Linear Regression

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Weight-Height example

Dataset: heights and weights of different people.

Task: build a model that predicts the height given the weight.

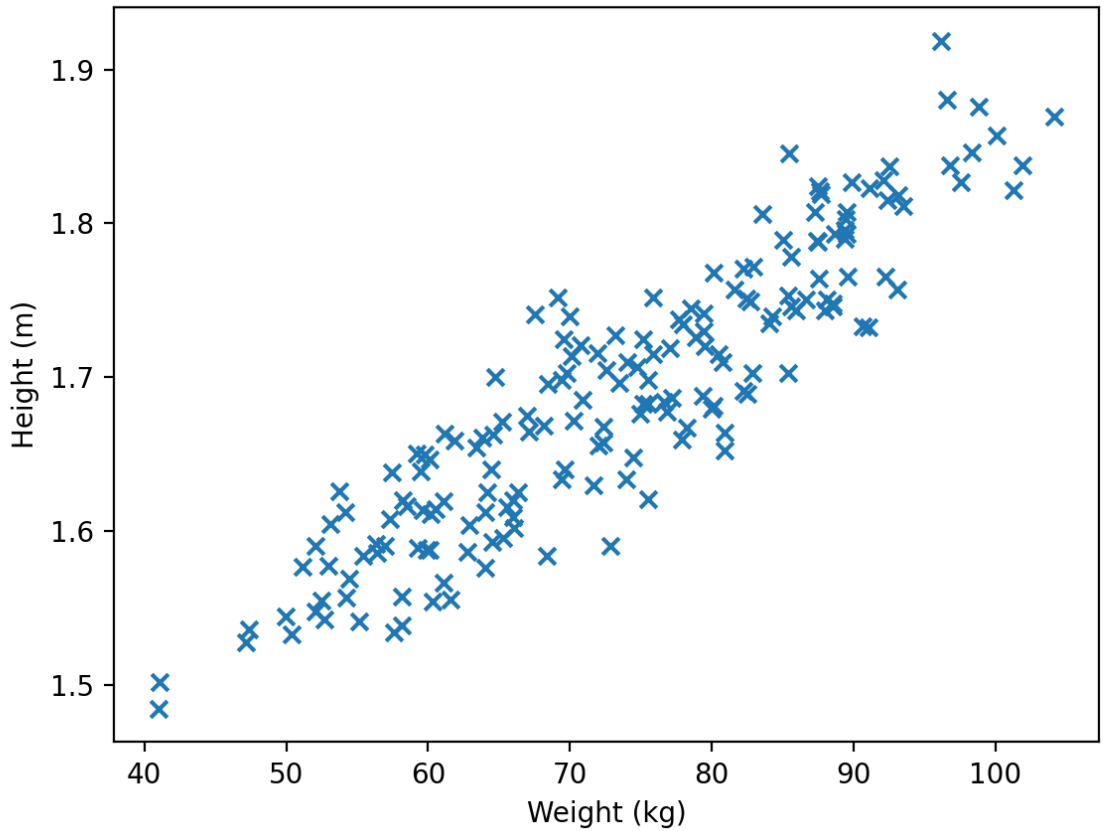


Figure: Plot of the dataset

A solution - Linear Regression model

Remarks:

- Regression problem (continuous output).
- Data with different orders of magnitude.

A possible solution to this problem may be represented by a linear model (represented in red in the figure below). This learning algorithm is called **Linear Regression** (LR).

