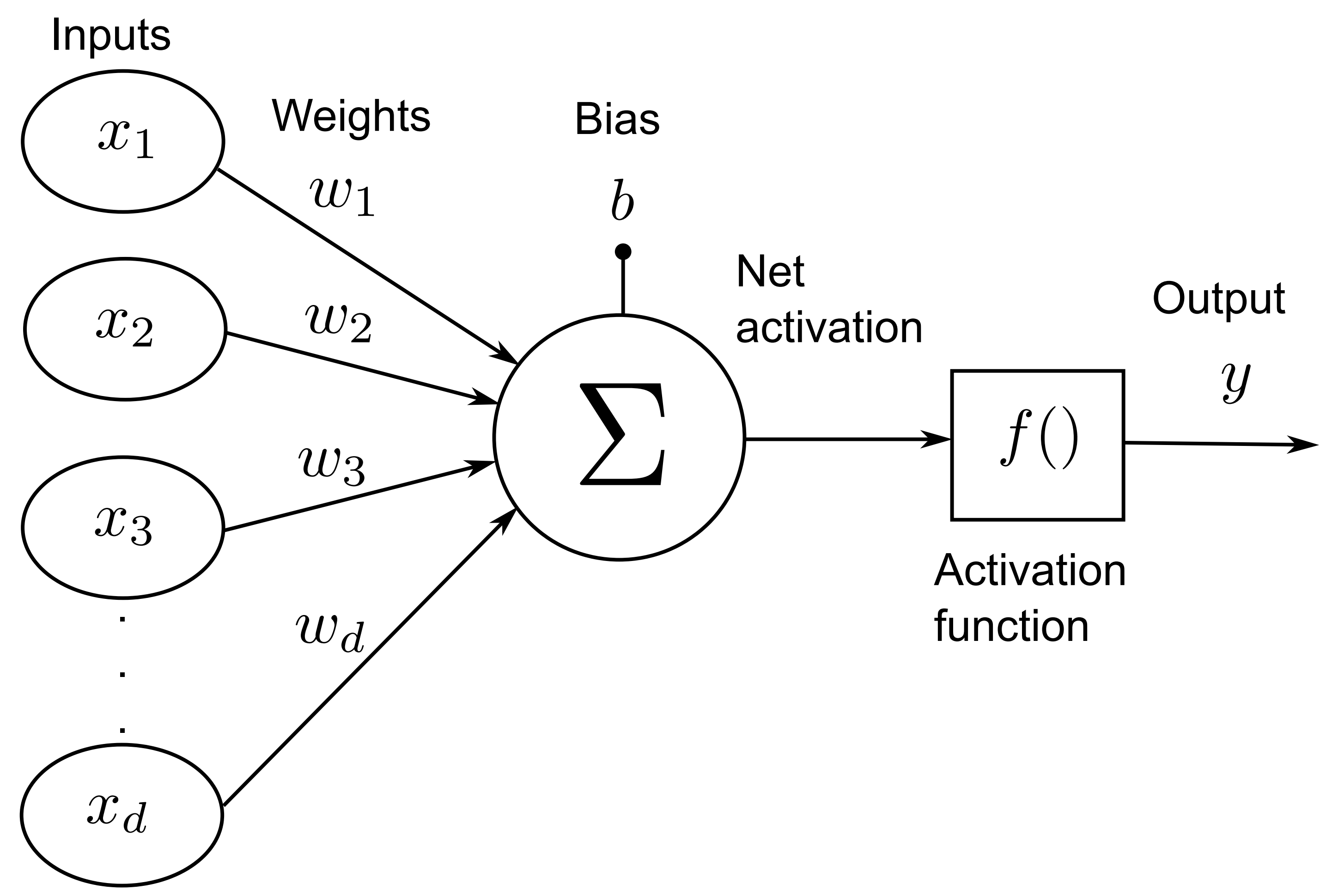


Overfitting



- When linear regression **underfits** (both training and test errors are high), the data is not linear: we need to use a **neural network**.
- When linear regression **overfits** (the test error is higher than the training error), we would like to **decrease its complexity**.

Complexity of a linear regression



- The problem is that the number of free parameters in linear regression only depends on the number of inputs (dimensions of the input space).

$$y = \sum_{i=1}^d w_i \, x_i + b$$

- For d inputs, there are $d+1$ free parameters: the d weights and the bias.

