TECHNISCHE UNIVERSITÄT
CHEMNITZ

Neurocomputing

Linear regression

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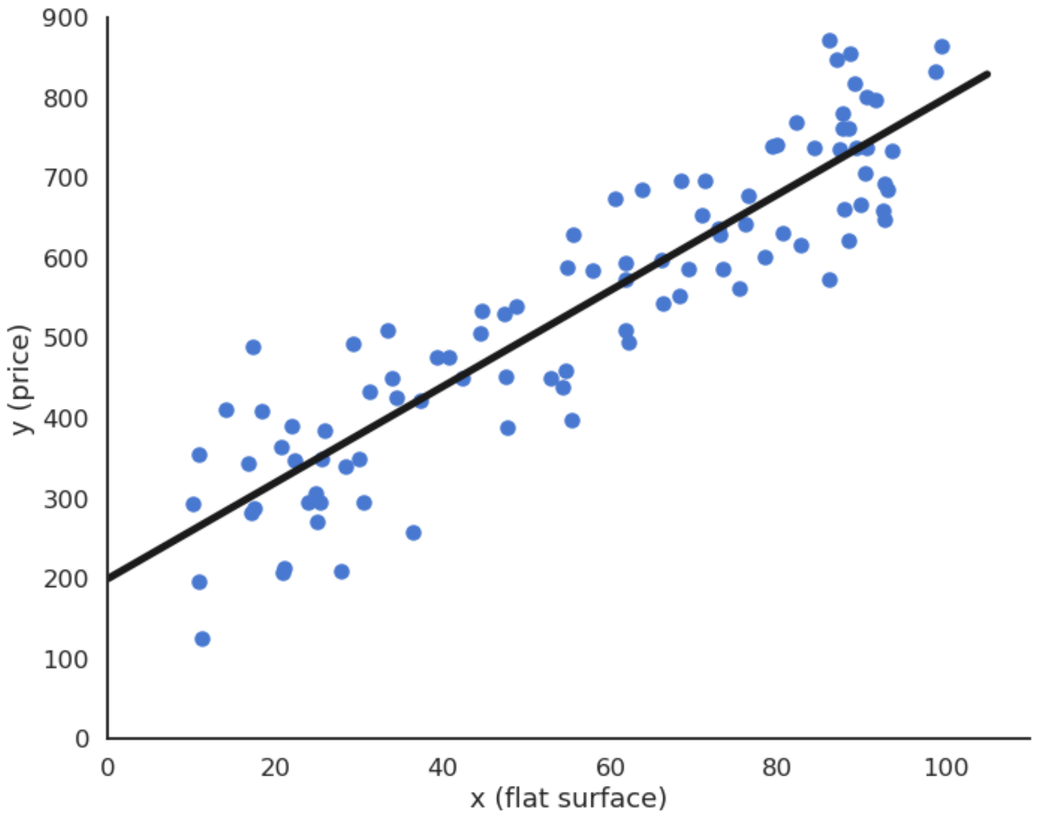
https://tu-chemnitz.de/informatik/KI/edu/neurocomputing

1 - Linear regression

Linear regression

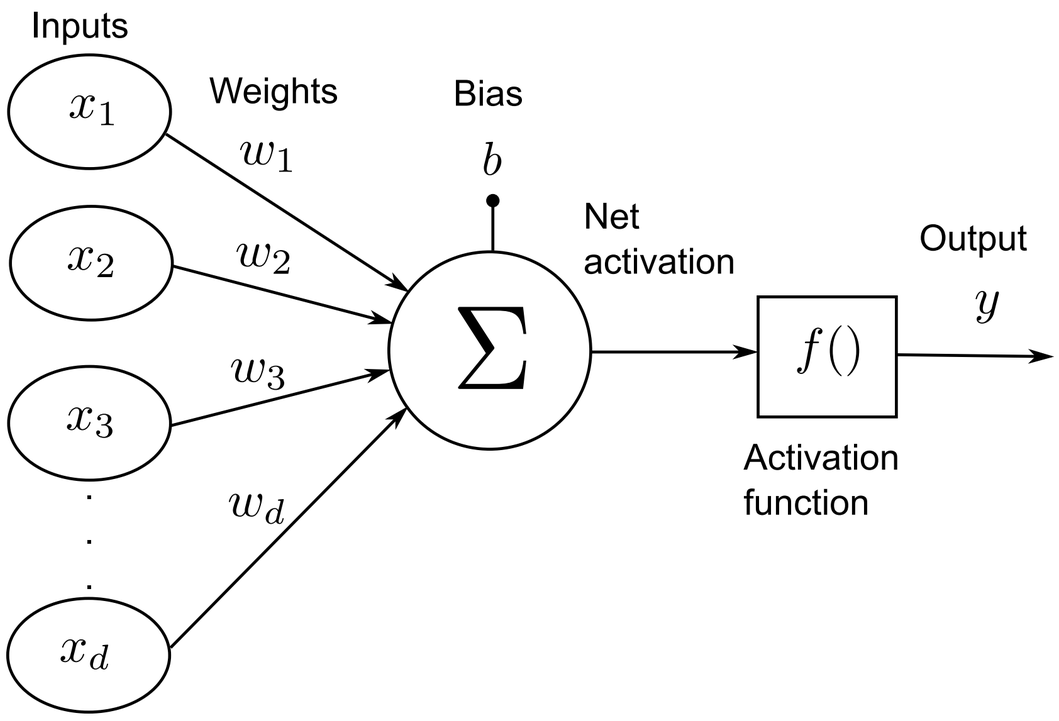


- We have a training set of N examples $\mathcal{D} = (x_i, t_i)_{i=1..N}$.
- In **linear regression**, we want to learn a linear model (hypothesis) y that is linearly dependent on the input x:

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

- 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:

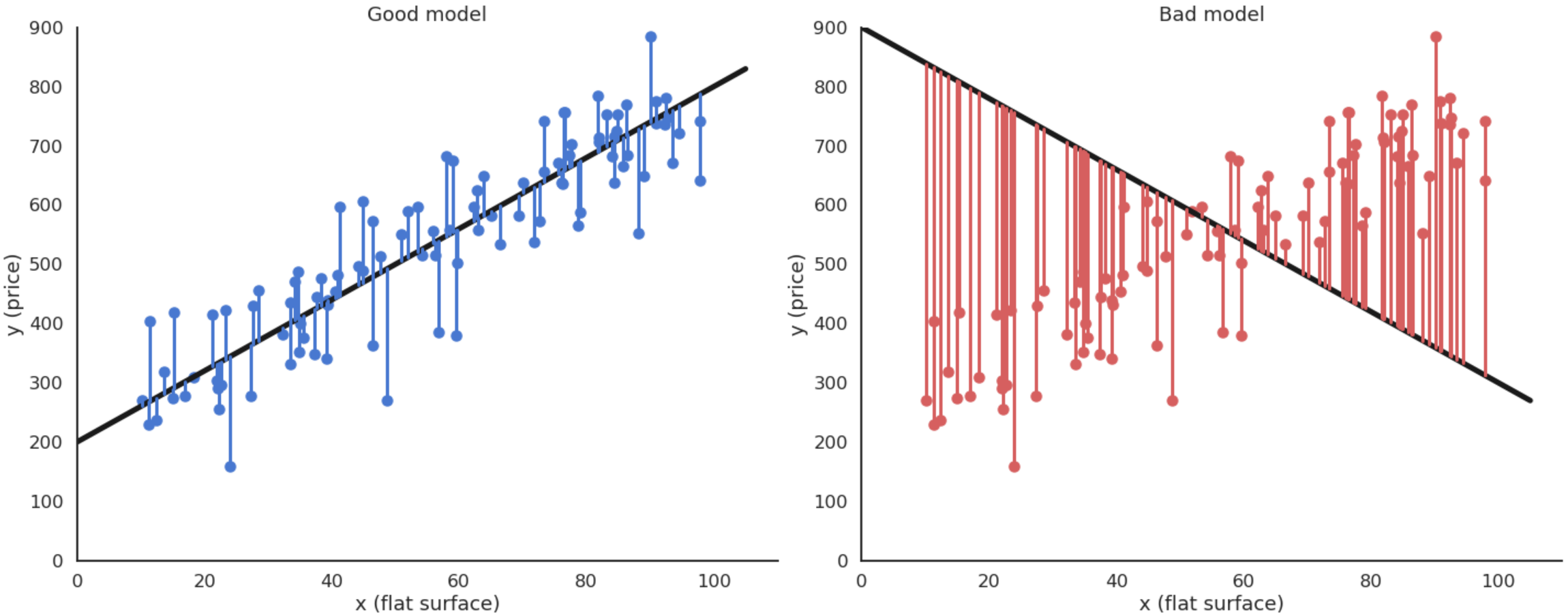
$$y = f_{w,b}(x) = w\,x + b$$

- 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:

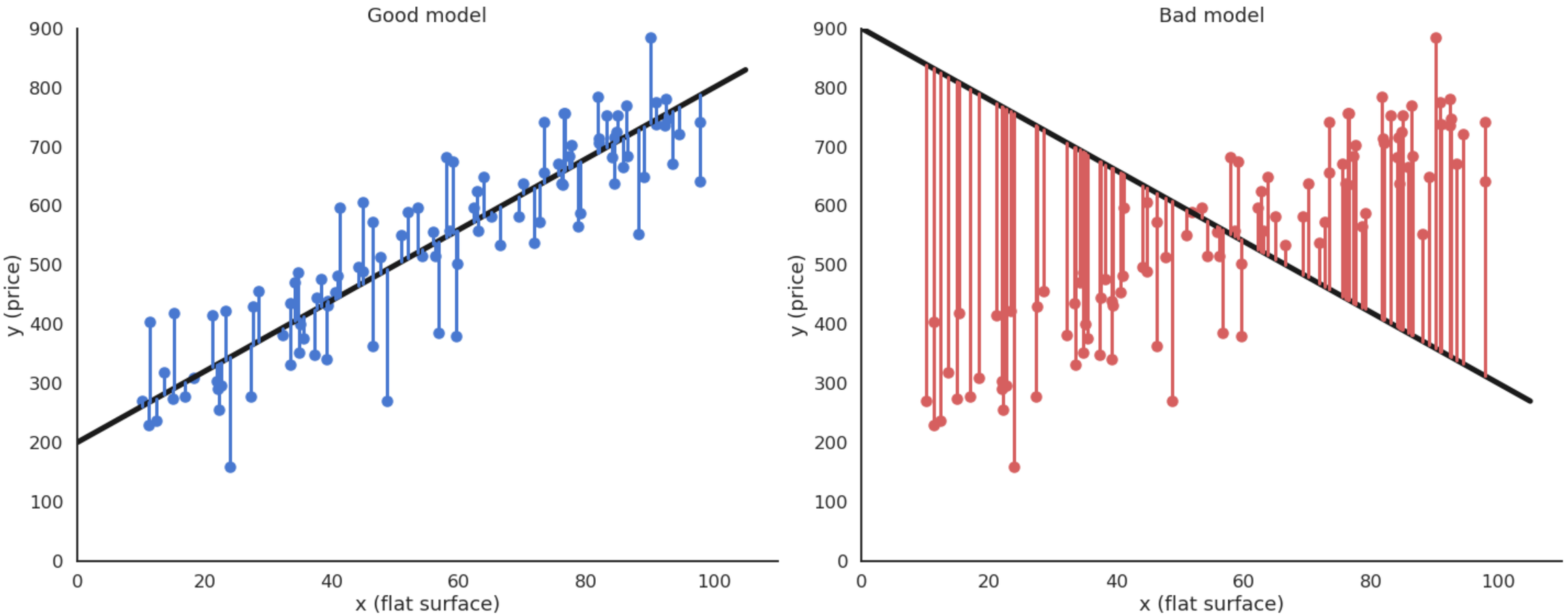
$$\mathcal{L}(w, b) = \mathbb{E}_{x_i, t_i \in \mathcal{D}}[(t_i - y_i)^2]$$



Linear regression

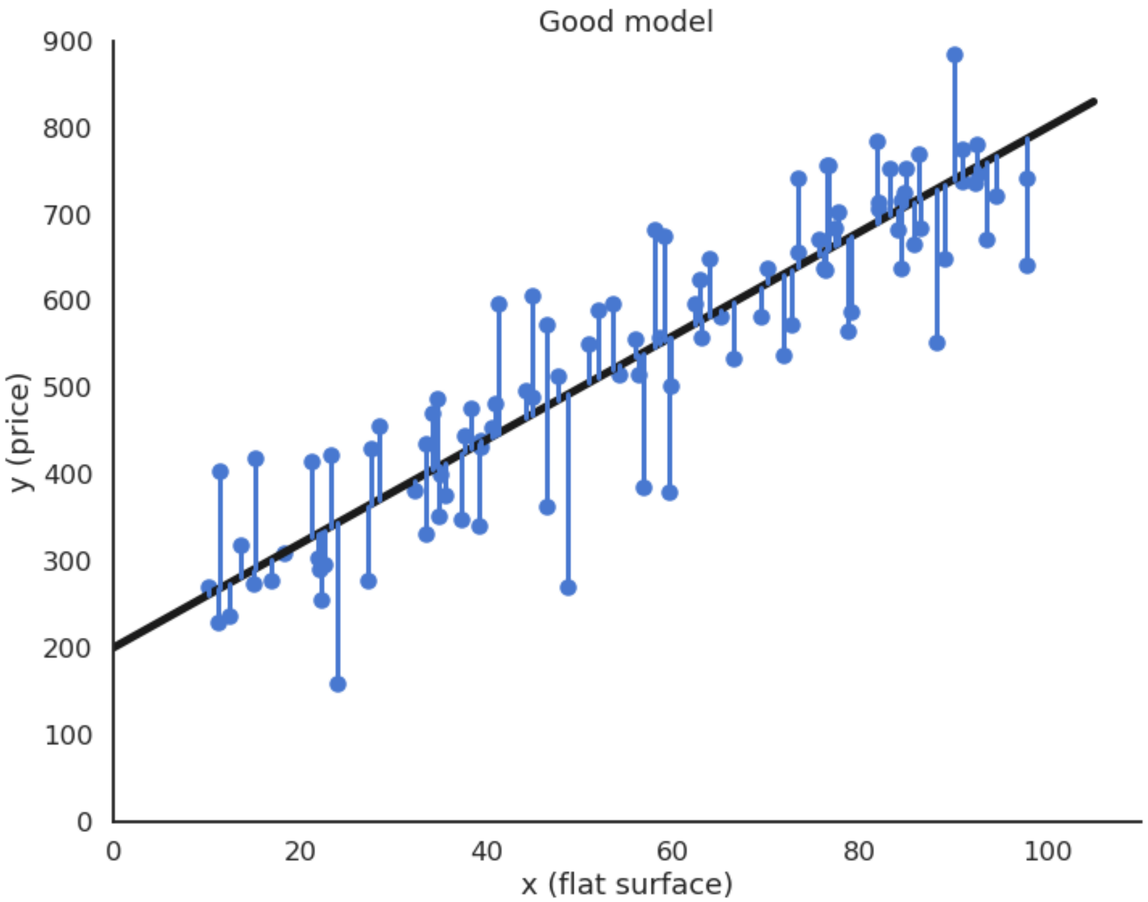
- The loss function is defined as the mathematical expectation of the quadratic error over the training set.
- As the training set is finite and the samples i.i.d, we can simply replace the expectation by an average:

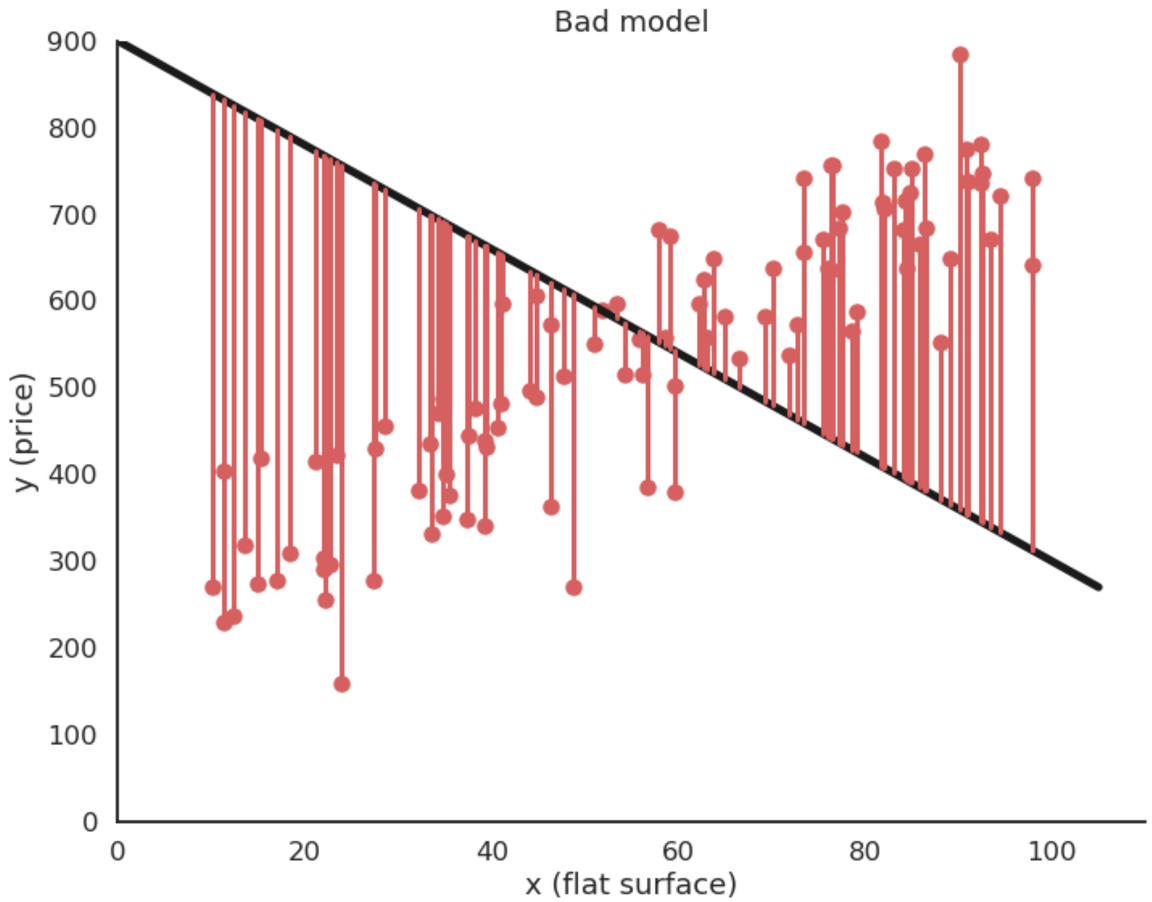
$$\mathcal{L}(w, b) = \frac{1}{N} \sum_{i=1}^{N} (t_i - y_i)^2$$



Linear regression

- The minimum of the mse is achieved when the **prediction** $y_i = f_{w,b}(x_i)$ is equal to the **true value** 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:

$$\frac{df(g(x))}{dx} = \frac{df(g(x))}{dg(x)} \times \frac{dg(x)}{dx} = \frac{df(y)}{dy} \times \frac{dg(x)}{dx}$$

- 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 gives 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.