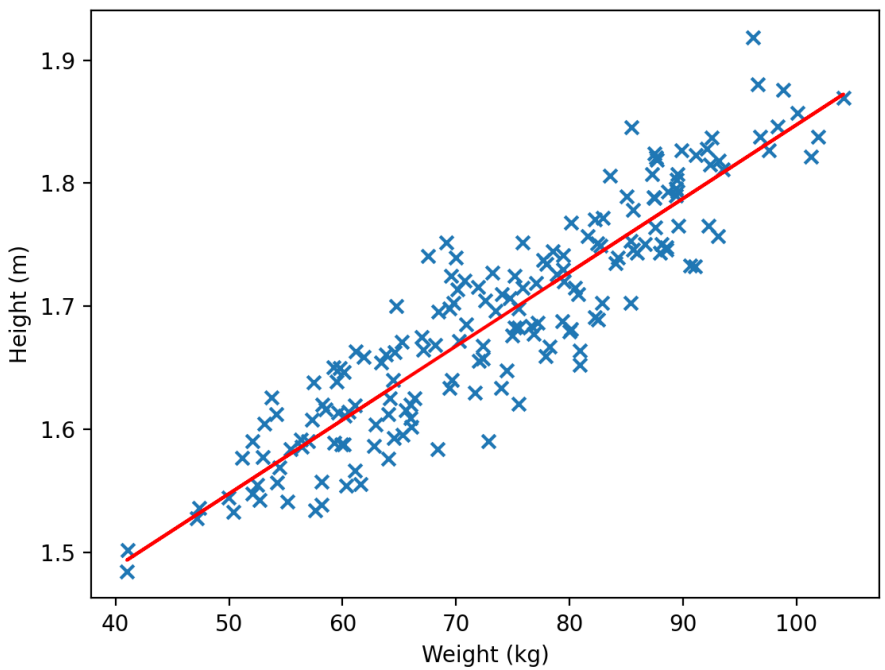


Figure: Trained model (in red)

General ingredients

Notation:

- $x^{(i)}$: a data sample.
- $y^{(i)}$: the data target corresponding to x
- N: number of samples.

Model/hypothesis: $h_{\boldsymbol{w}}(x^{(i)}) = w_1 x^{(i)} + w_0$, where $\boldsymbol{w} = [w_0, w_1]$ is the vector of parameter that has to be learned.
In our example, $x^{(i)}$ is the weight of a single sample and $h_{\boldsymbol{w}}(x^{(i)})$ corresponds to the prediction of its height.

The set $\mathcal{H} := \{h_{\boldsymbol{w}} | \boldsymbol{w} \in \mathbb{R}^2\}$ is called **hypothesis space**.

How to learn $\boldsymbol{w}$ from data?

Performance measure: Mean Squared Error (MSE)

To evaluate how good is the prediction we compute the error $(h_{\boldsymbol{w}}(x^{(i)}) - y^{(i)})^2$.

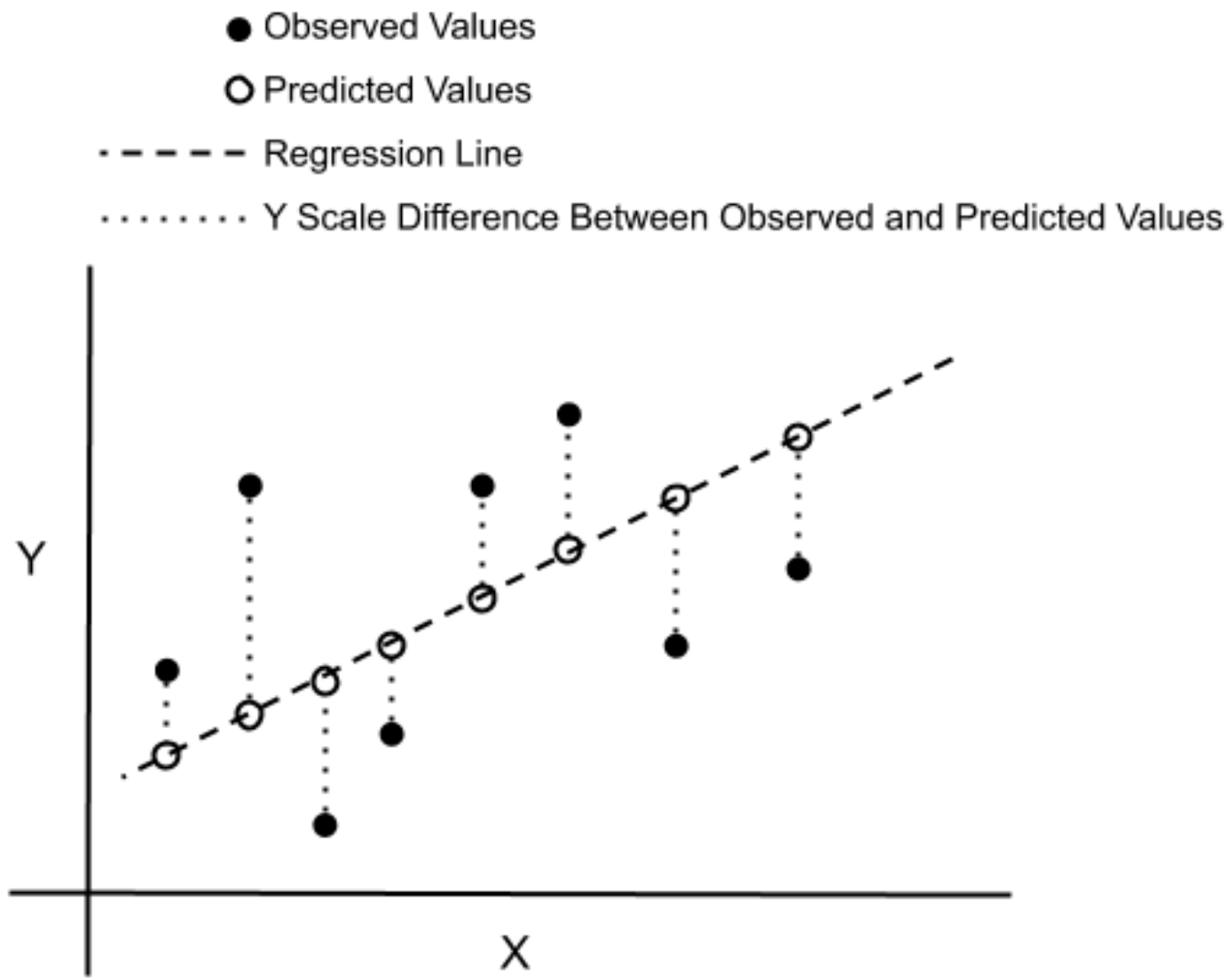
Notice that: $(h_{\boldsymbol{w}}(x^{(i)}) - y^{(i)})^2 \geq 0$ and $(h_{\boldsymbol{w}}(x^{(i)}) - y^{(i)})^2 = 0$ if and only if $h_{\boldsymbol{w}}(x^{(i)}) = y^{(i)}$. The **mean squared error** (MSE) is:

$$E(\boldsymbol{w}) := \frac{1}{N} \sum_{i=1}^{N} (h_{\boldsymbol{w}}(x^{(i)}) - y^{(i)})^2.$$

To find the parameters of the best model we minimize the MSE.

$$\boldsymbol{w} \in \arg\min_{\tilde{\boldsymbol{w}} \in \mathbb{R}^2} E(\tilde{\boldsymbol{w}}).$$

MSE - Visualization



n-dimensional LR

Dataset samples.
Previous case: $x^{(i)} \in \mathbb{R}, y^{(i)} \in \mathbb{R}$.
Now: $\boldsymbol{x}^{(i)} \in \mathbb{R}^n, y^{(i)} \in \mathbb{R}$.
Notation: $x_j^{(i)}$ is the j-th coordinate of the i-th sample.

Candidate hypothesis.

$$\begin{aligned} h_{\boldsymbol{w}}(\boldsymbol{x}) &= w_n x_n + w_{n-1} x_{n-1} + \cdots + w_1 x_1 + w_0 \\ &= \sum_{i=0}^{n} w_i \tilde{x}_i = \boldsymbol{w}^T \tilde{\boldsymbol{x}}, \end{aligned}$$

where $\boldsymbol{w} = [w_0, \ldots, w_n]^T$ and $\tilde{\boldsymbol{x}} = [1, x_1, \ldots, x_n]^T$.

n-dimensional LR

MSE.

$$
\begin{aligned}
E(\boldsymbol{w}) &= \frac{1}{N}\sum_{i=1}^{N}(h_w(\boldsymbol{x}^{(i)}) - y^{(i)})^2 \\
&= \frac{1}{N}(\mathrm{X}\boldsymbol{w} - \boldsymbol{y})^T(\mathrm{X}\boldsymbol{w} - \boldsymbol{y}) \\
&= \frac{1}{N}||\mathrm{X}\boldsymbol{w} - \boldsymbol{y}||^2
\end{aligned}
$$

where

$$
\mathrm{X} := \begin{bmatrix} \tilde{\boldsymbol{x}}^{(1)} \\ \vdots \\ \tilde{\boldsymbol{x}}^{(N)} \end{bmatrix} \quad \boldsymbol{y} = \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(N)} \end{bmatrix}.
$$

In particular, $\mathrm{X} \in \mathbb{R}^{N\times(n+1)}$ and $\boldsymbol{y} \in \mathbb{R}^N$.