- We must find a way to reduce the complexity of the linear regression without changing the number of parameters, which is impossible.
- The solution is to **constrain** the values that the parameters can take: **regularization**.
- Regularization reduces the variance at the cost of increasing the bias.

L2 regularization - Ridge regression

- Using **L2 regularization** for linear regression leads to the **Ridge regression** algorithm.
- The individual loss function is defined as:

$$l_i(\mathbf{w}, b) = (t_i - y_i)^2 + \lambda \, ||\mathbf{w}||^2$$

- The first part of the loss function is the classical **mse** on the training set: its role is to reduce the **bias**.
- The second part minimizes the L2 norm of the weight vector (or matrix), reducing the variance:

$$||\mathbf{w}||^2 = \sum_{i=1}^{d} w_i^2$$

- Deriving the regularized delta learning rule is straightforward:

$$\Delta w_i = \eta \, ((t_i - y_i) \, x_i - \lambda \, w_i)$$

- Ridge regression is also called **weight decay**: even if there is no error, all weights will decay to 0.

L1 regularization - LASSO regression

- Using **L1 regularization** for linear regression leads to the **LASSO regression** algorithm (least absolute shrinkage and selection operator).
- The individual loss function is defined as:

$$l_i(\mathbf{w}, b) = (t_i - y_i)^2 + \lambda \, |\mathbf{w}|$$

- The second part minimizes this time the L1 norm of the weight vector, i.e. its absolute value:

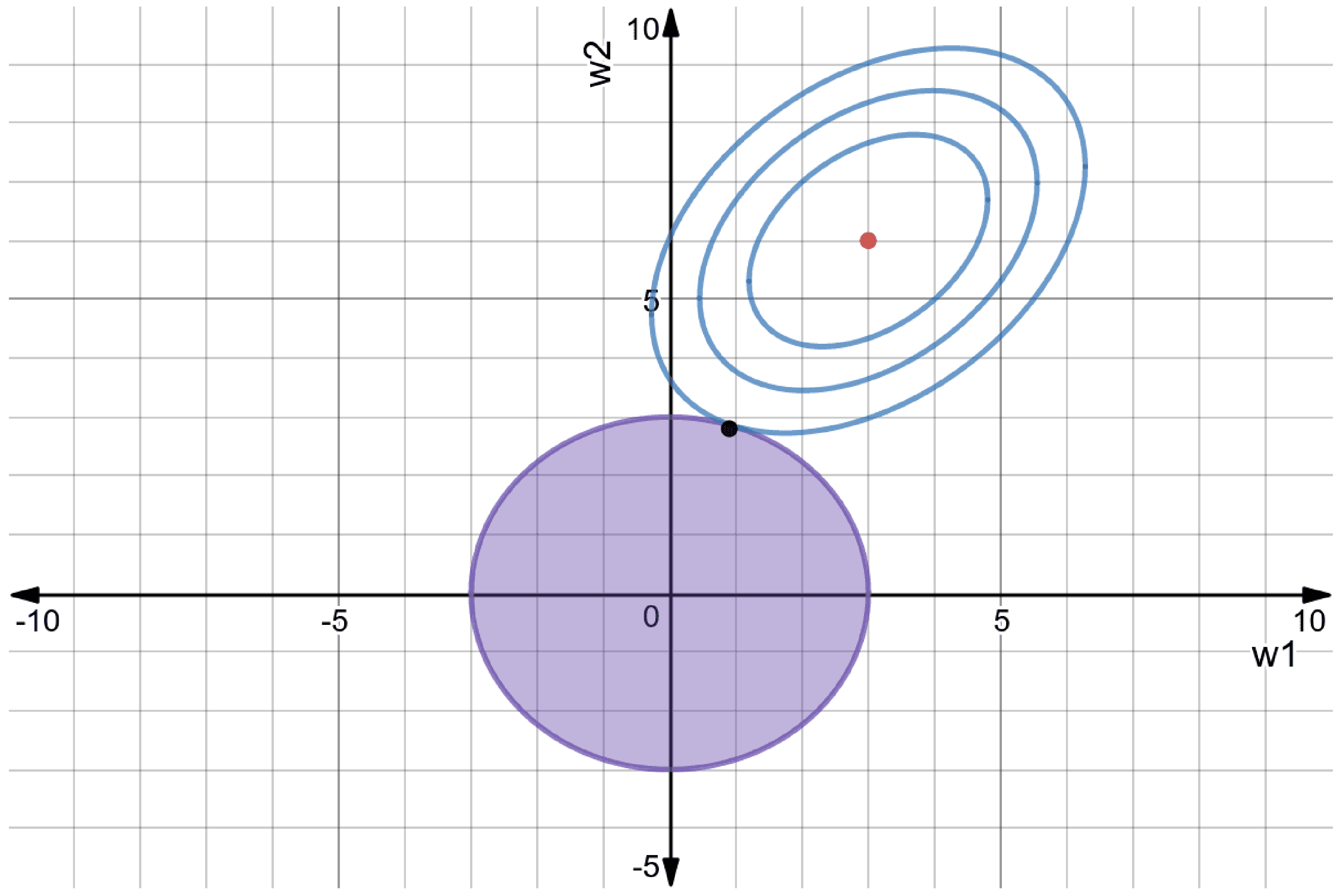
$$|\mathbf{w}| = \sum_{i=1}^{d} |w_i|$$

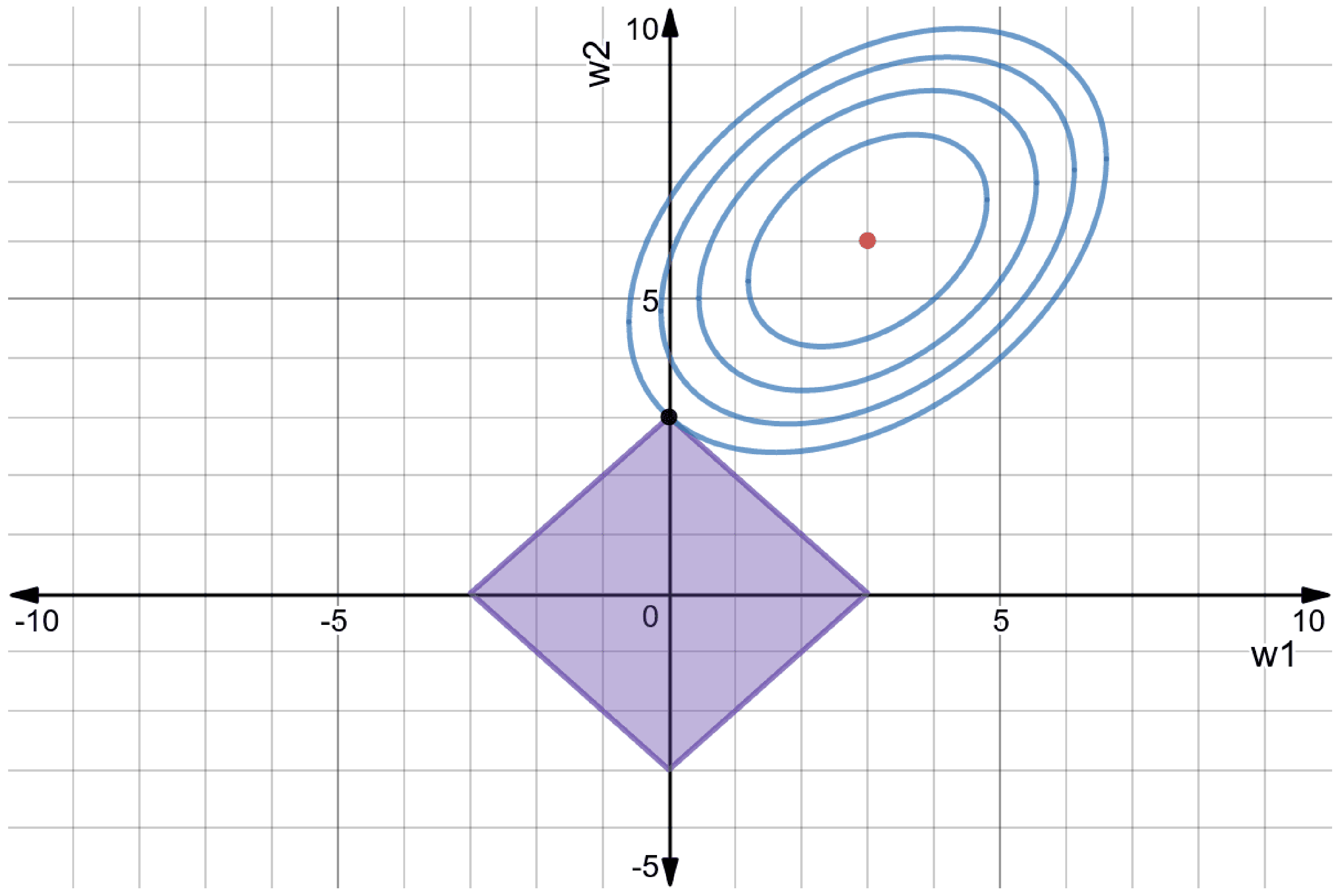
- Regularized delta learning rule with LASSO:

$$\Delta w_i = \eta \, ((t_i - y_i) \, x_i - \lambda \, \text{sign}(w_i))$$

- **Weight decay** does not depend on the value of the weight, only its sign. Weights can decay very fast to 0.

Ridge and Lasso regression



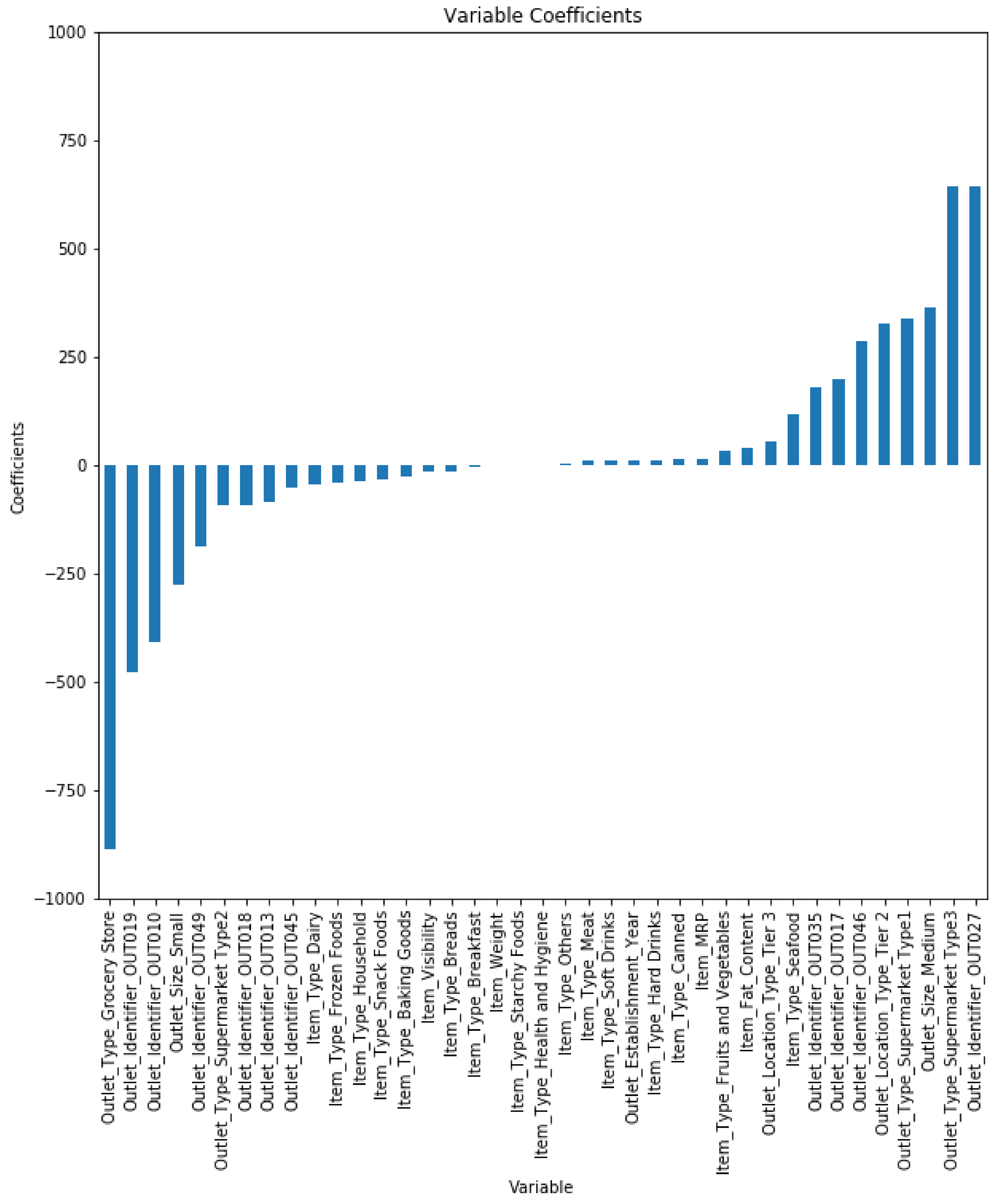


- **Ridge regression** finds the smallest value for the weights that minimize the mse.
- **LASSO regression** tries to set as many weight to 0 as possible (sparse code).