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

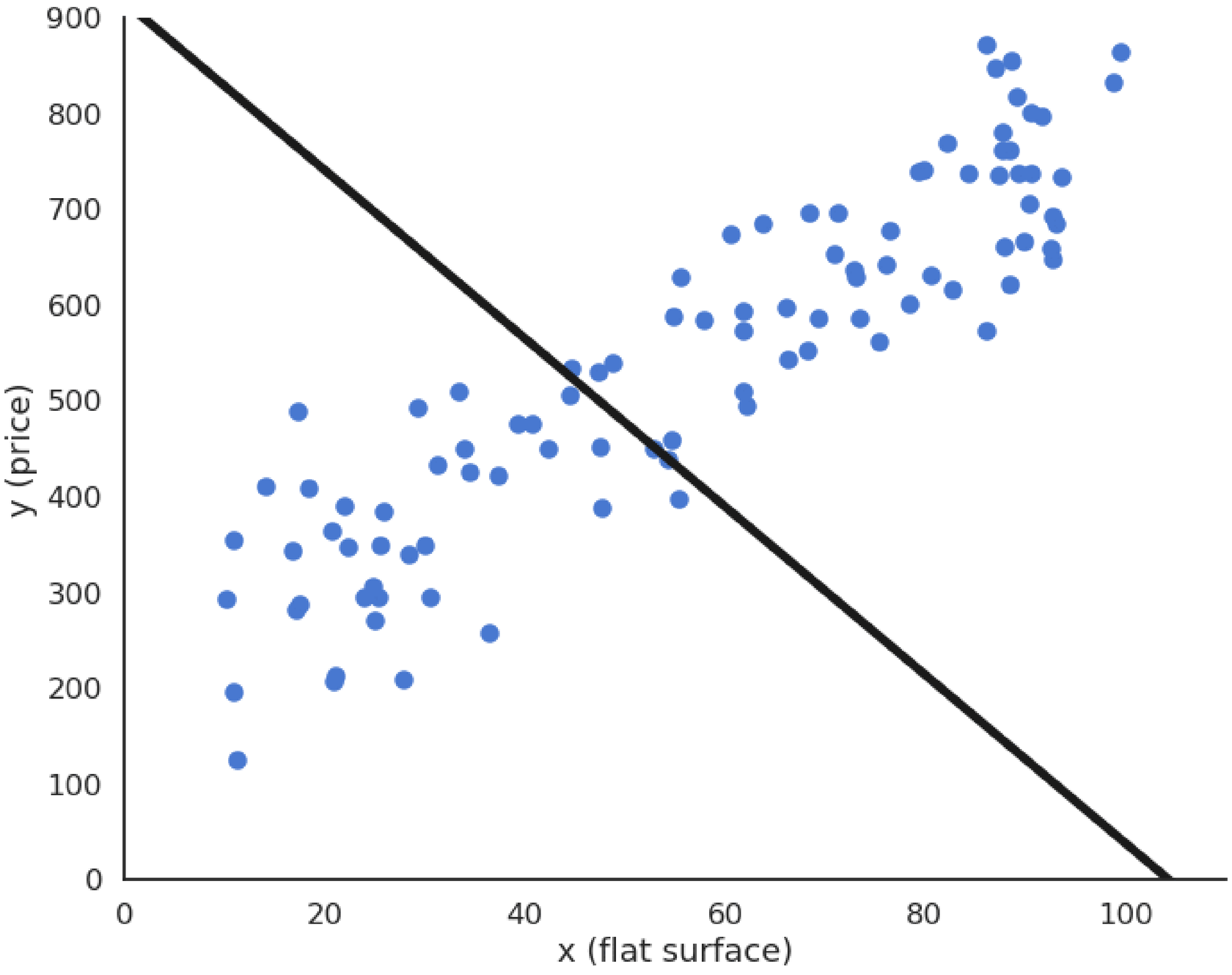
$$\Delta b = \eta \, \frac{1}{N} \sum_{i=1}^{N} (t_i - y_i)$$

- 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

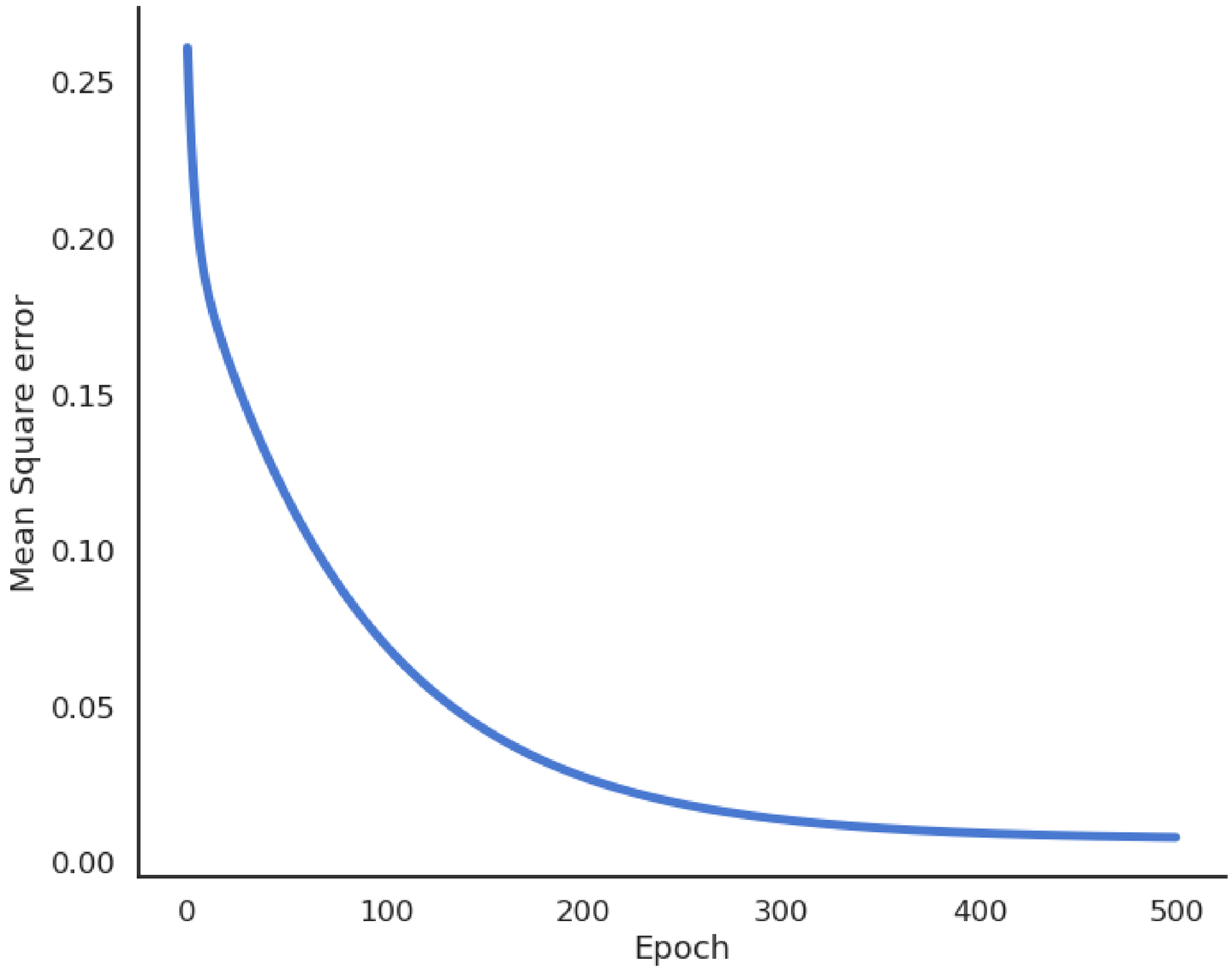
- $w = 0 \quad ; \quad b = 0$
- **for** M epochs:
  - $dw = 0 \quad ; \quad db = 0$
  - **for** each sample (x_i, t_i):
    - $y_i = w \, x_i + b$
    - $dw = dw + (t_i - y_i) \, x_i$
    - $db = db + (t_i - y_i)$
  - $\Delta w = \eta \, \frac{1}{N} dw$
  - $\Delta b = \eta \, \frac{1}{N} db$

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

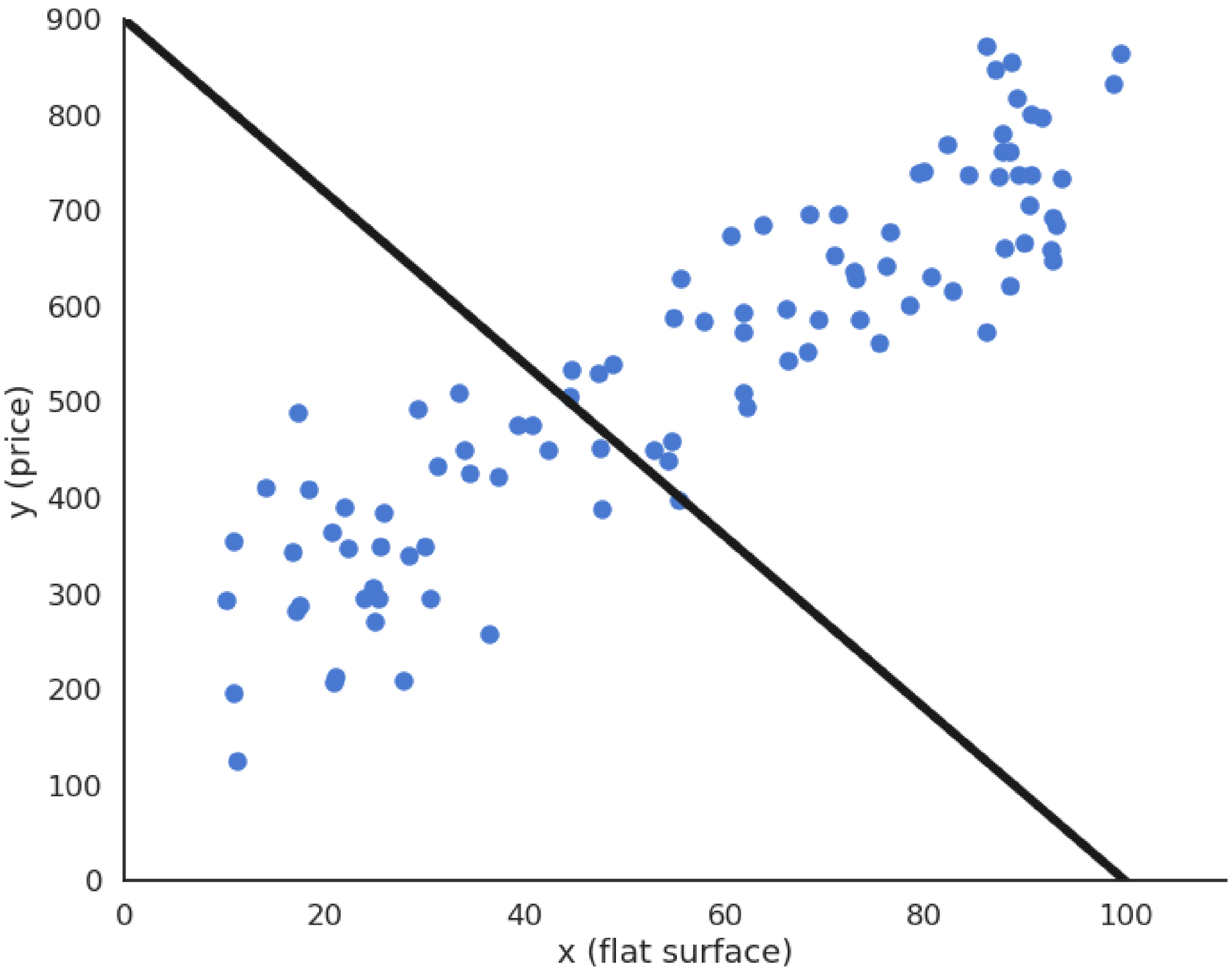
- $w = 0 \quad ; \quad b = 0$
- **for** M epochs:
  - **for** each sample (x_i, t_i):
    - $y_i = w \, x_i + b$
    - $\Delta w = \eta \, (t_i - y_i) \, x_i$
    - $\Delta b = \eta \, (t_i - y_i)$

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

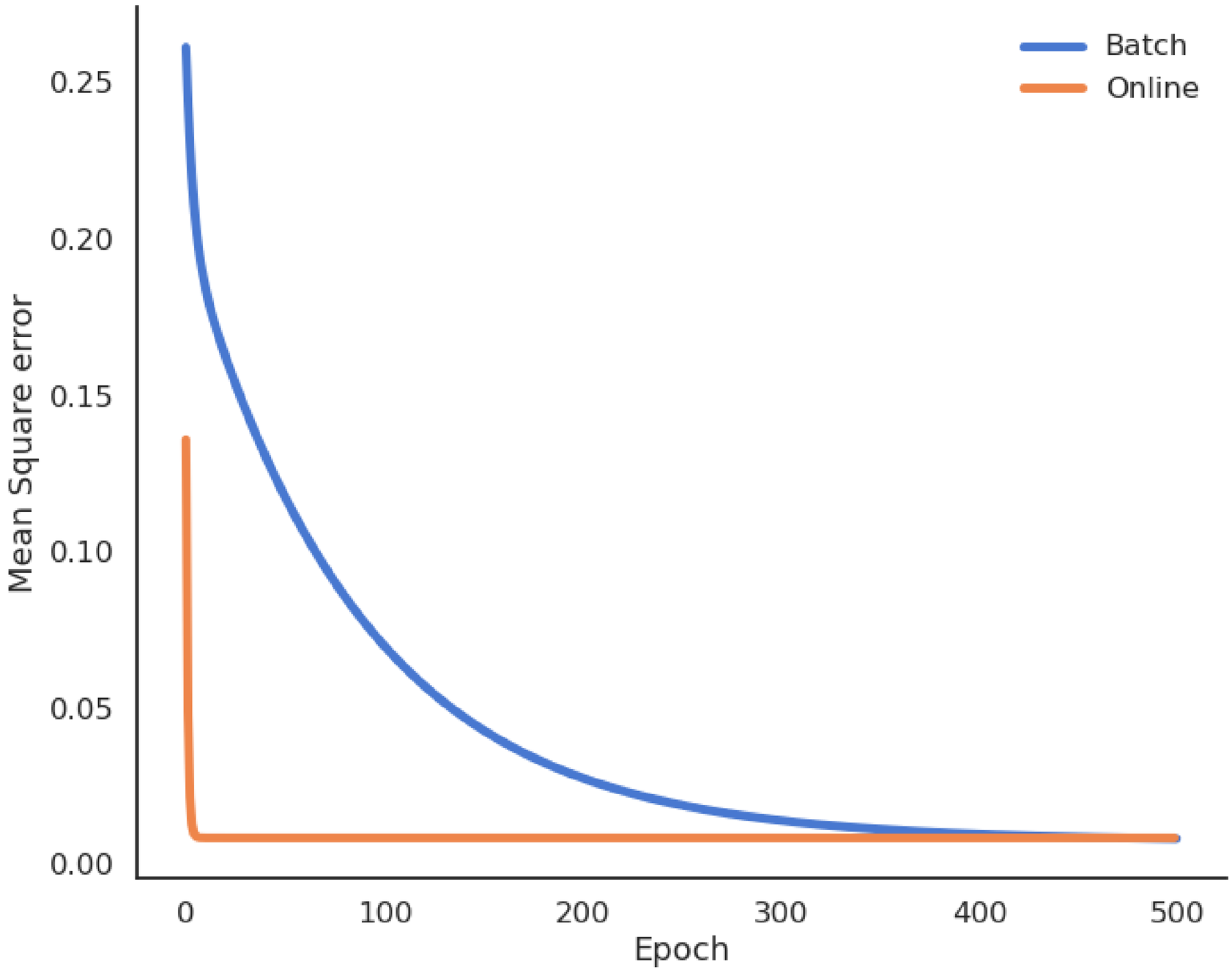
$$\begin{cases} \Delta w = \eta \, (t_i - y_i) \, x_i \\ \\ \Delta b = \eta \, (t_i - y_i) \end{cases}$$

- 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

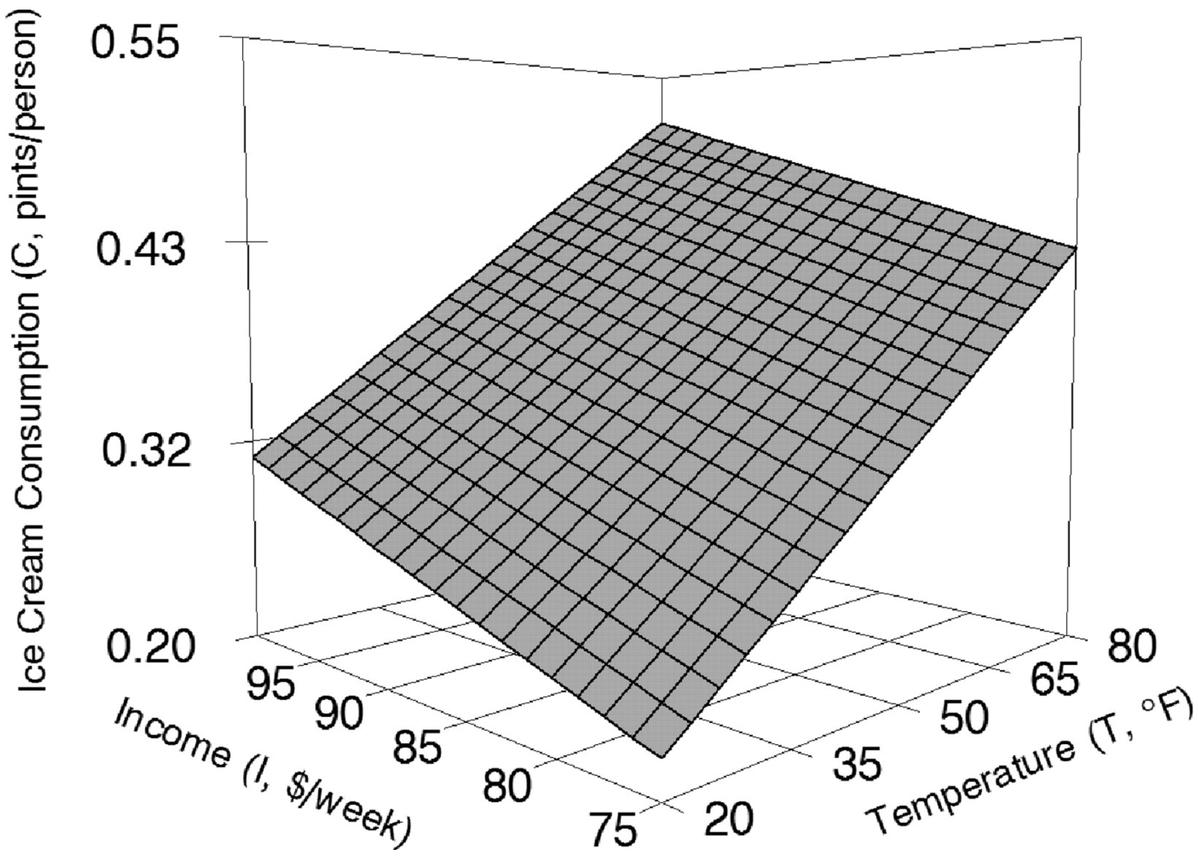
Multiple linear regression

- 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.