Spot the minimum - Gradient descent

How to find $\boldsymbol{w} \in \arg\min_{\tilde{\boldsymbol{w}} \in \mathbb{R}^2} E(\tilde{\boldsymbol{w}})$?

Main idea: geometrically, the gradient of a scalar function represents the direction of maximum slope. Hence, following the direction opposite to the gradient leads closer to the minimum of the function.

Formally:

- Start with an initial guess $\boldsymbol{w}^0$ (random).
- For $j \geq 0$, update $\boldsymbol{w}^{j+1} := \boldsymbol{w}^j + \boldsymbol{d}^j$, where $\boldsymbol{d}^j$ is such that

$$E(\boldsymbol{w}^{j+1}) \leq E(\boldsymbol{w}^j)$$

Gradient descent: $\boldsymbol{d}^j = -\alpha \nabla E(\boldsymbol{w}^j)$; $\alpha > 0$ is called **learning rate**.

Gradient descent - 3D visualization

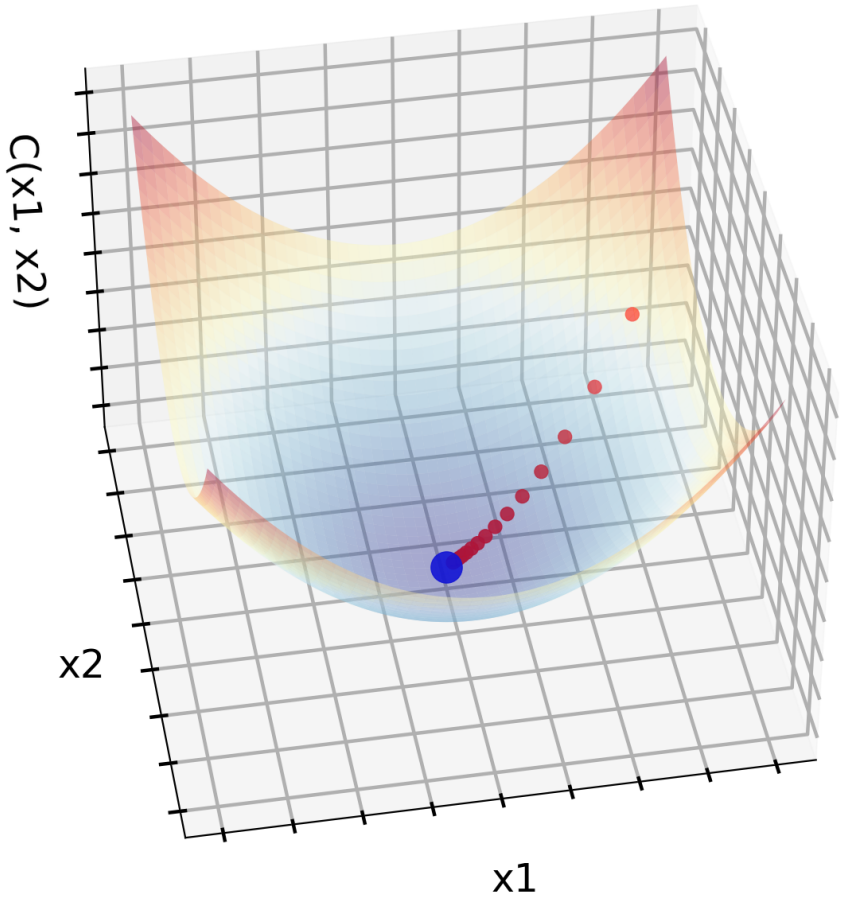


Figure: In blue the global minimum, in red the iteration points.