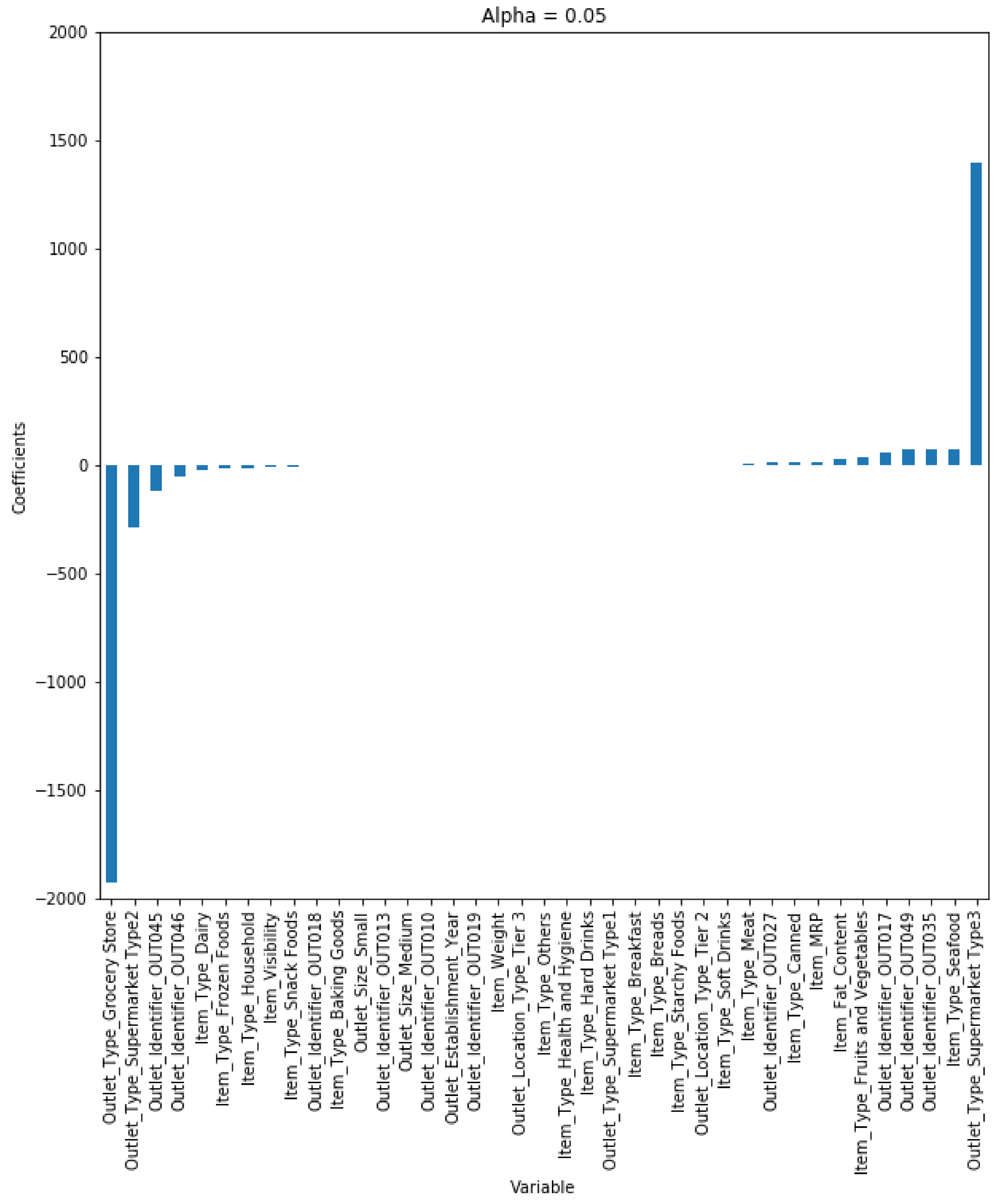
- Both methods depend on the **regularization parameter** λ. Its value determines how important the regularization term should.
- Regularization introduce a **bias**, as the solution found is **not** the minimum of the mse, but reduces the variance of the estimation, as small weights are less sensible to noise.