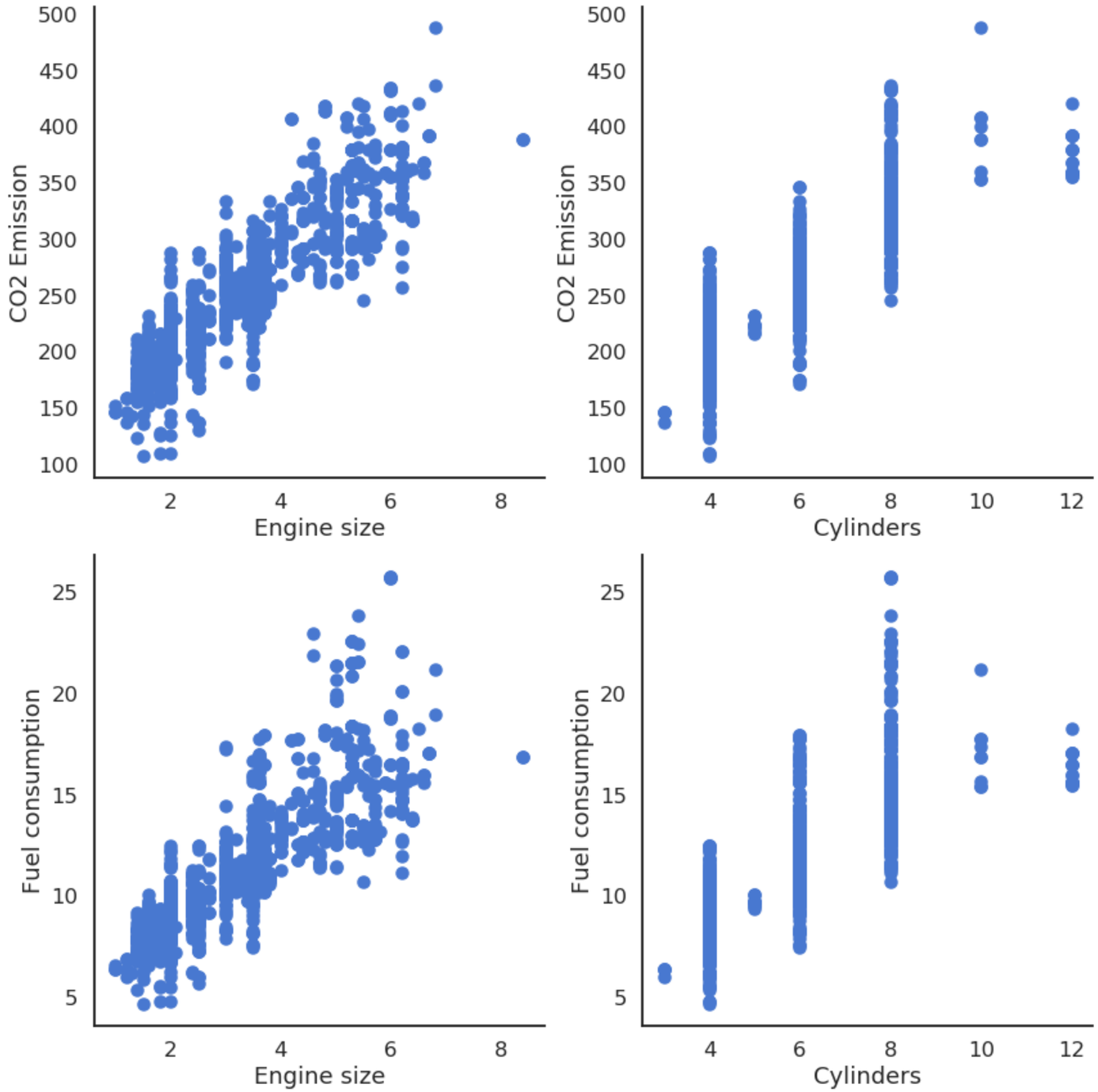


MLR example: fuel consumption and CO2 emissions

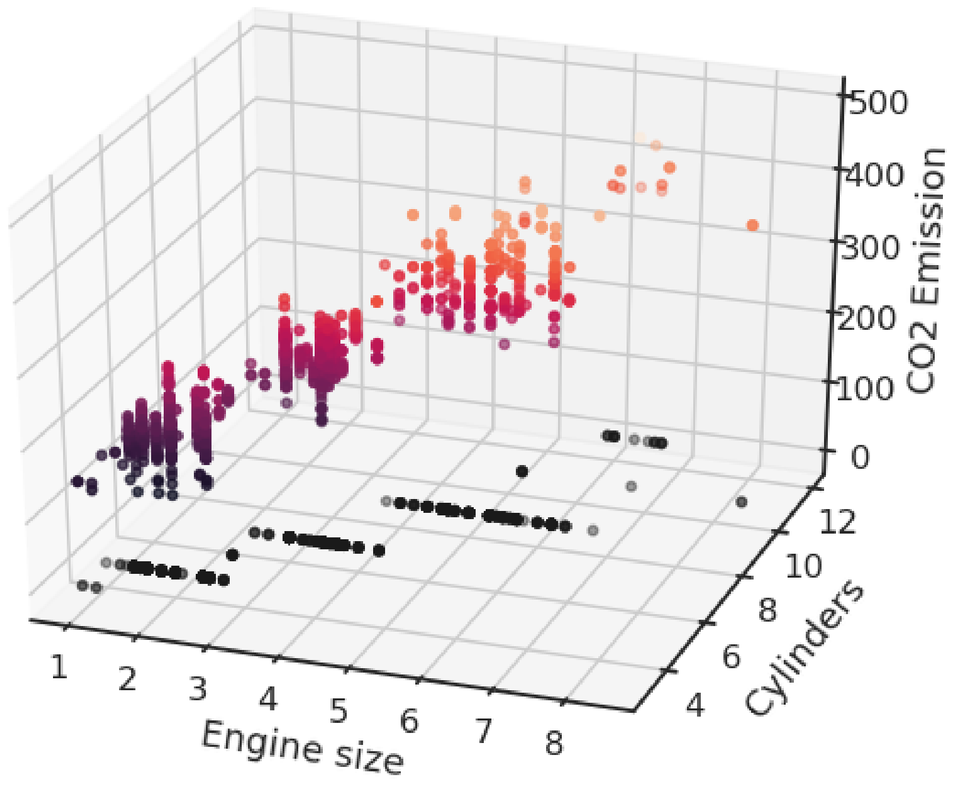
- Let’s suppose you have 13971 measurements in some Excel file, linking engine size, number of cylinders, fuel consumption and CO2 emissions of various cars.
- You want to predict fuel consumption and CO2 emissions when you know the engine size and the number of cylinders.

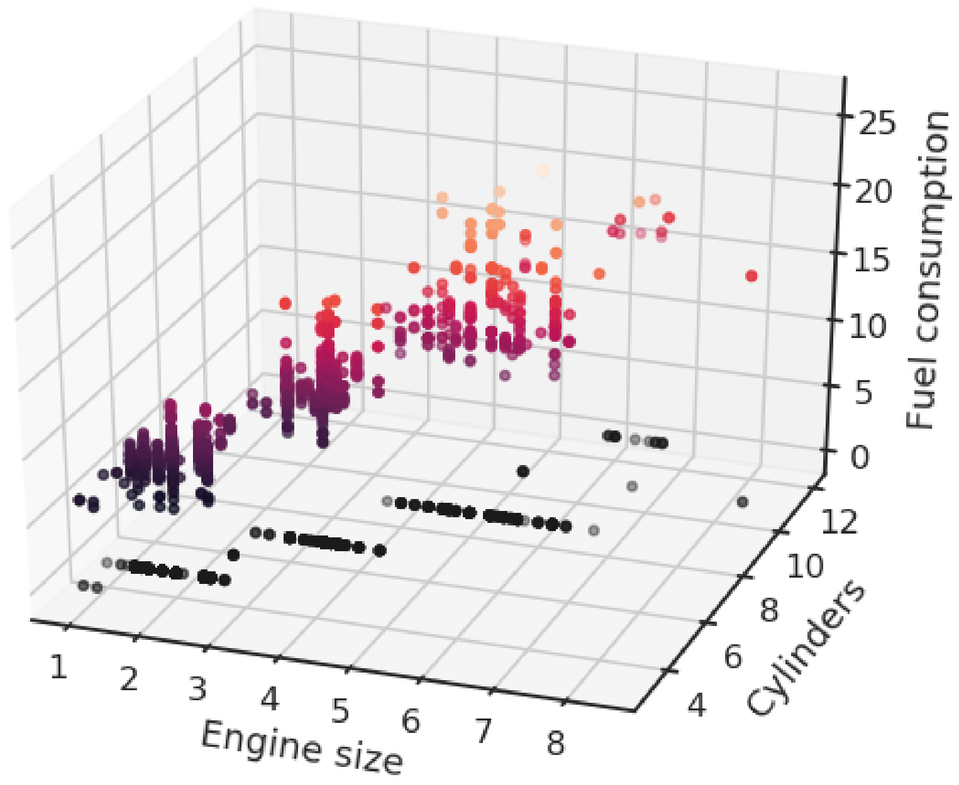
Engine size	Cylinders	Fuel consumption	CO2 emissions
2	4	8.5	196
2.4	4	9.6	221
1.5	4	5.9	136
3.5	6	11	255
3.5	6	11	244
3.5	6	10	230
3.5	6	10	232
3.7	6	11	255
3.7	6	12	267
…	…	…	…