Gradient descent - 2D visualization

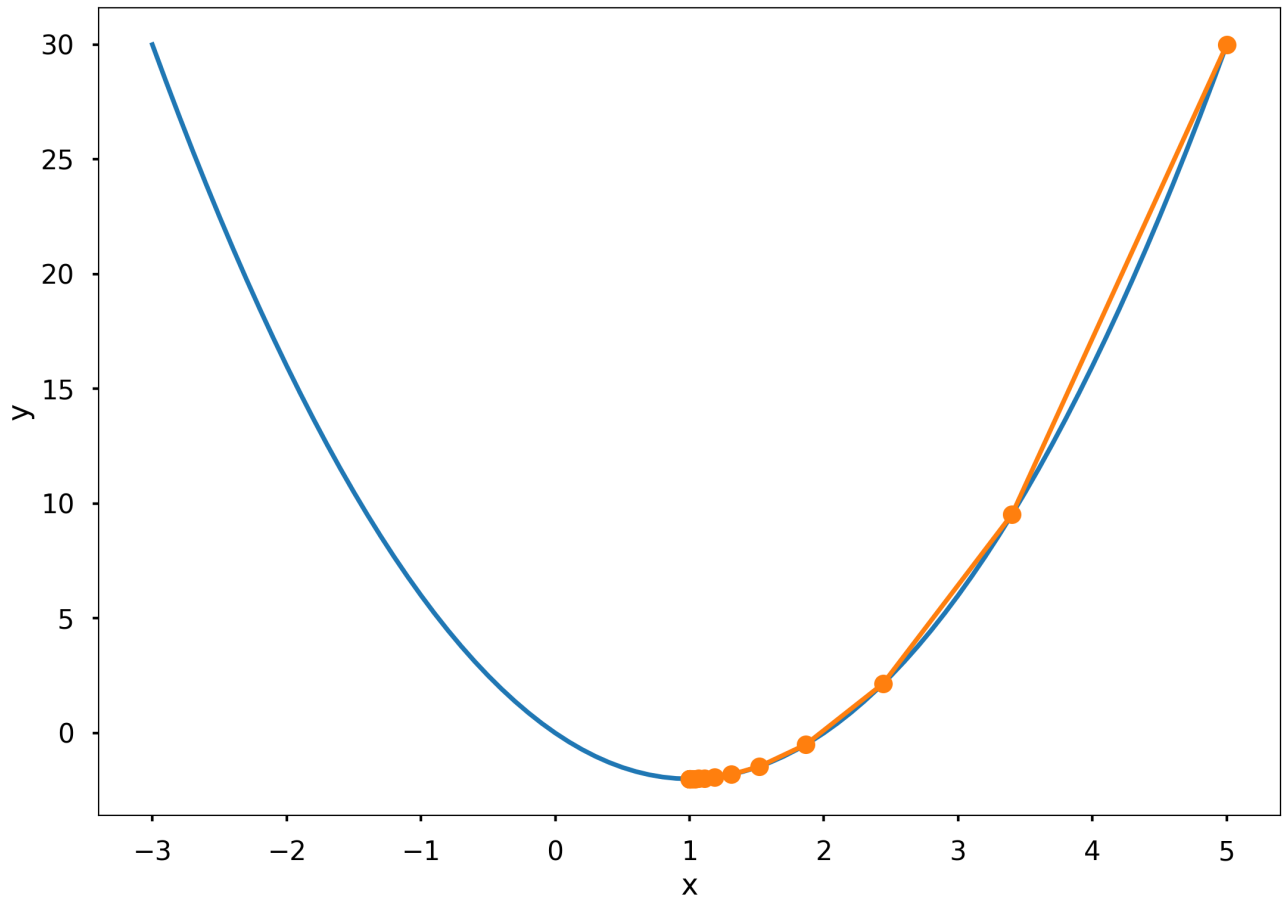


Figure: Learning rate = 0.1

Gradient descent - 2D visualization

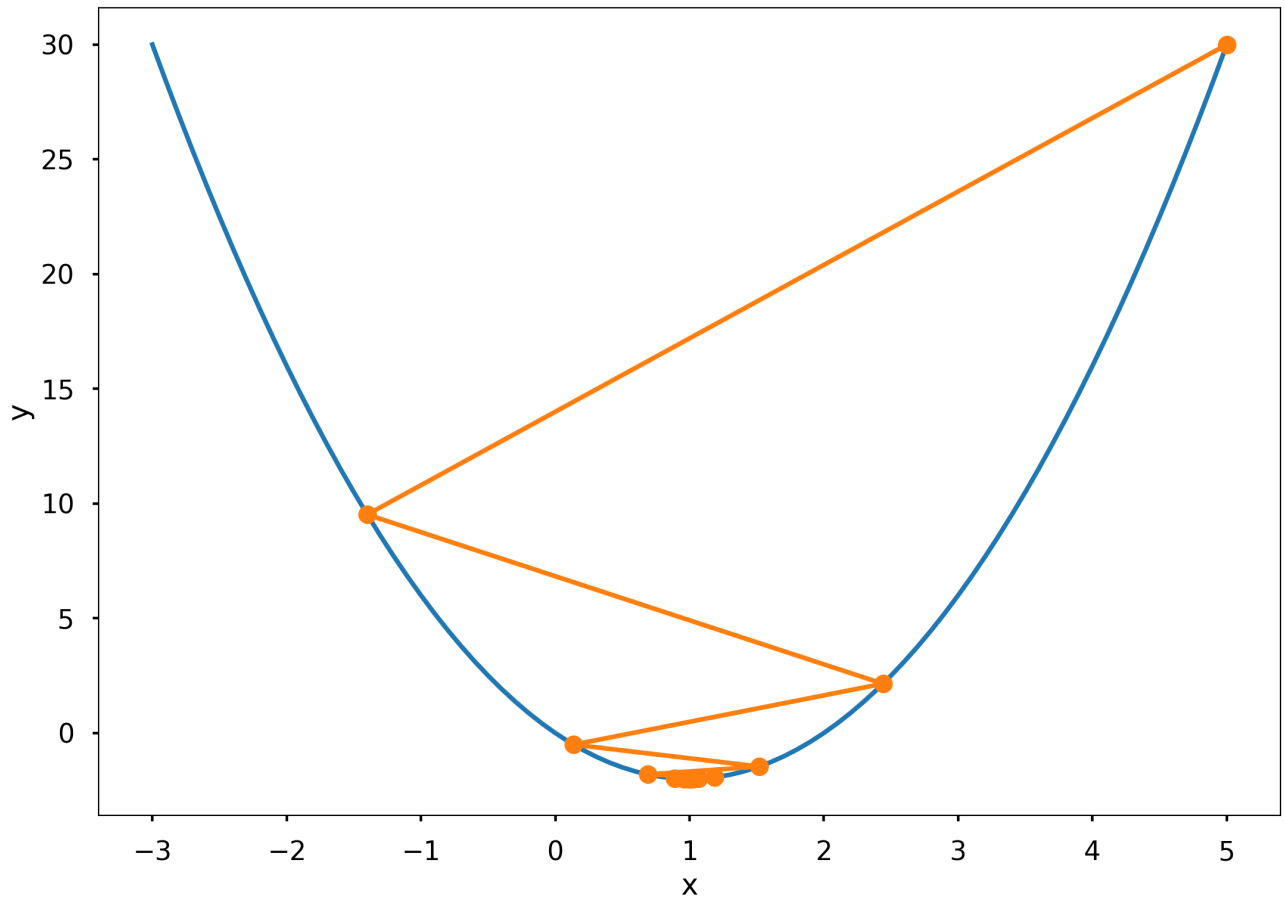


Figure: Learning rate = 0.4

Gradient descent - 2D visualization

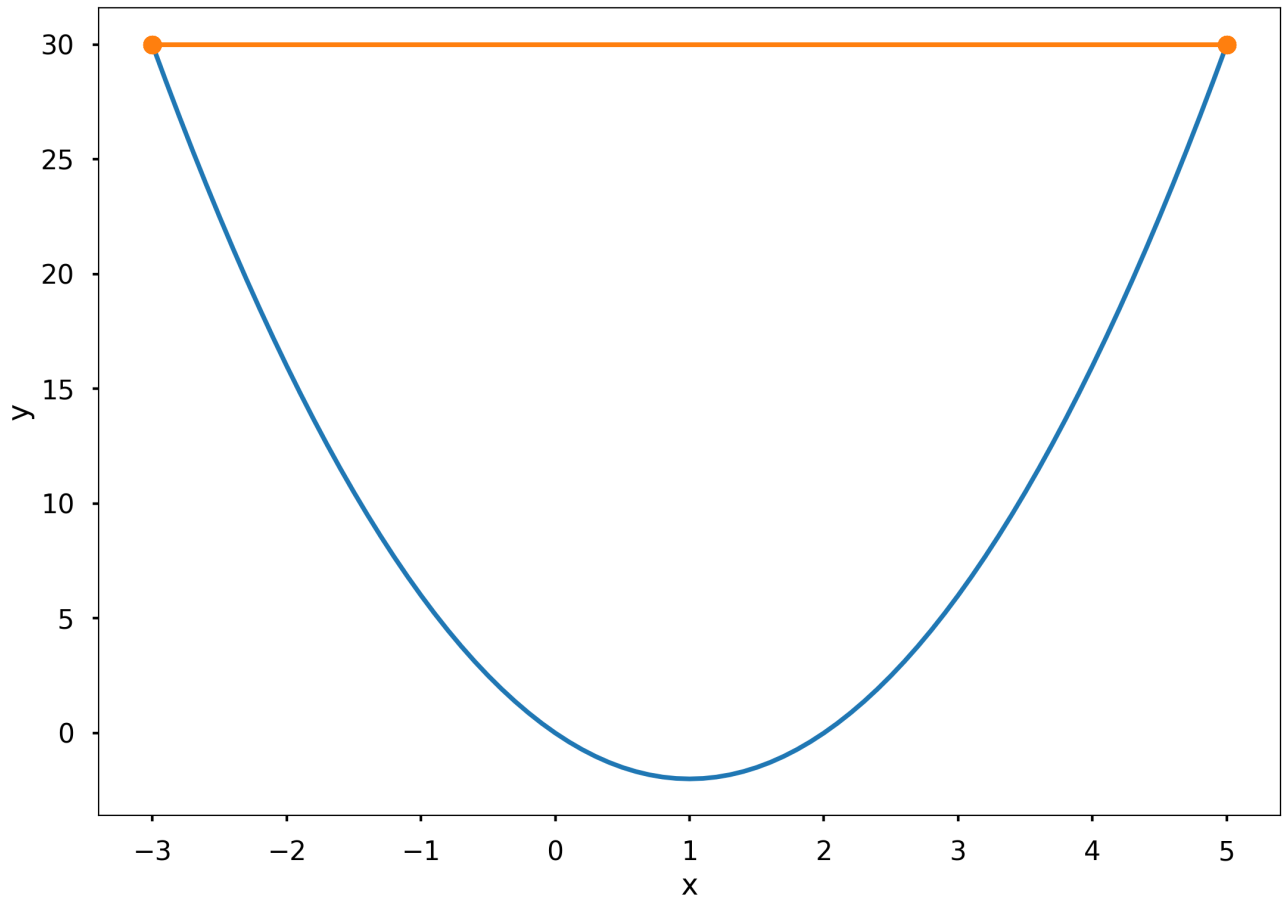


Figure: Learning rate = 0.5

Batch, SGD and Mini-Batch - Intuition

Notation: $E(\boldsymbol{w}) = 1/N \sum_{i=1}^{N} E_i(\boldsymbol{w})$

The classical gradient descent update rule, i.e. update the weights vector computing the gradient of the entire cost function $E(\boldsymbol{w})$, is called **batch version**. However, for