- LASSO allows **feature selection**: features with a zero weight can be removed from the training set.

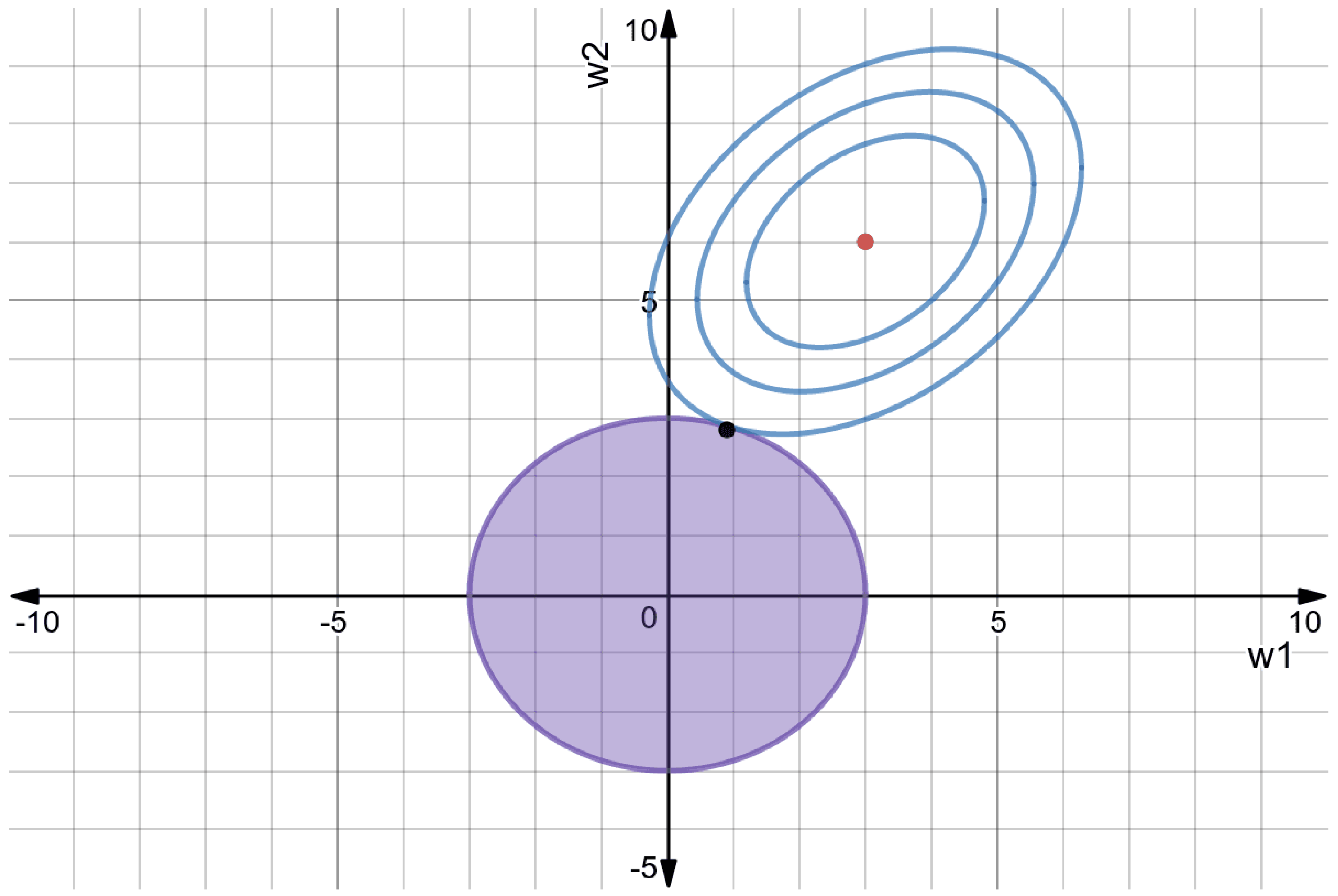
Linear regression

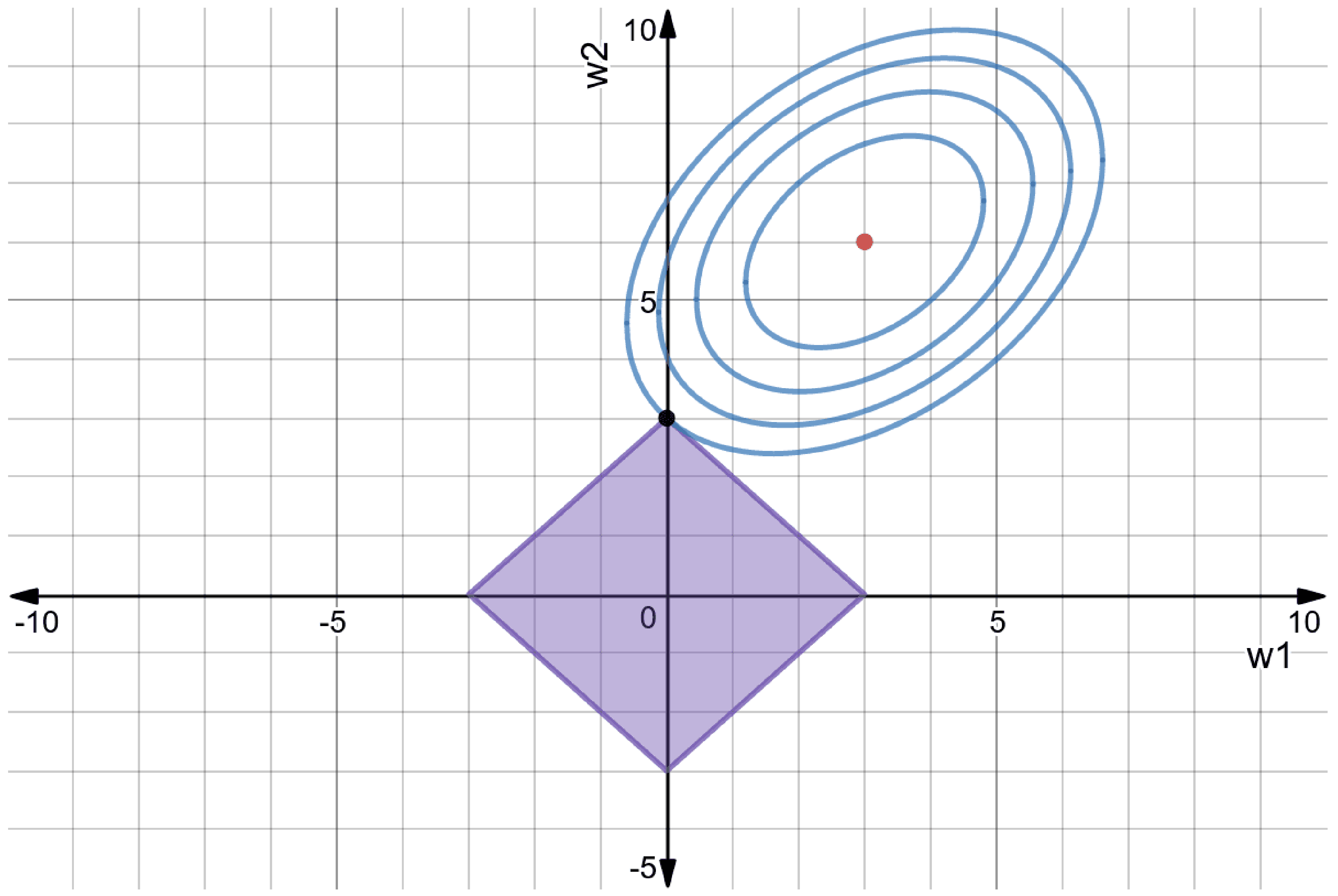


LASSO



L1+L2 regularization - ElasticNet





- An **ElasticNet** is a linear regression using both L1 and L2 regression:

$$l_i(\mathbf{w}, b) = (t_i - y_i)^2 + \lambda_1 \, |\mathbf{w}| + \lambda_2 \, ||\mathbf{w}||^2$$

- It combines the advantages of Ridge and LASSO, at the cost of having now two regularization parameters to determine.