MLR example: fuel consumption and CO2 emissions



MLR example: fuel consumption and CO2 emissions



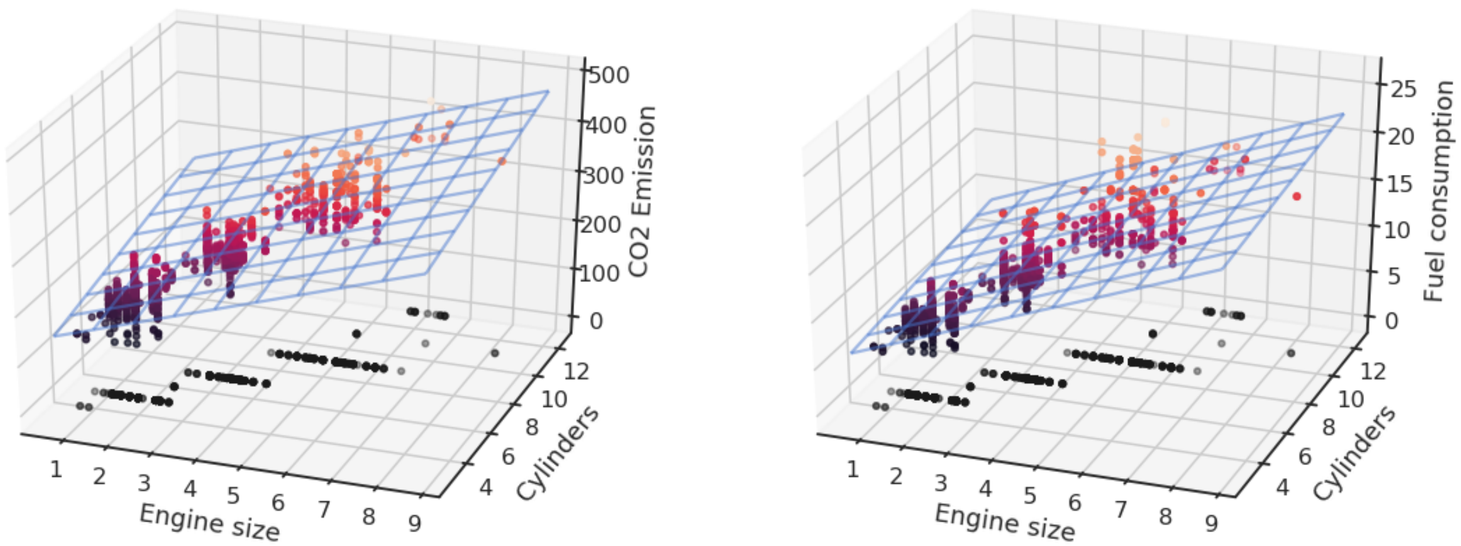


MLR example: fuel consumption and CO2 emissions

- 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:

```
1 from sklearn.linear_model import LinearRegression
2 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:

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

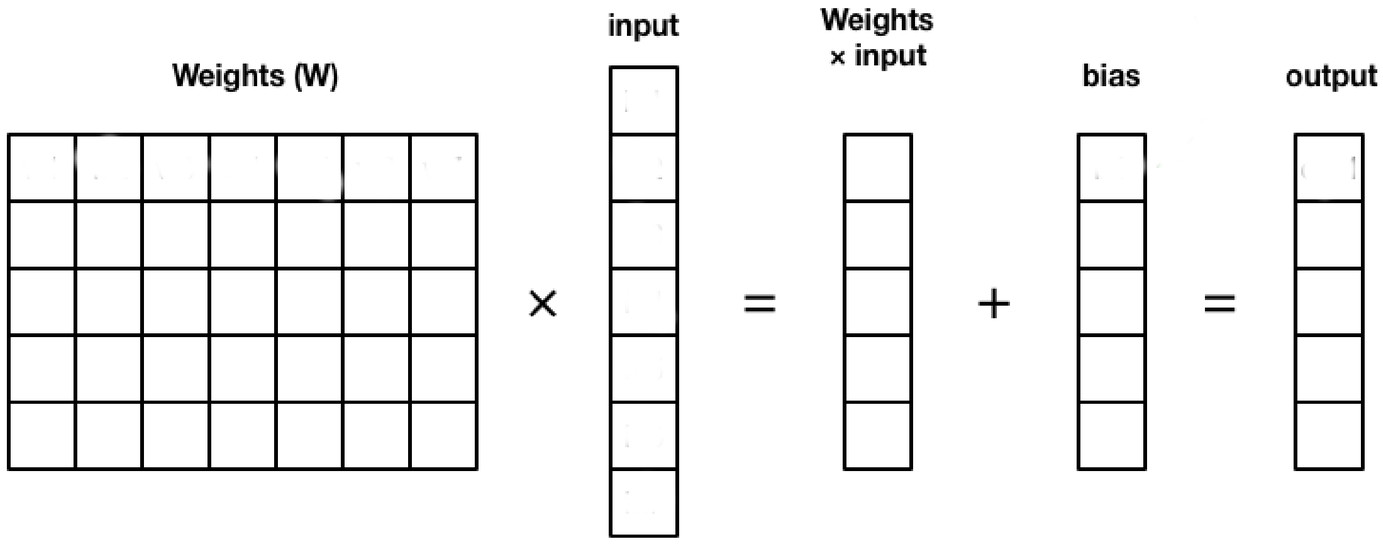
- We simply create the corresponding vectors and matrices:

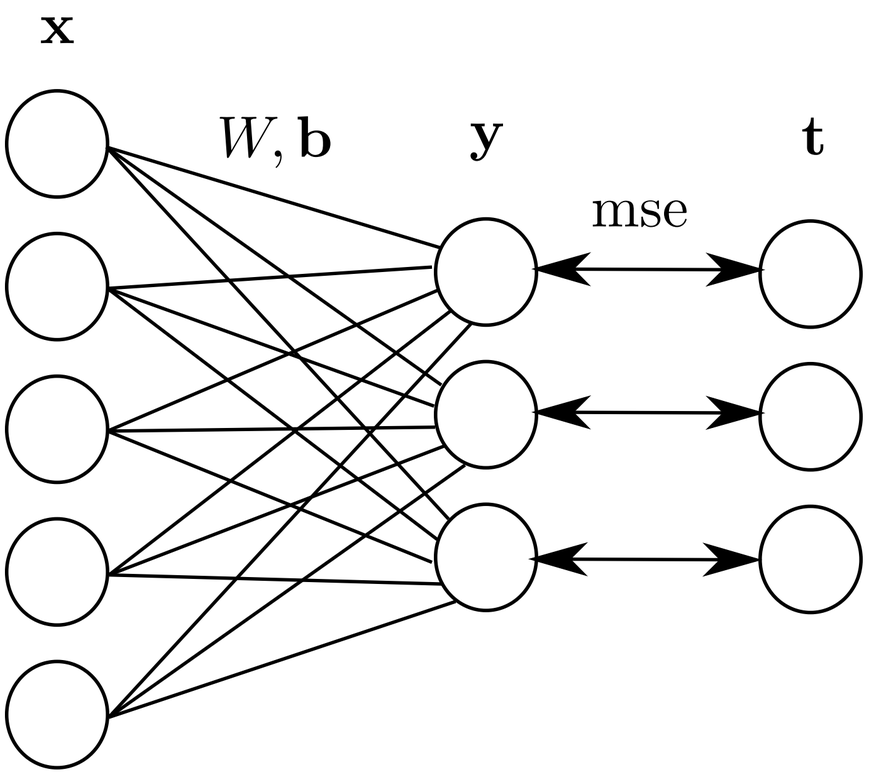
$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \qquad \mathbf{t} = \begin{bmatrix} t_1 \\ t_2 \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \qquad W = \begin{bmatrix} w_1 & w_2 \\ w_3 & w_4 \end{bmatrix}$$

- $\mathbf{x}$ 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:

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

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 $(f \times g)' = f' \, g + f \, g'$:

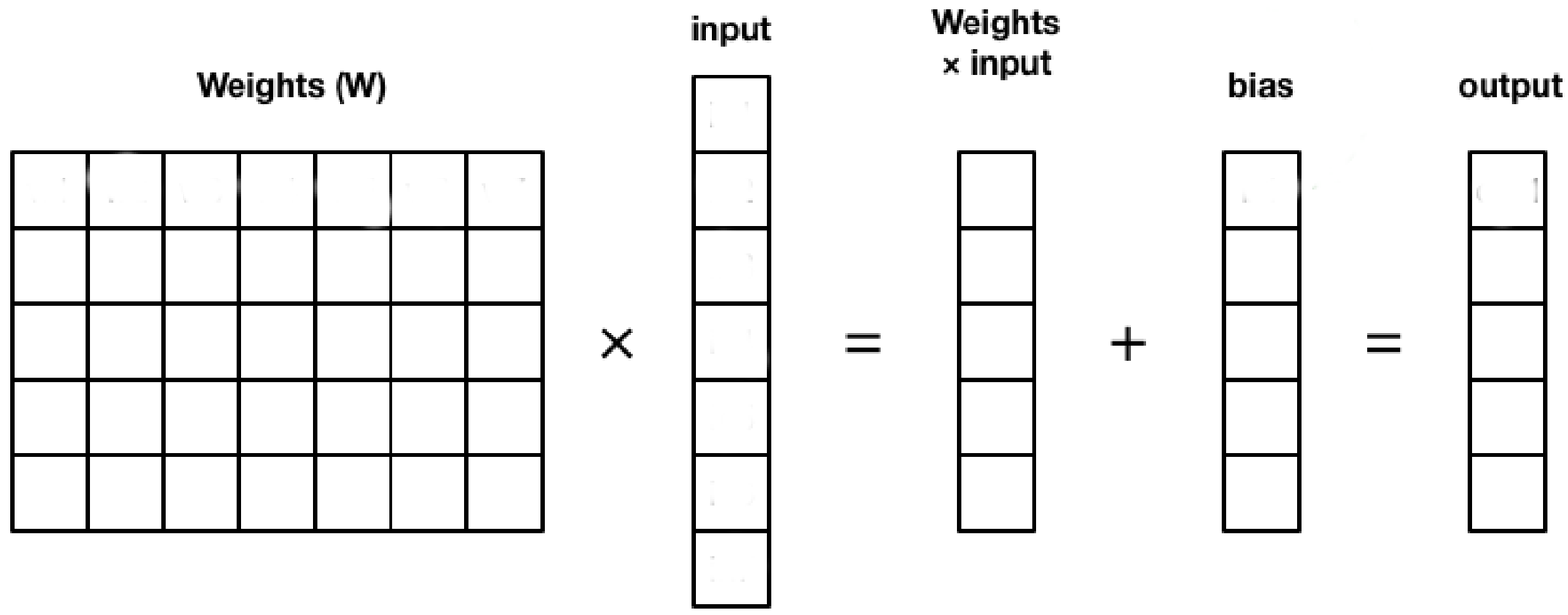
$$\nabla_{\mathbf{y}_i} \, (\mathbf{t}_i - \mathbf{y}_i)^T \times (\mathbf{t}_i - \mathbf{y}_i) = (\nabla_{\mathbf{y}_i} \, (\mathbf{t}_i - \mathbf{y}_i)) \times (\mathbf{t}_i - \mathbf{y}_i) + (\mathbf{t}_i - \mathbf{y}_i) \times \nabla_{\mathbf{y}_i} \, (\mathbf{t}_i - \mathbf{y}_i)$$

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

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

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:

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

- 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:

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

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

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

Example

- Let’s prove it element per element:

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

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

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

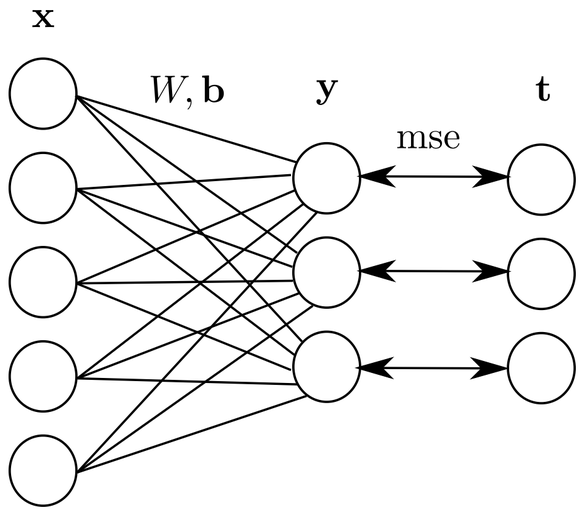
- The Jacobian w.r.t W can be explicitly formed using partial derivatives:

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

- 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



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

$$\begin{cases} \Delta w_1 = \eta \left(t_1 - y_1 \right) x_1 \\ \Delta w_2 = \eta \left(t_1 - y_1 \right) x_2 \\ \Delta w_3 = \eta \left(t_2 - y_2 \right) x_1 \\ \Delta w_4 = \eta \left(t_2 - y_2 \right) x_2 \end{cases} \qquad \begin{cases} \Delta b_1 = \eta \left(t_1 - y_1 \right) \\ \Delta b_2 = \eta \left(t_2 - y_2 \right) \end{cases}$$

- Batch version:

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

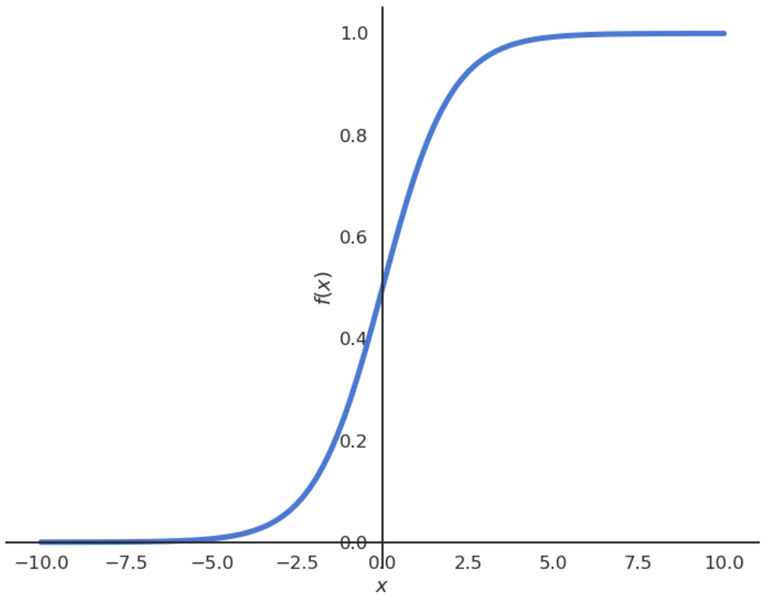
- Online version (**delta learning rule**):

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

- 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:

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

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

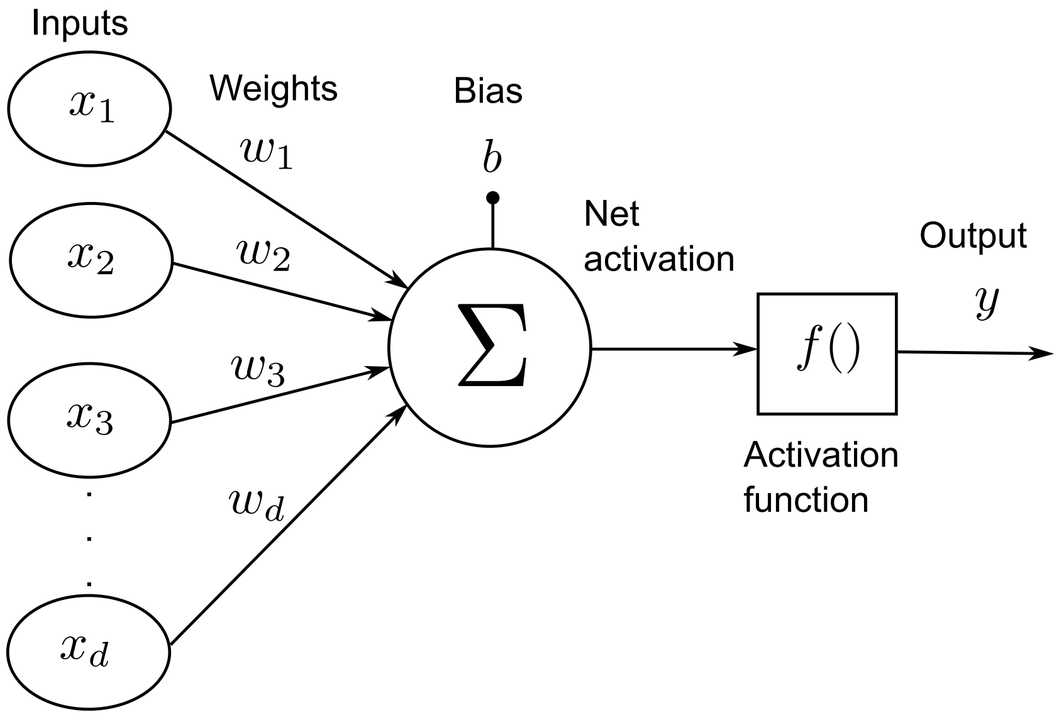
$$\Delta w = \eta\,(t_i - y_i)\,\sigma'(w\, x_i + b)\, x_i$$

- 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



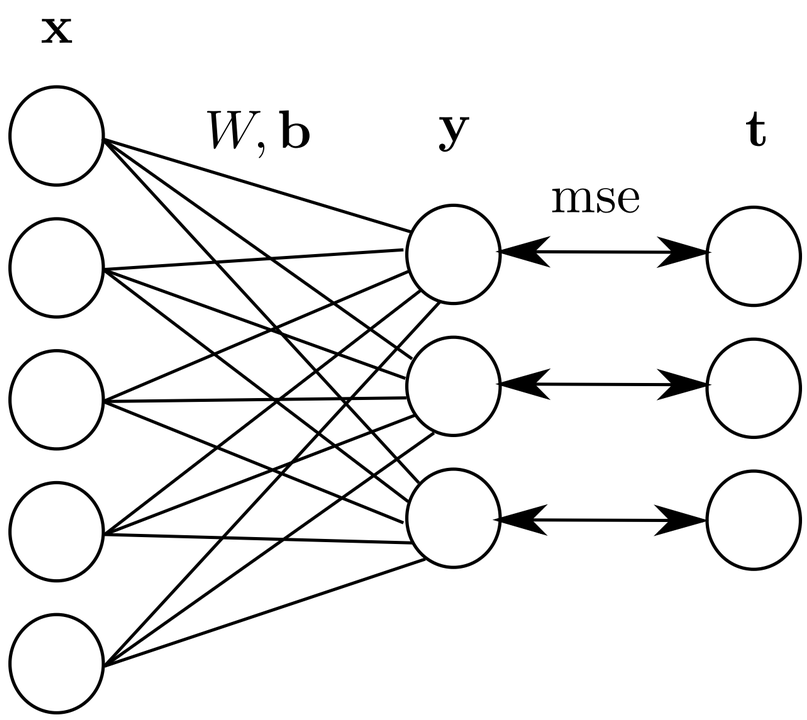
- Model:

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

- 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):

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

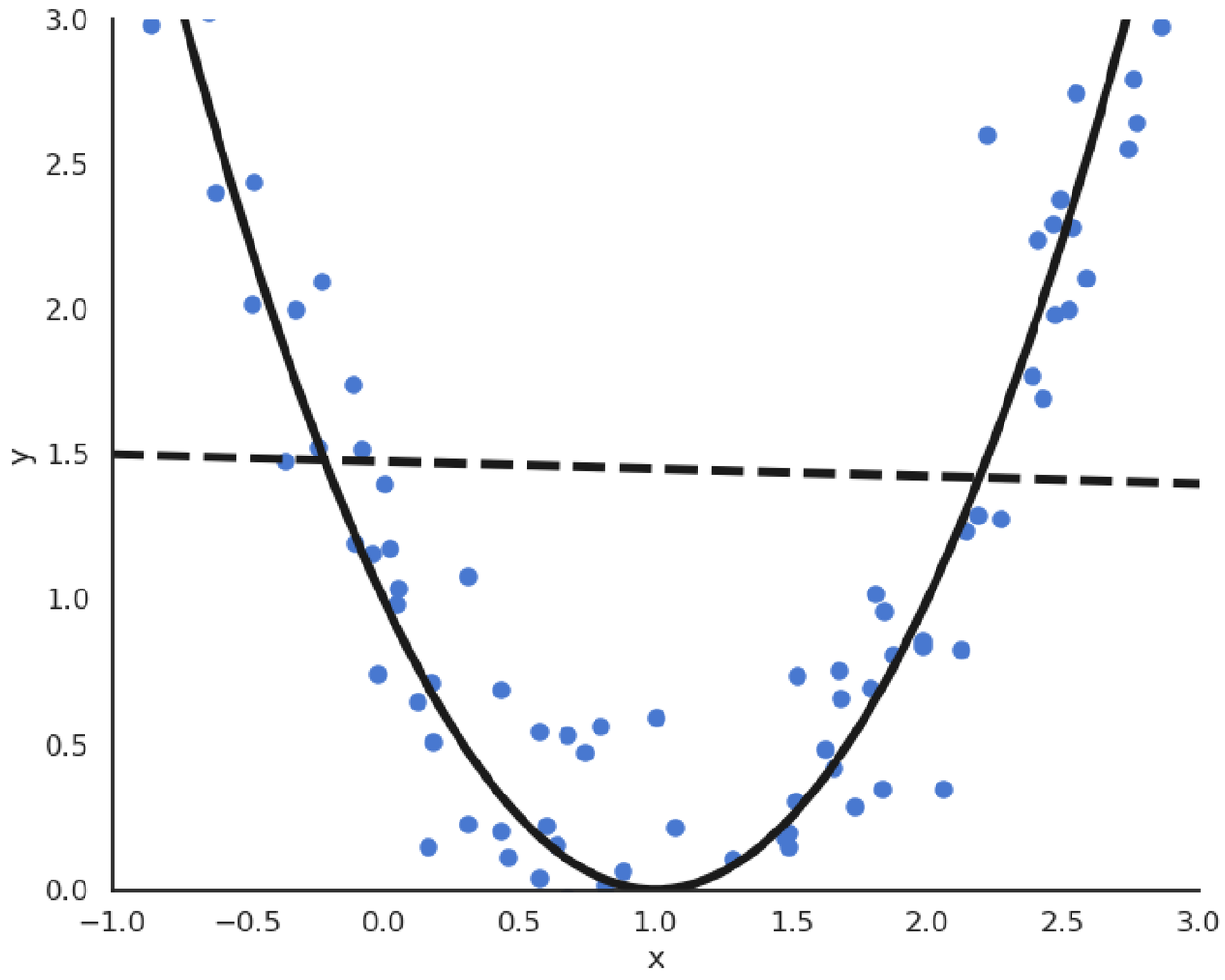
- Delta learning rule:

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

- 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 is better modeled by a second-order polynomial:

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

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:

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

$$\Delta b = \eta\, (t - y)$$

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:

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

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

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

$$\Delta b = \eta\,(t - y)$$

- 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?

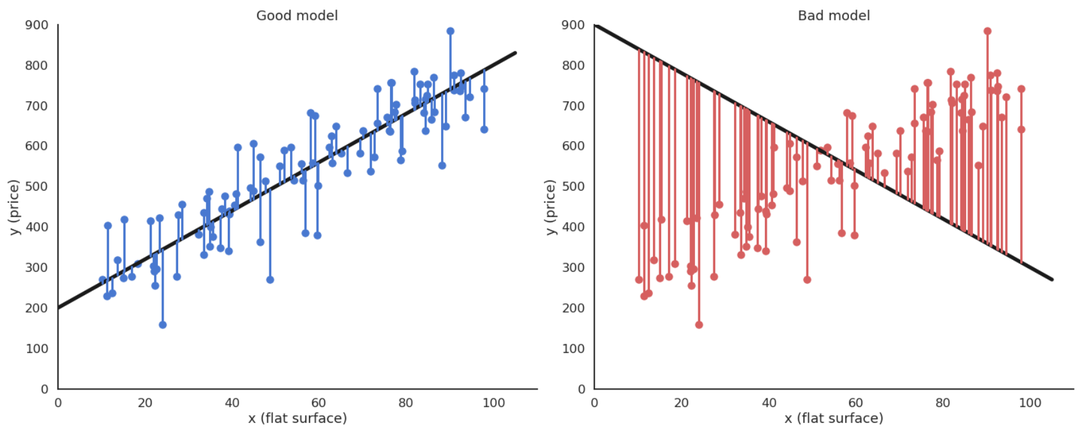