large number of samples (N) computing $\nabla E(\boldsymbol{w})$ is very time consuming.

To speed-up the update rule we approximate $\nabla E(\boldsymbol{w})$ with $\nabla E_i(\boldsymbol{w})$. This is the idea behind the so-called **Stochastic Gradient Descent** (SGD) or **online version**.

A trade-off between GD and SGD is called **mini-batch version**.

Batch, SGD and Mini-Batch - Formal

Batch

- Start with a random $\boldsymbol{w}^0$.
- For $j \geq 0$, update $\boldsymbol{w}^{j+1} := \boldsymbol{w}^j - \alpha \nabla E(\boldsymbol{w}^j)$.

Stochastic Gradient Descent (SGD or online)

- Start with a random $\boldsymbol{w}^0$.
- For each epoch $j \geq 0$:
  - shuffle the dataset to prevent cycles;
  - for each $1 \leq i \leq N$ update $\boldsymbol{w} := \boldsymbol{w} - \alpha \nabla E_i(\boldsymbol{w})$.

Mini-Batch. Fix an integer $1 \leq \text{mb} \leq N$(mini-batch size).

- Start with a random $\boldsymbol{w}^0$.
- For each epoch $j \geq 0$:
  - shuffle the dataset to prevent cycles;
  - for each $0 \leq i < \frac{N}{\text{mb}}$ update

$$\boldsymbol{w} := \boldsymbol{w} - \alpha \nabla \sum_{k=i\cdot \text{mb}+1}^{(i+1)\cdot \text{mb}} E_k(\boldsymbol{w}).$$

Tips and Tricks - How to choose?