- Before going further, let's think about what we have been doing so far. We had a bunch of data samples $\mathcal{D} = (x_i, t_i)_{i=1..N}$ (the **training set**) and we decided to apply a (linear) model on it:

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

- 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?

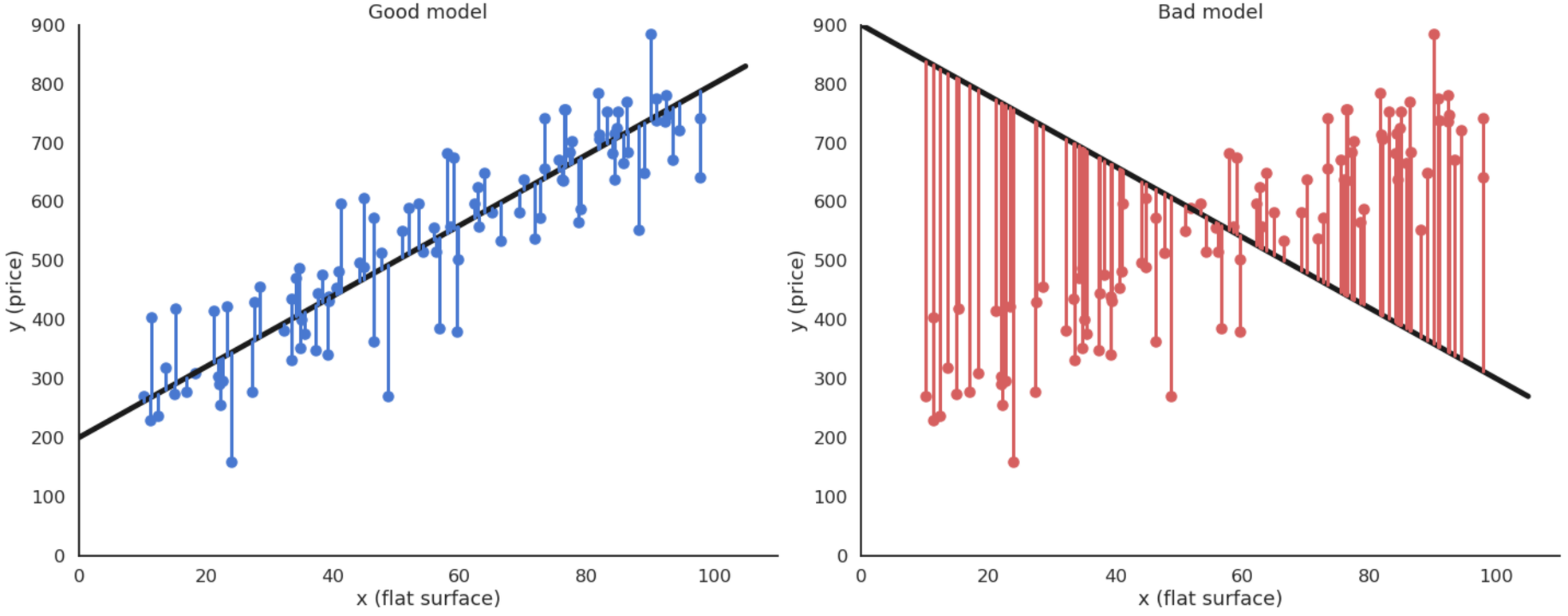


Regression error

- 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 model.

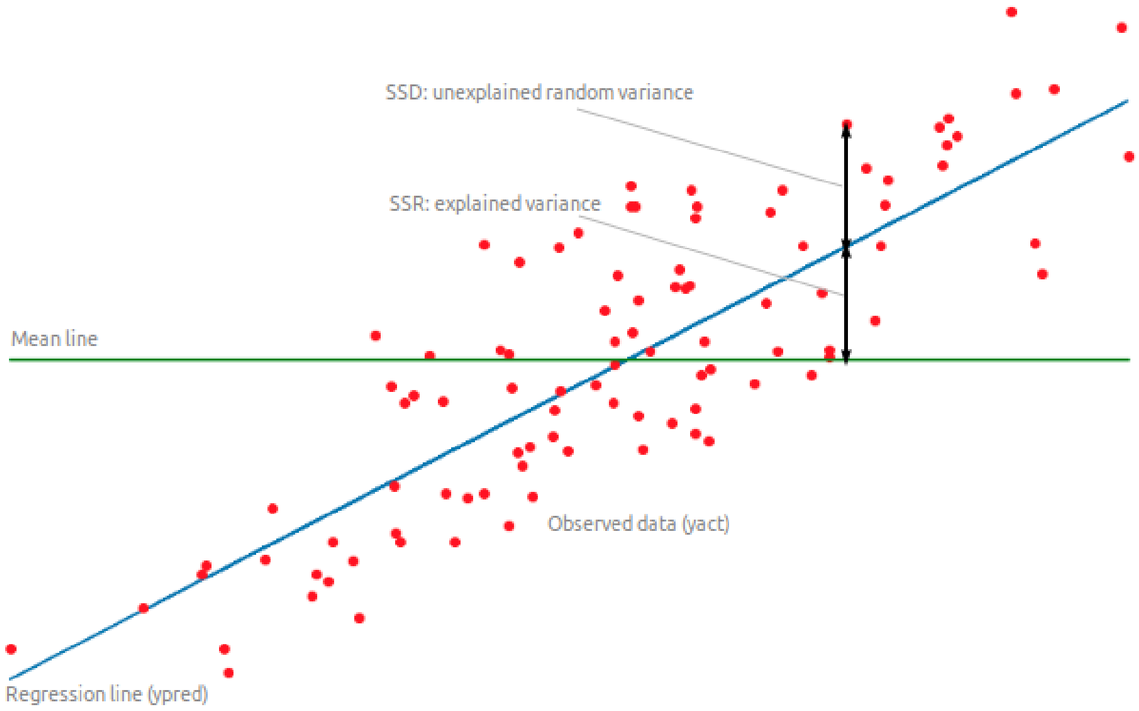


Coefficient of determination

- 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 $\hat{t}$:

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

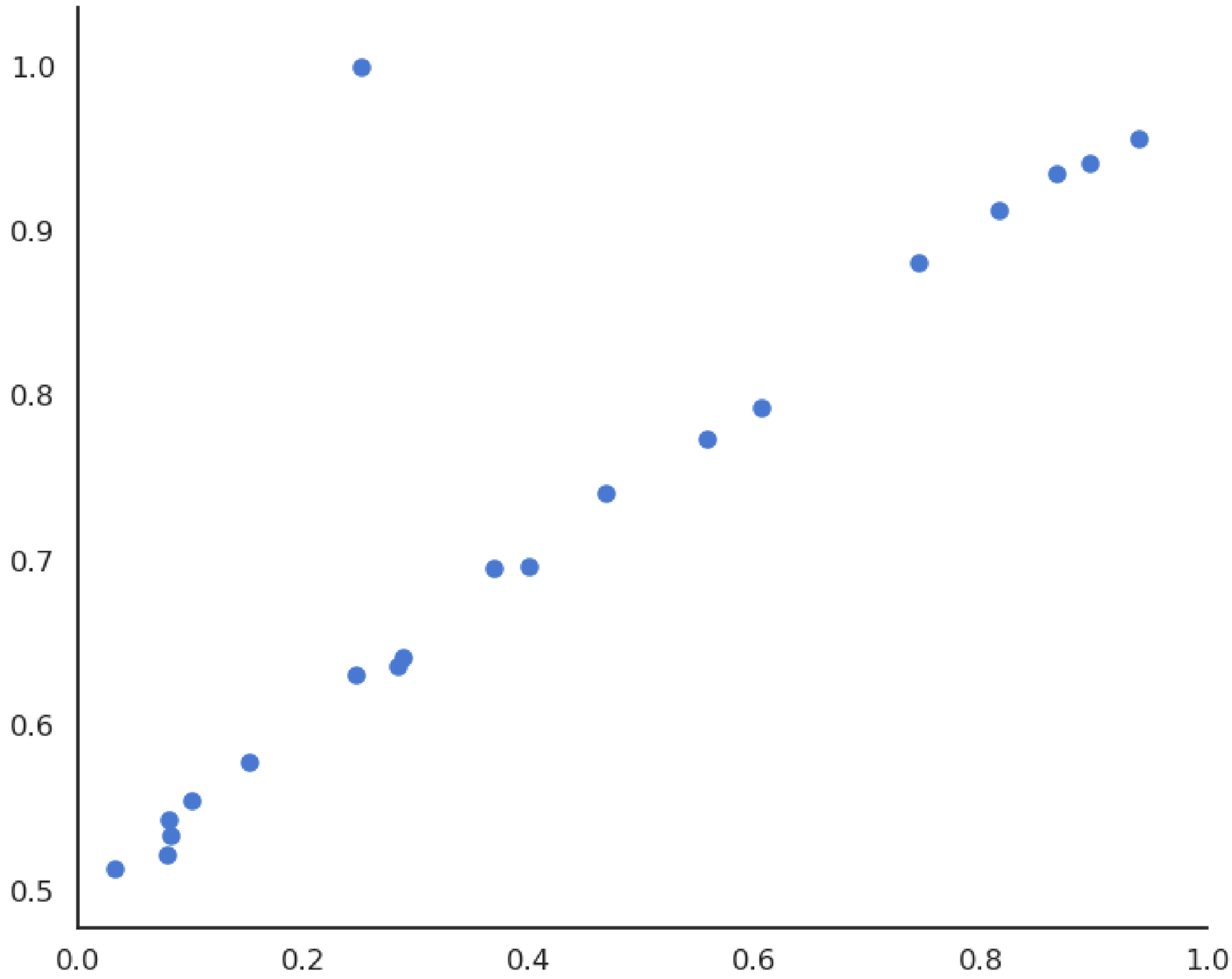
- R^2 should be as close from 1 as possible. For example, if $R^2 = 0.8$, we can say that the **model explains 80% of the variance of the data**.



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

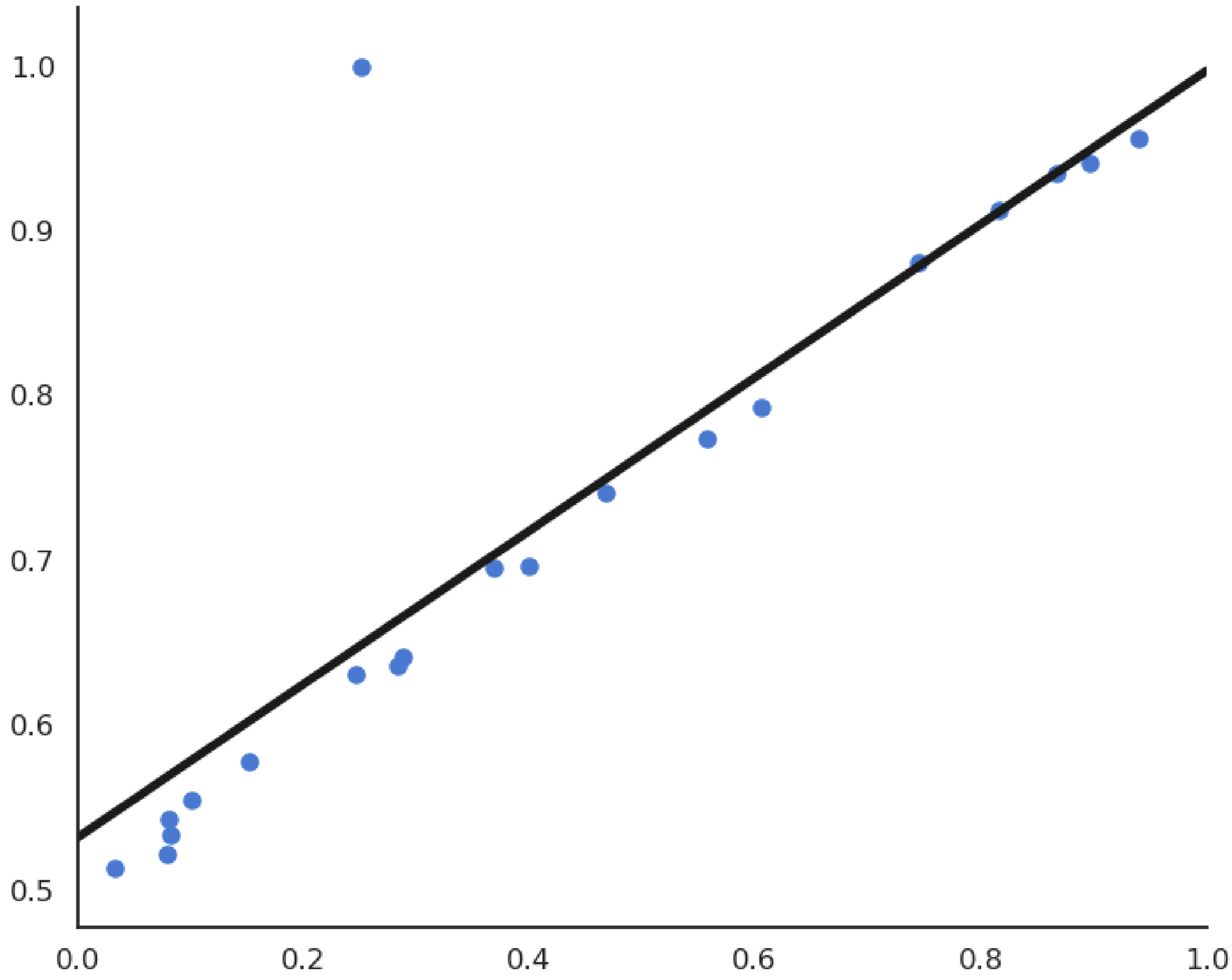
Sensibility to outliers

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



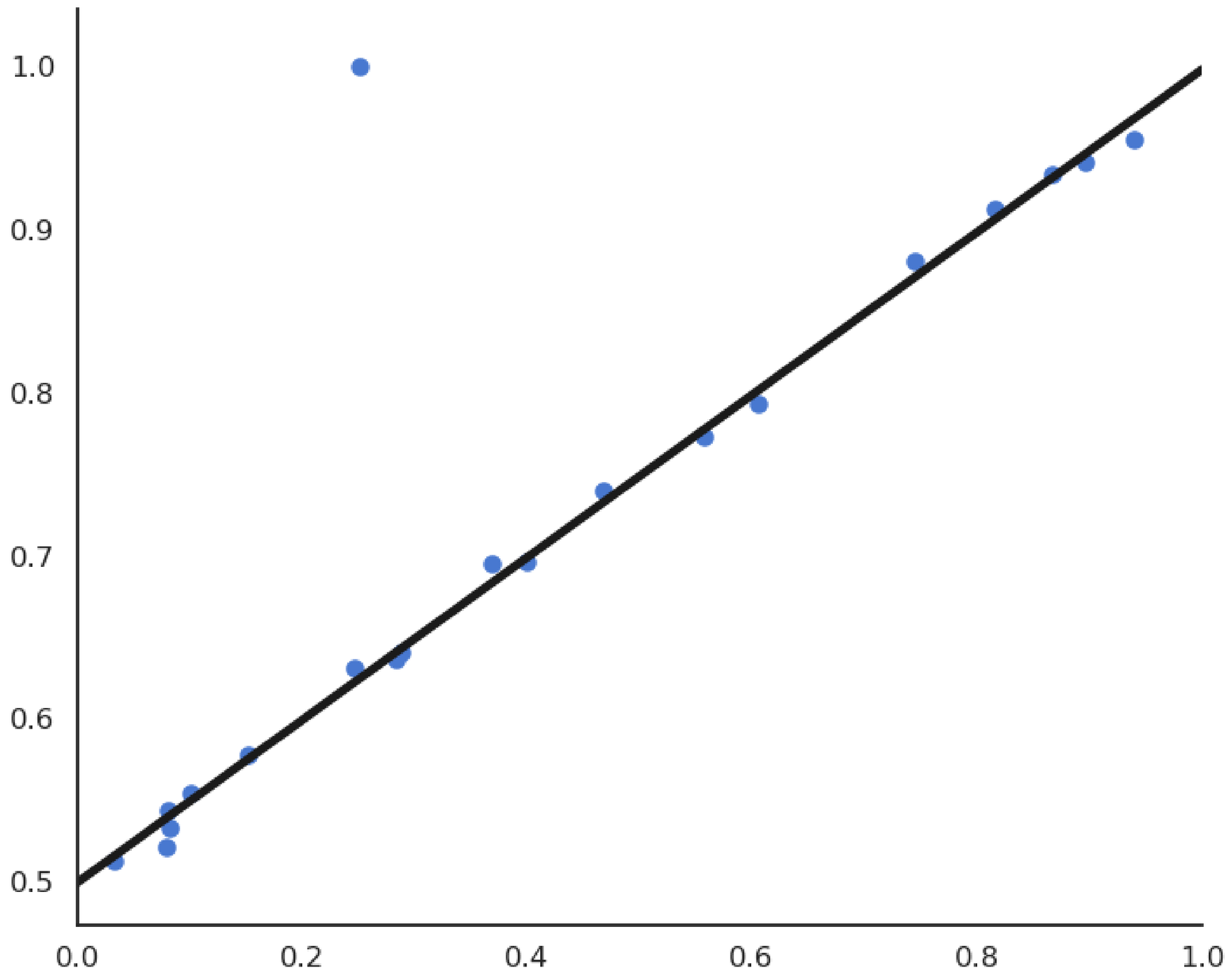
Sensibility to outliers

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

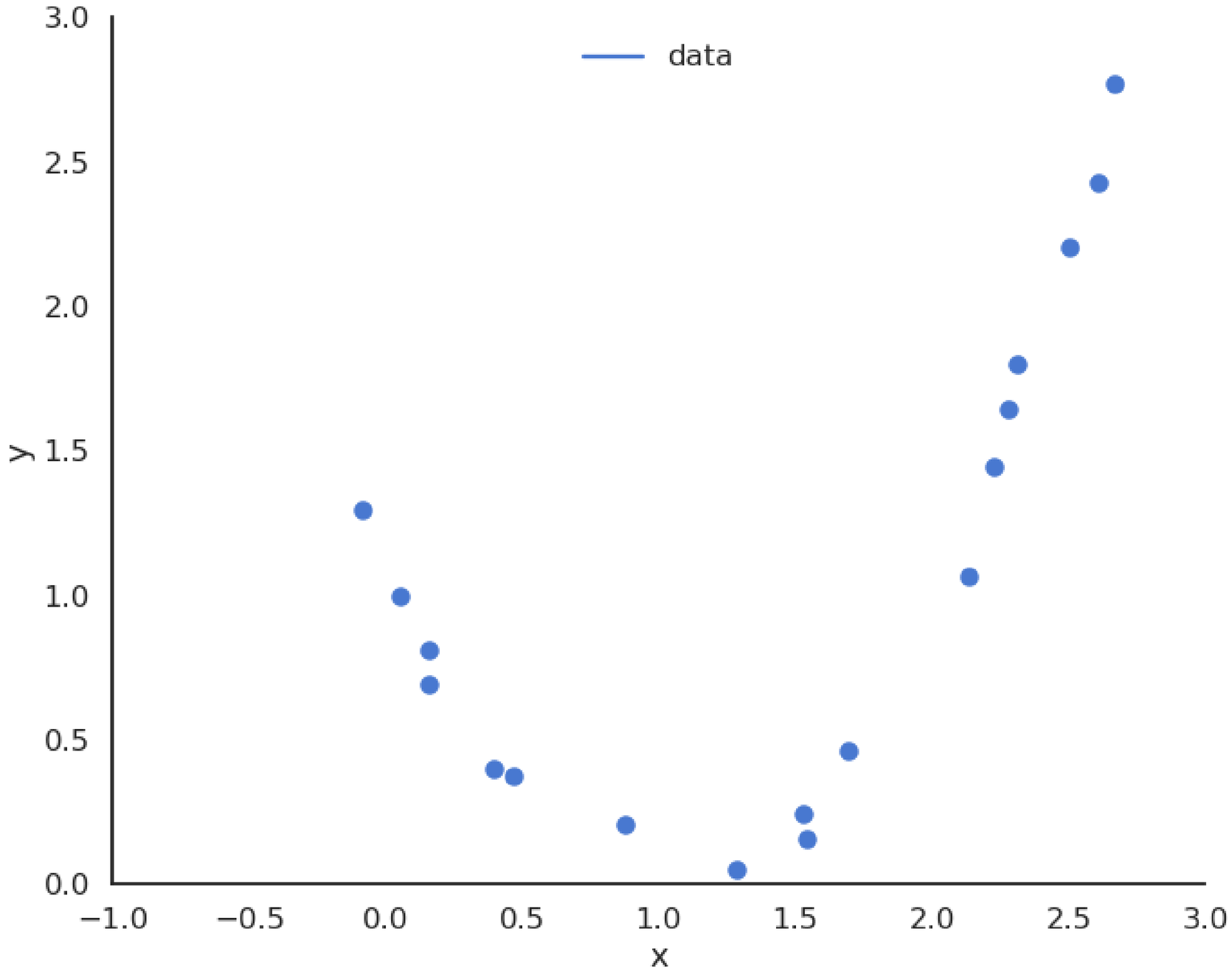


Sensibility to outliers

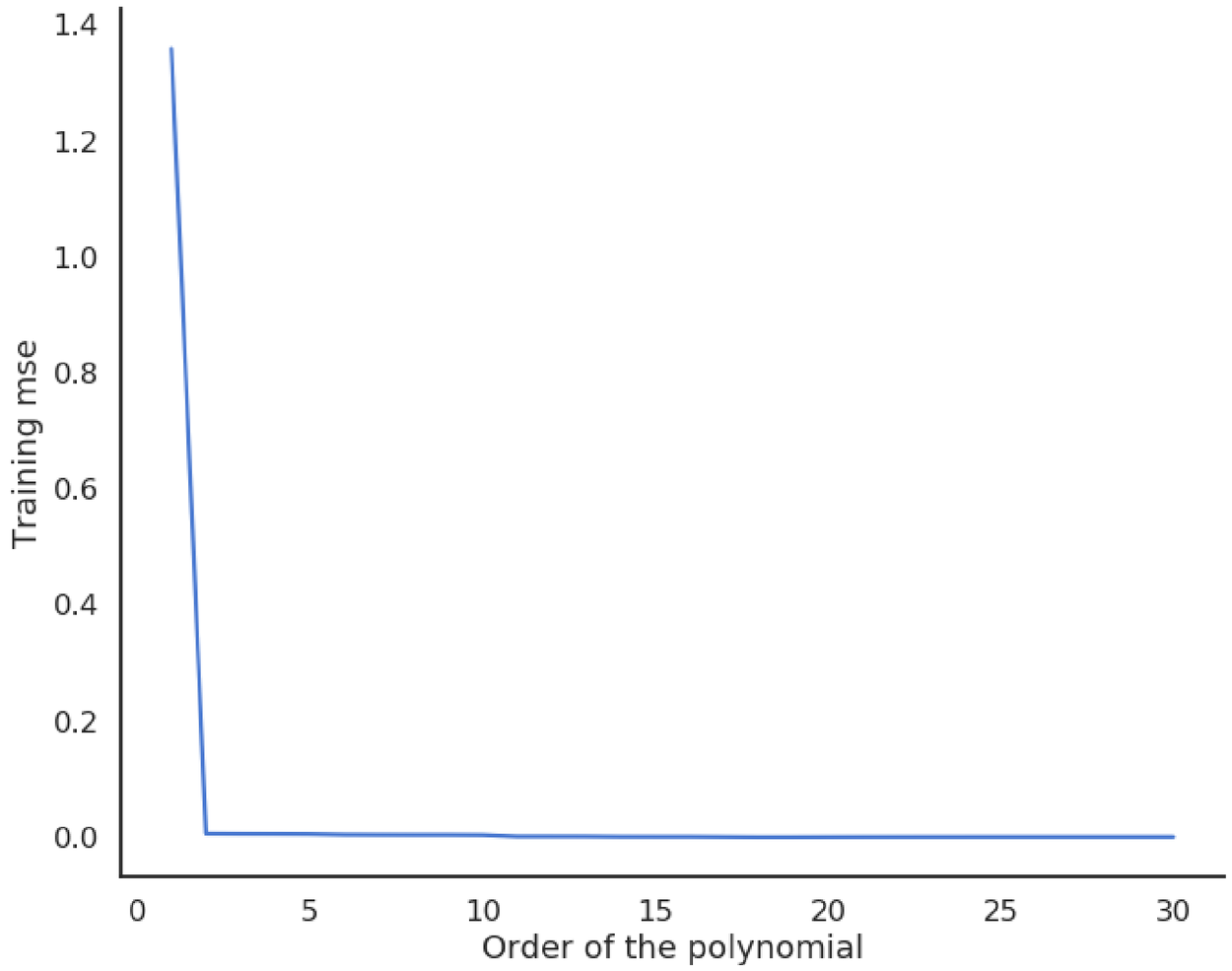
- This model feels much better, but its residual mse is higher…



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!

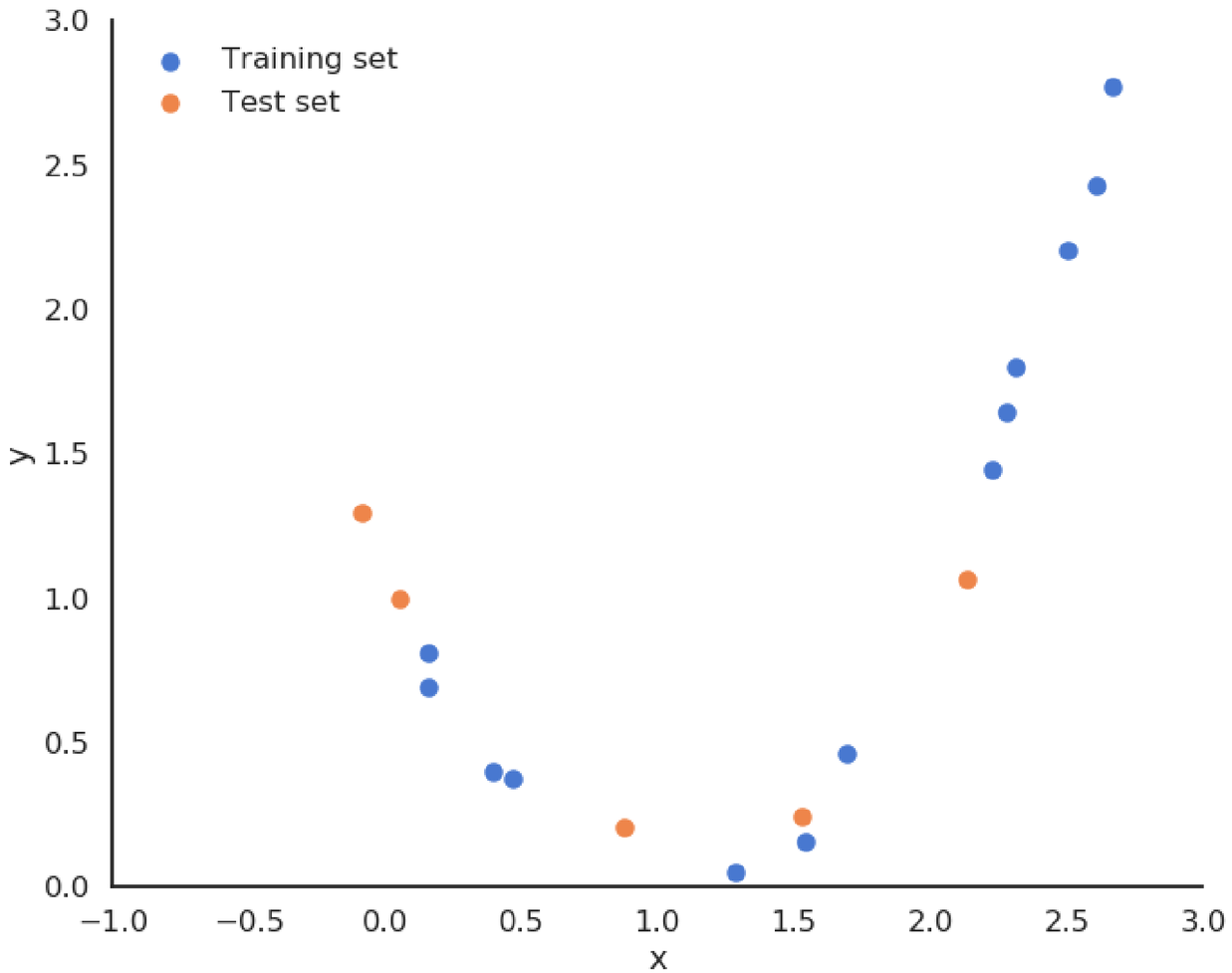
- For all models M_i:
  - Train M_i on $\mathcal{D}$ to obtain an hypothesis h_i.
  - Compute the training error $\epsilon_{\mathcal{D}}(h_i)$ of h_i on $\mathcal{D}$:

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

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

- 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 $\mathcal{S}_{\text{test}}$:

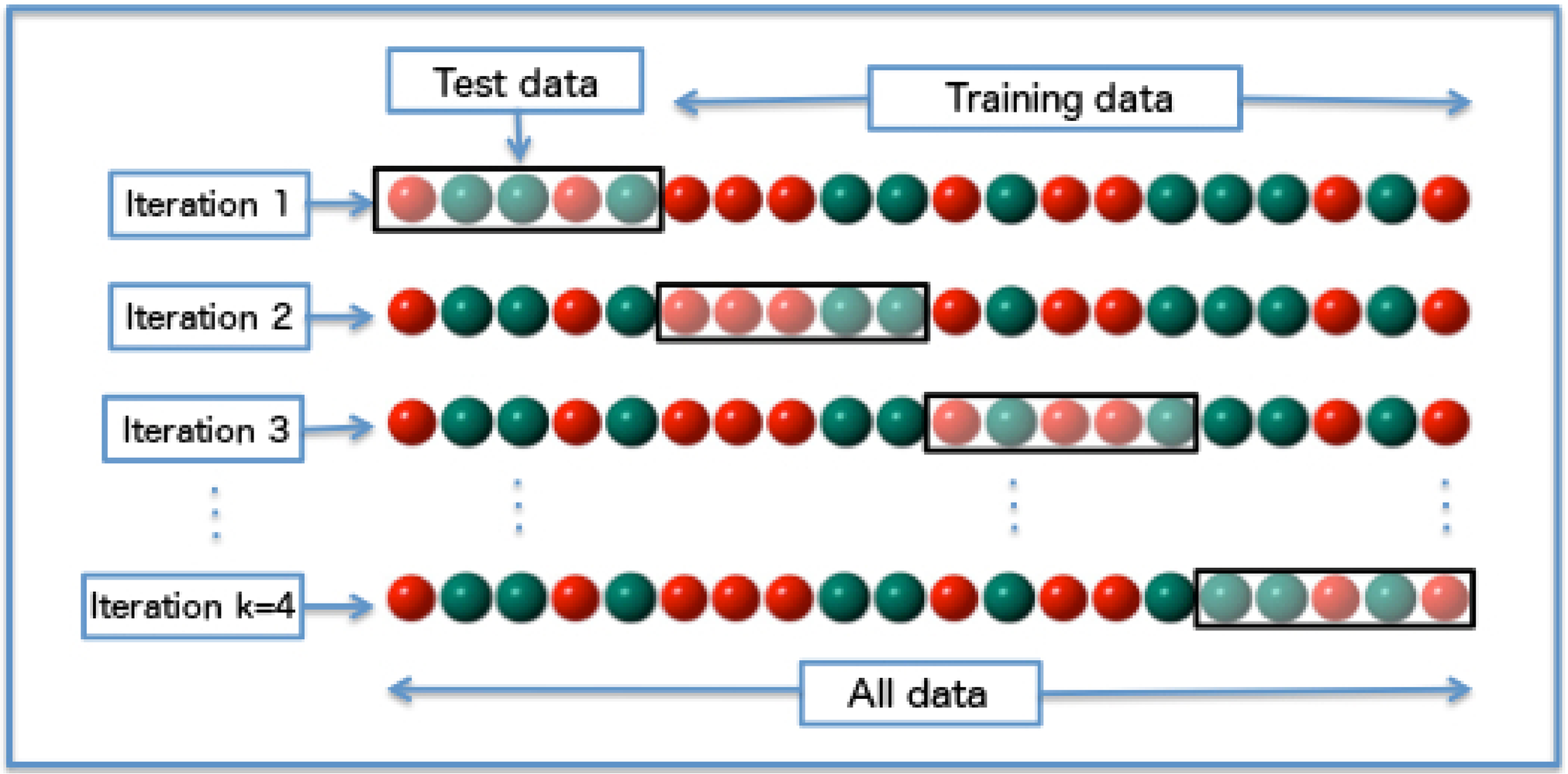
$$\epsilon_{\text{test}}(h_i) = \mathbb{E}_{(\mathbf{x},t)\in\mathcal{S}_{\text{test}}}\left[(h_i(\mathbf{x}) - t)^2\right]$$

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

- Disadvantage: 20 or 30% of the data is wasted and not used for learning. It may be a problem when data is rare or expensive.

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.



Source https://upload.wikimedia.org/wikipedia/commons/1/1c/K-fold_cross_validation_EN.jpg

k-fold cross-validation

Algorithm

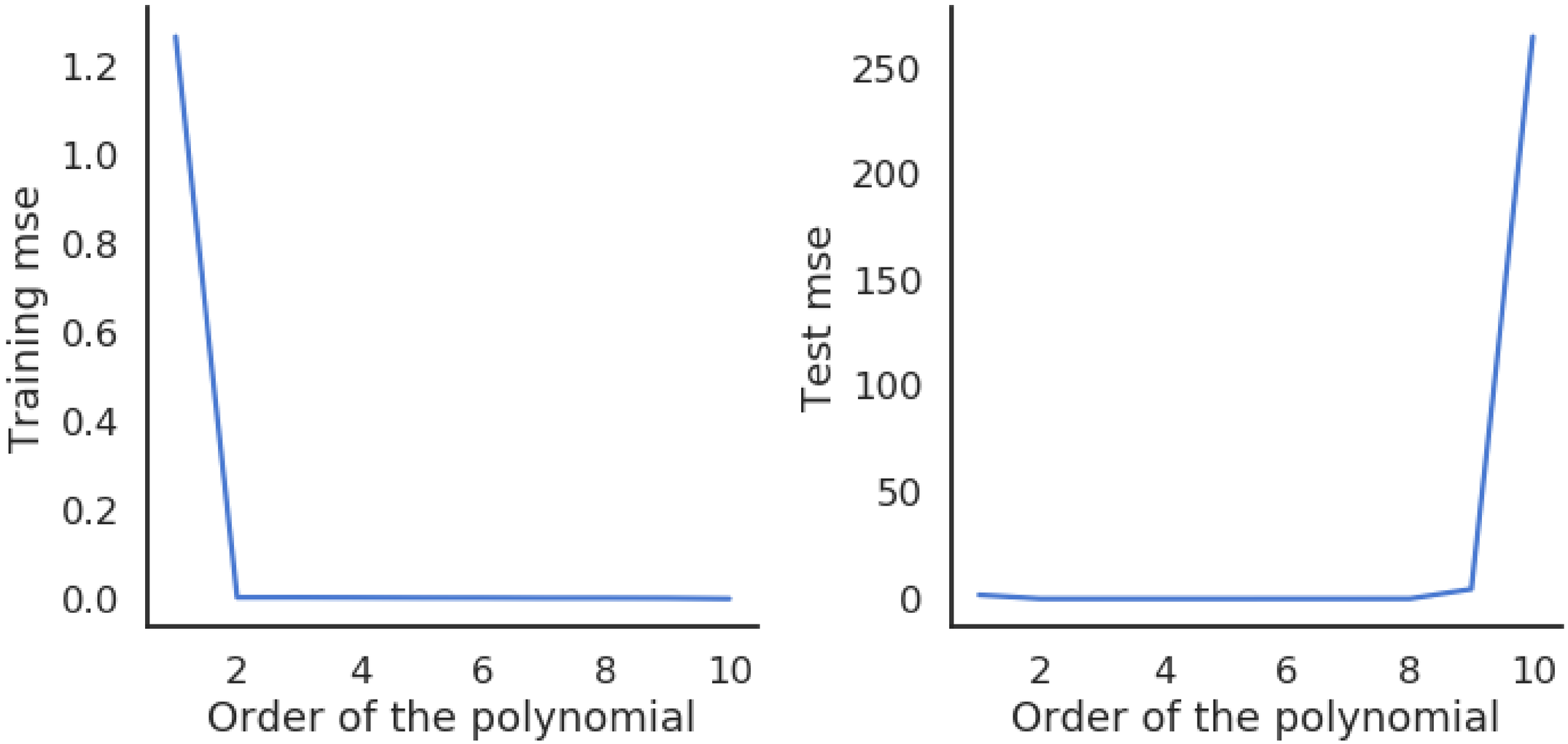
- Randomly split the data $\mathcal{D}$ into k subsets of $\frac{N}{k}$ examples $\{\mathcal{S}_1, \ldots, \mathcal{S}_k\}$
- For all models M_i:
  - For all k subsets $\mathcal{S}_j$:
    - Train M_i on $\mathcal{D} - \mathcal{S}_j$ to obtain an hypothesis h_{ij}
    - Compute the empirical error $\epsilon_{\mathcal{S}_j}(h_{ij})$ 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 $\mathcal{D}$.

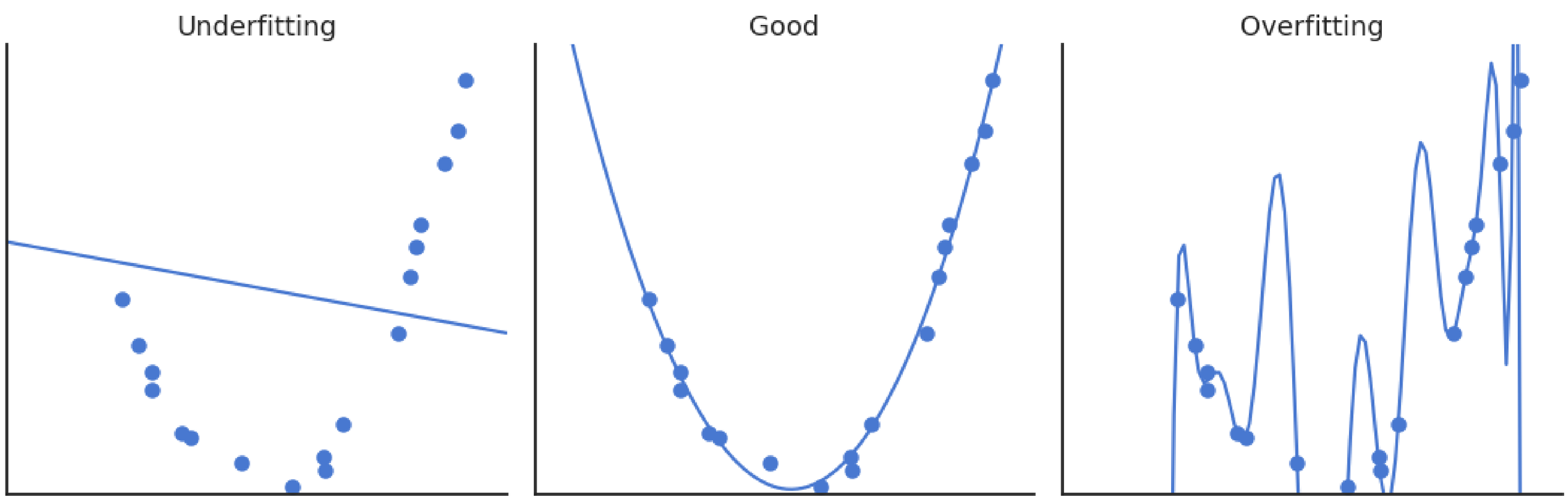
- In general $k = 10$. Extreme cases take $k = N$: **leave-one-out cross-validation**.
- k-fold cross-validation works well, but needs a lot of repeated learning.

Training and test errors



- While the training mse always decrease with more complex models, the 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?

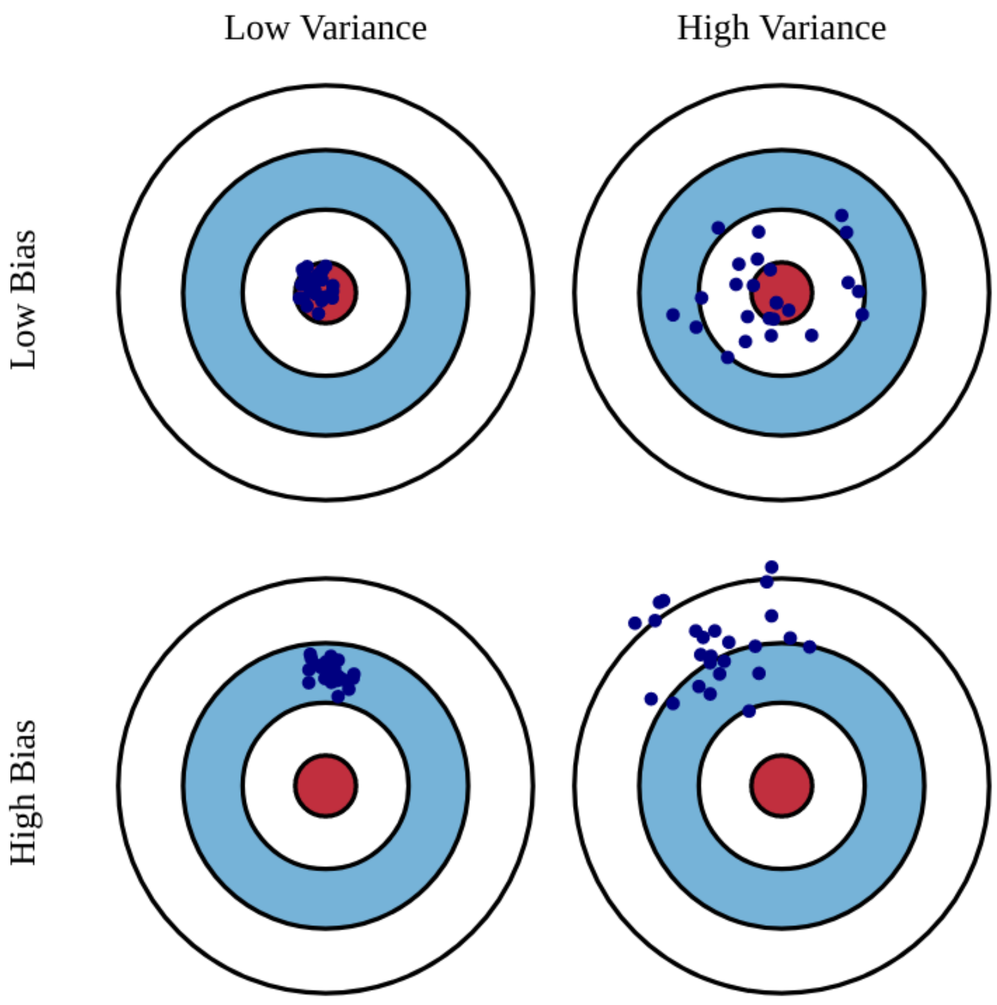
- In polynomial regression, the complexity is related to the order of the polynomial, i.e. the number of coefficients to estimate:

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

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

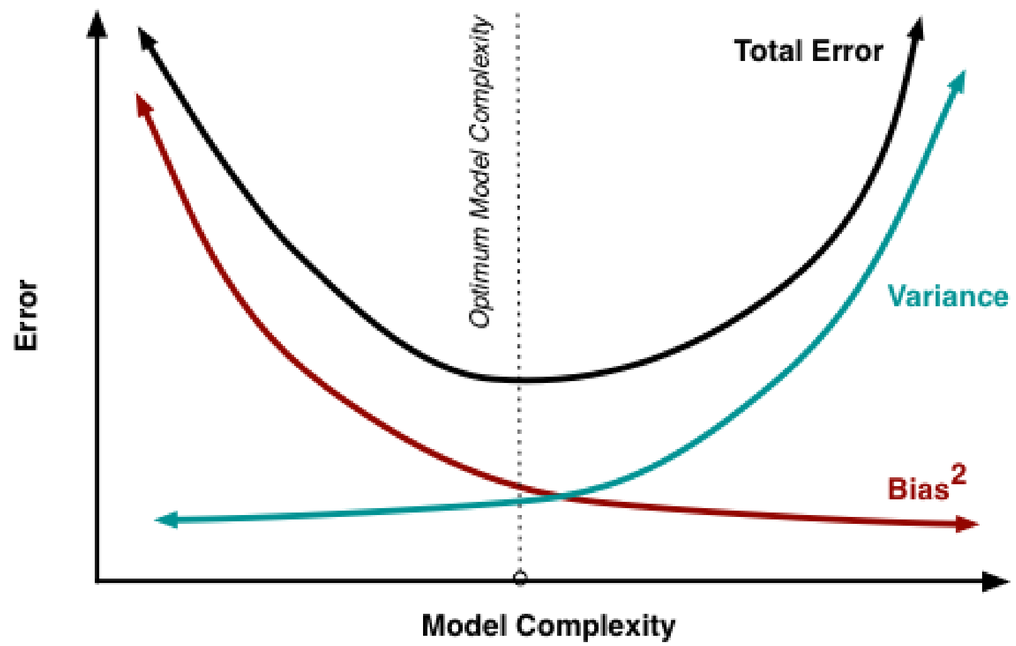
- A polynomial of order p has $p + 1$ unknown parameters (**free parameters**): the p weights and the bias.
- Generally, the **complexity of a model** relates to its **number of free parameters**:
  - **The more free parameters, the more complex the model is, the more likely it will overfit.**

Bias - variance trade-off



- Under-/Over-fitting relates to the statistical concept of **bias-variance trade-off**.
- The **bias** is the training error that the hypothesis would make if the training set was infinite (accuracy, flexibility of the model).
  - A model with high bias is underfitting.
- The **variance** is the error that will be made by the hypothesis on new examples taken from the same distribution (spread, the model is correct on average, but not for individual samples).
  - A model with high variance is overfitting.

Bias - variance trade-off



- The bias decreases when the model becomes complex.
- The variance increases when the model becomes complex.
- The **generalization error** is a combination of the bias and variance:

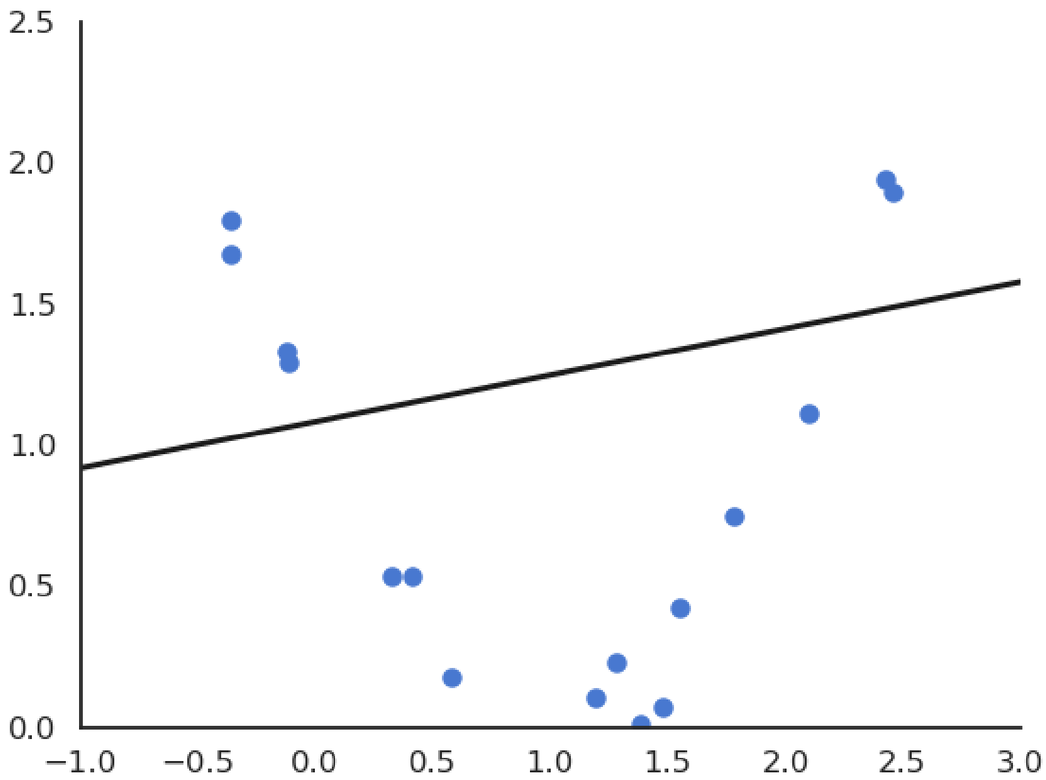
$$\text{generalization error} = \text{bias}^2 + \text{variance}$$

- We search for the model with the **optimum complexity** realizing the trade-off between bias and variance.
- It is better to have a model with a slightly higher bias (training error) but with a smaller variance (generalization error).

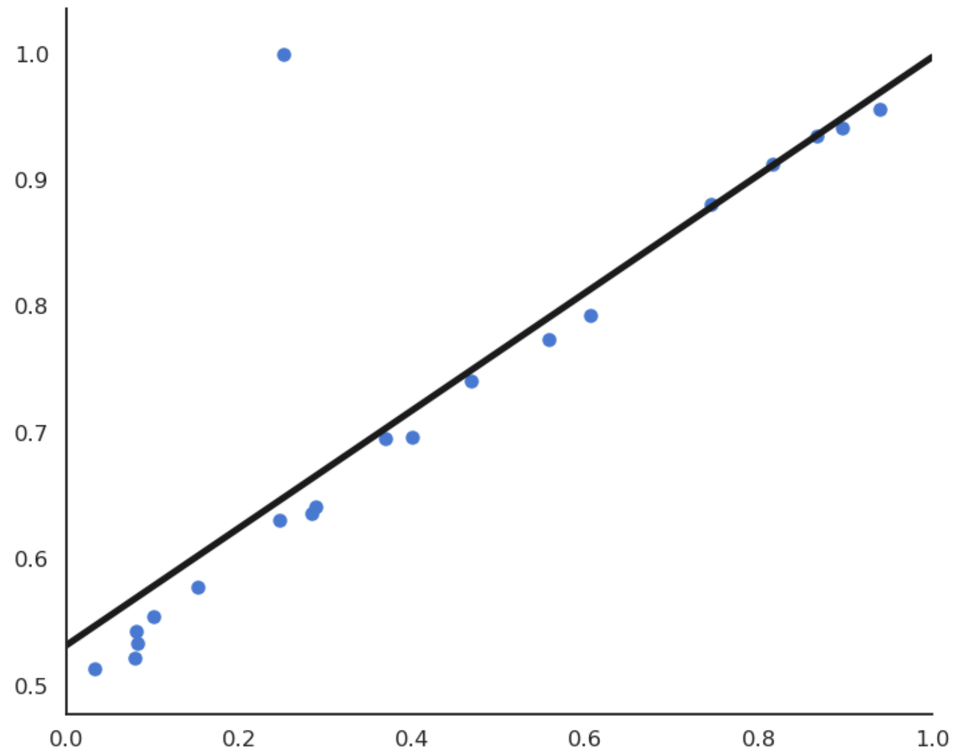
6 - Regularized regression

Linear regression can either underfit or overfit depending on the data

Underfitting

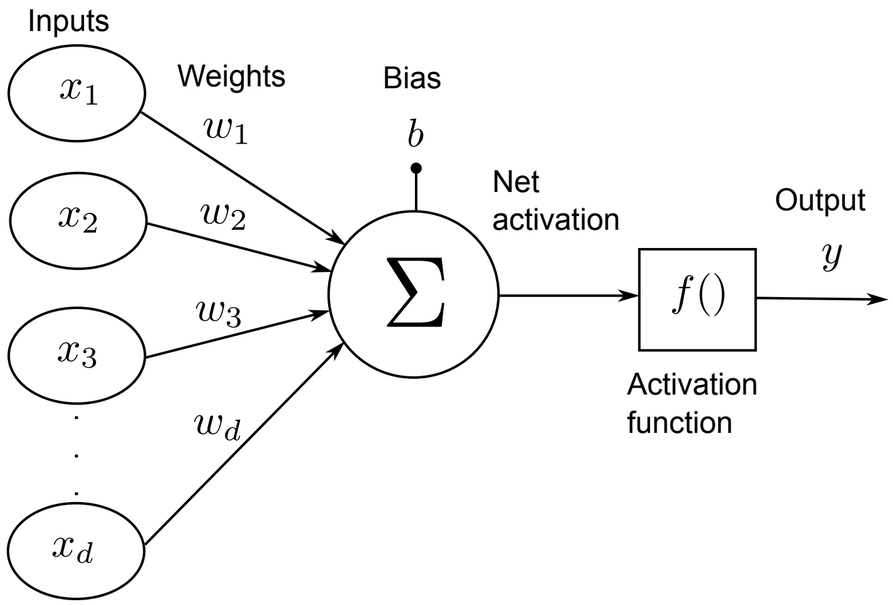


Overfitting



- 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:

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

- 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:

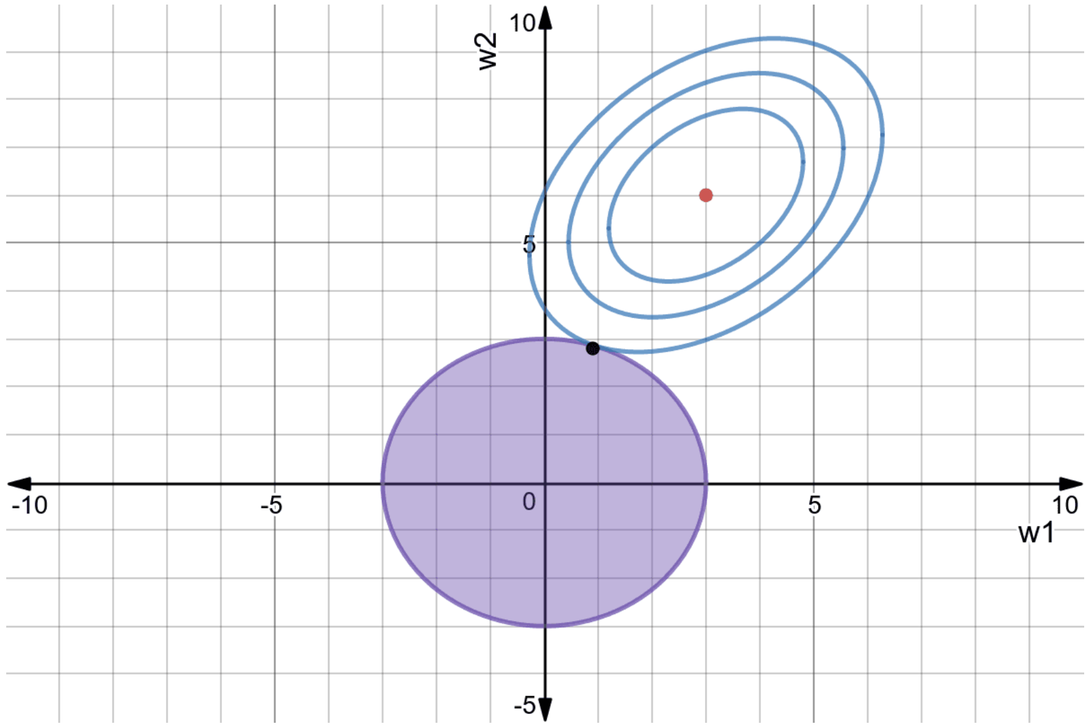
$$|\mathbf{w}| = \sum_{i=1}^{d} |w_i|$$

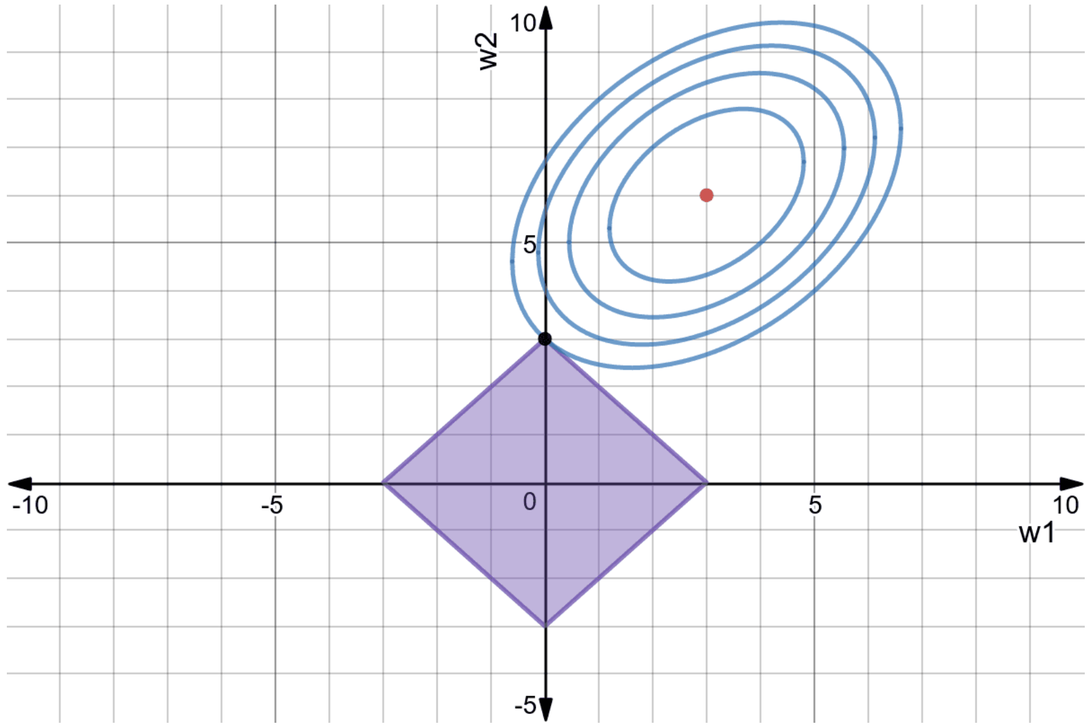
- Regularized delta learning rule with LASSO:

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

- **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



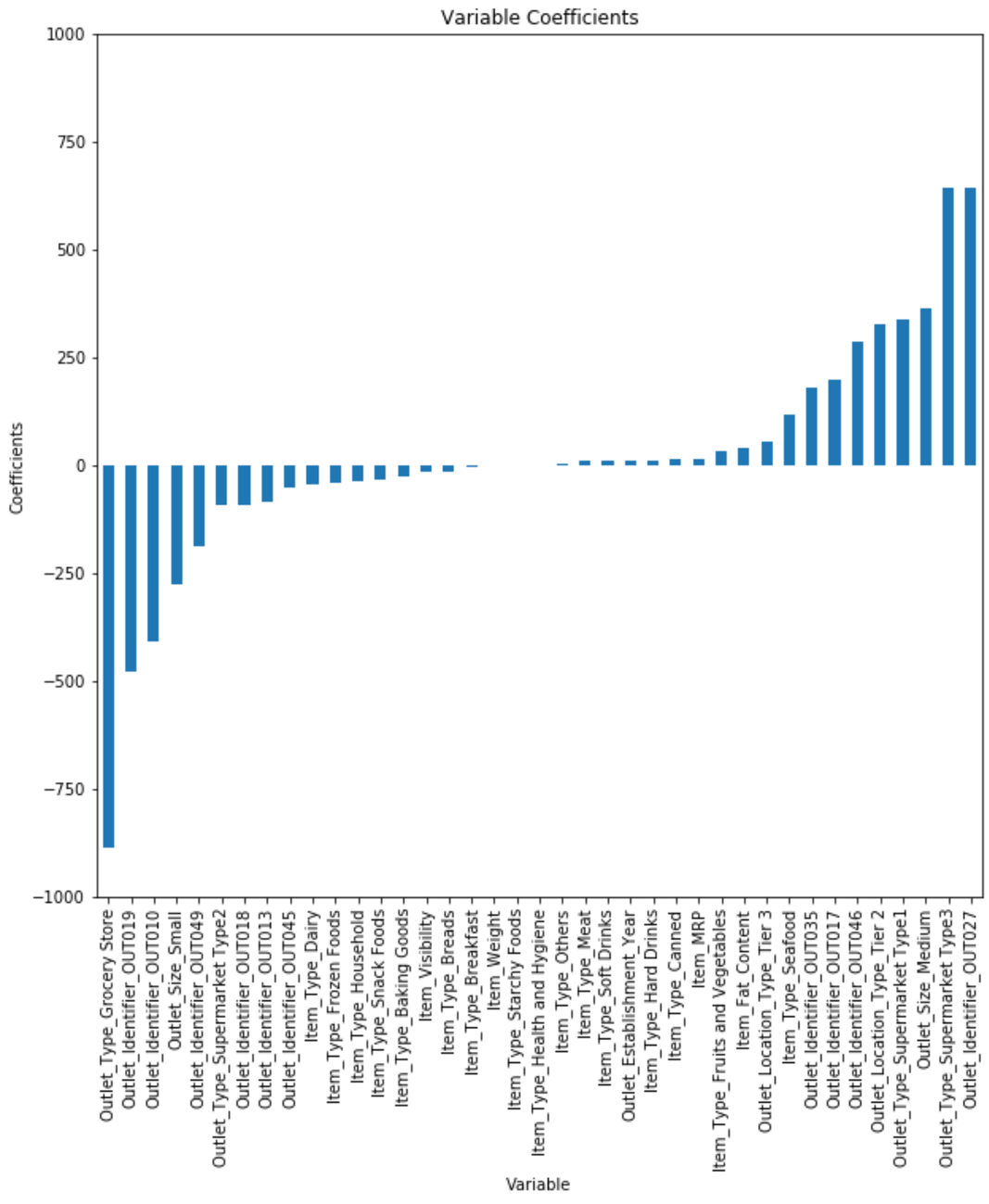


- **Ridge regression** finds the smallest value for the weights that minimize the mse.
- **LASSO regression** tries to set as many weight to 0 as possible (sparse code).

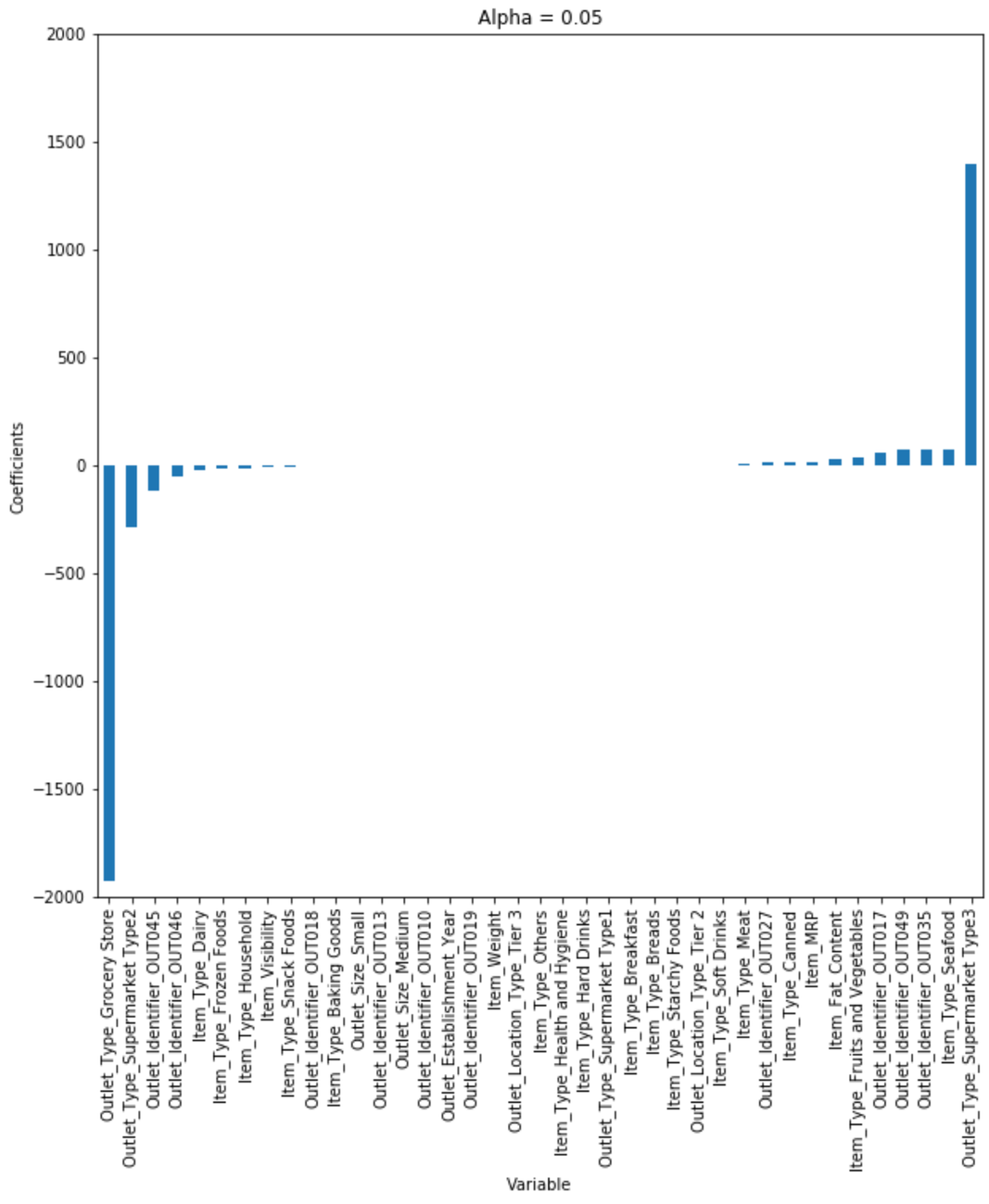
- Both methods depend on the **regularization parameter** λ. Its value determines how important the regularization term should.
- Regularization introduce a **bias**, as the solution found is **not** the minimum of the mse, but reduces the variance of the estimation, as small weights are less sensible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

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

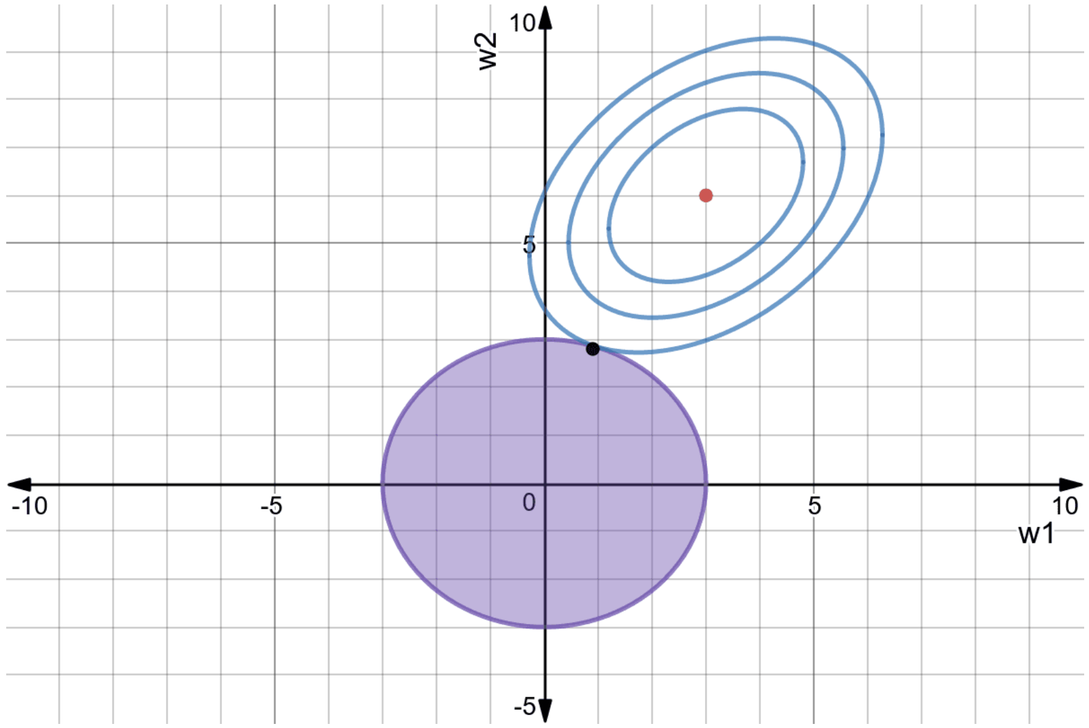
Linear regression

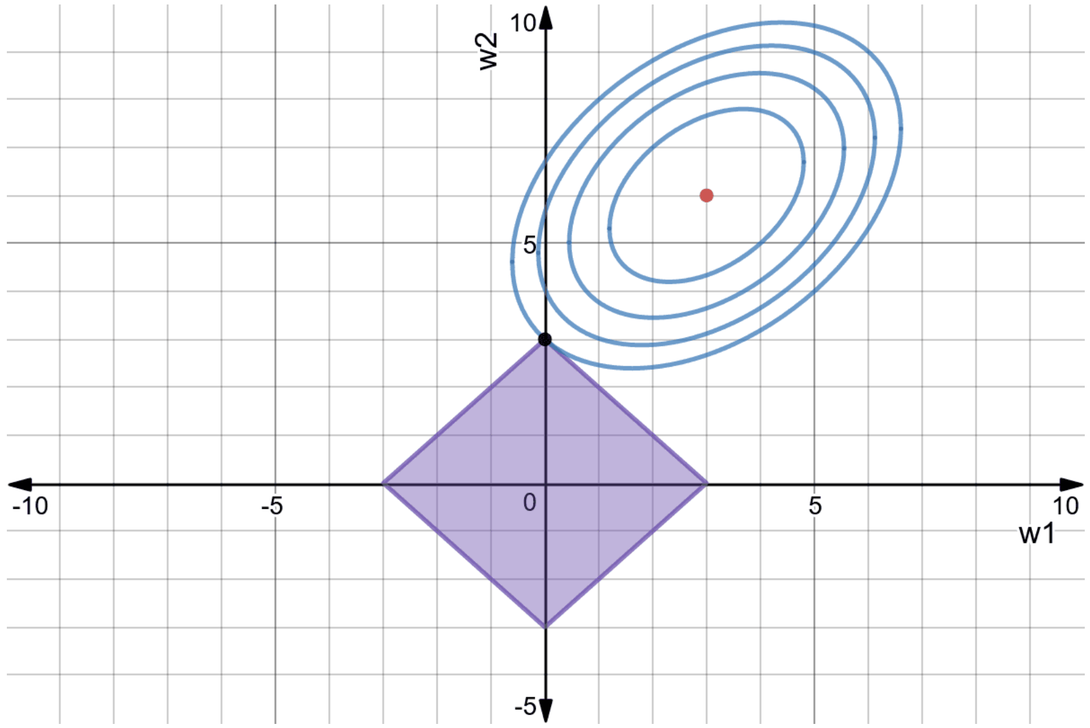


LASSO



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.