- Batch: usually more stable and provide a more accurate estimation of the gradient, but very slow.
- SGD: very fast, stochastic approximation of the gradient implies possible instability (Zig-zag effect)
- Mini-Batch: a trade-off (parallelism available).

In practice, through SGD and mini-batch we may not even reach the minimum, but it is enough to get close to it.

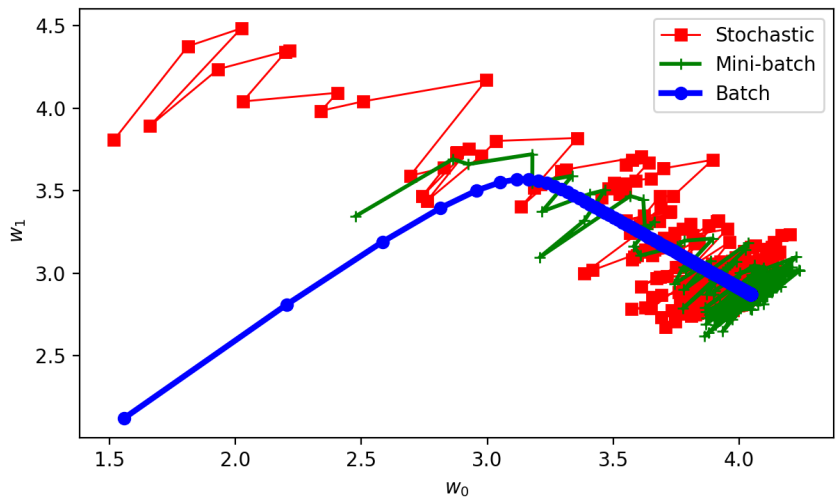


Figure: Batch vs SGD vs Mini-batch

Gradient descent and normal equation for LR

We have $E(\boldsymbol{w}) = \frac{1}{N}||\mathrm{X}\boldsymbol{w} - \boldsymbol{y}||^2$, hence

$$\nabla E(\boldsymbol{w}) = \frac{1}{N}\nabla(||\mathrm{X}\boldsymbol{w} - \boldsymbol{y}||^2) = \frac{2}{N}\mathrm{X}^T(\mathrm{X}\boldsymbol{w} - \boldsymbol{y})$$

Normal equation ($\Longleftrightarrow$ holds if $\mathrm{X}^T\mathrm{X}$ is invertible):

$$\begin{aligned}\nabla E(\boldsymbol{w}) = 0 &\Longleftrightarrow \frac{2}{N}\mathrm{X}^T(\mathrm{X}\boldsymbol{w} - \boldsymbol{y}) = 0 \\ &\Longleftrightarrow \mathrm{X}^T\mathrm{X}\boldsymbol{w} = \mathrm{X}^T\boldsymbol{y} \\ &\Longleftrightarrow \boldsymbol{w} = (\mathrm{X}^T\mathrm{X})^{-1}\mathrm{X}^T\boldsymbol{y}\end{aligned}$$

Gradient descent main iteration for LR:

$$\boldsymbol{w}^{j+1} := \boldsymbol{w}^j - \frac{2\alpha}{N}\mathrm{X}^T(\mathrm{X}\boldsymbol{w}^j - \boldsymbol{y})$$

Tips and Tricks - Invertibility of $X^T X$

Invertibility of $X^T X \iff$ columns of X linearly independent (preprocessing information).

What happens when $X^T X$ is not invertible?

If two columns are linearly dependent, then those features are correlated (**redundant**).

Solution: discard one of those features.

Normal equation vs gradient descent

Normal equation:

- No hyperparameter (explicit solution).
- No need to iterate.
- $\mathcal{O}(N^3)$, since this is the cost to invert a dense matrix. In particular, it is slow when N is large.

Gradient descent:

- Need to choose the learning rate α.
- Needs many iterations.
- $\mathcal{O}(N^2)$, hence faster when N is large.

Tips and Tricks - Standardization

General (not only for LR): features must be on a similar scale!

- Speed up the convergence of gradient descent.
- Try to have (on average) $-1 \leq \boldsymbol{x}^{(i)} \leq 1$.

Common techniques:

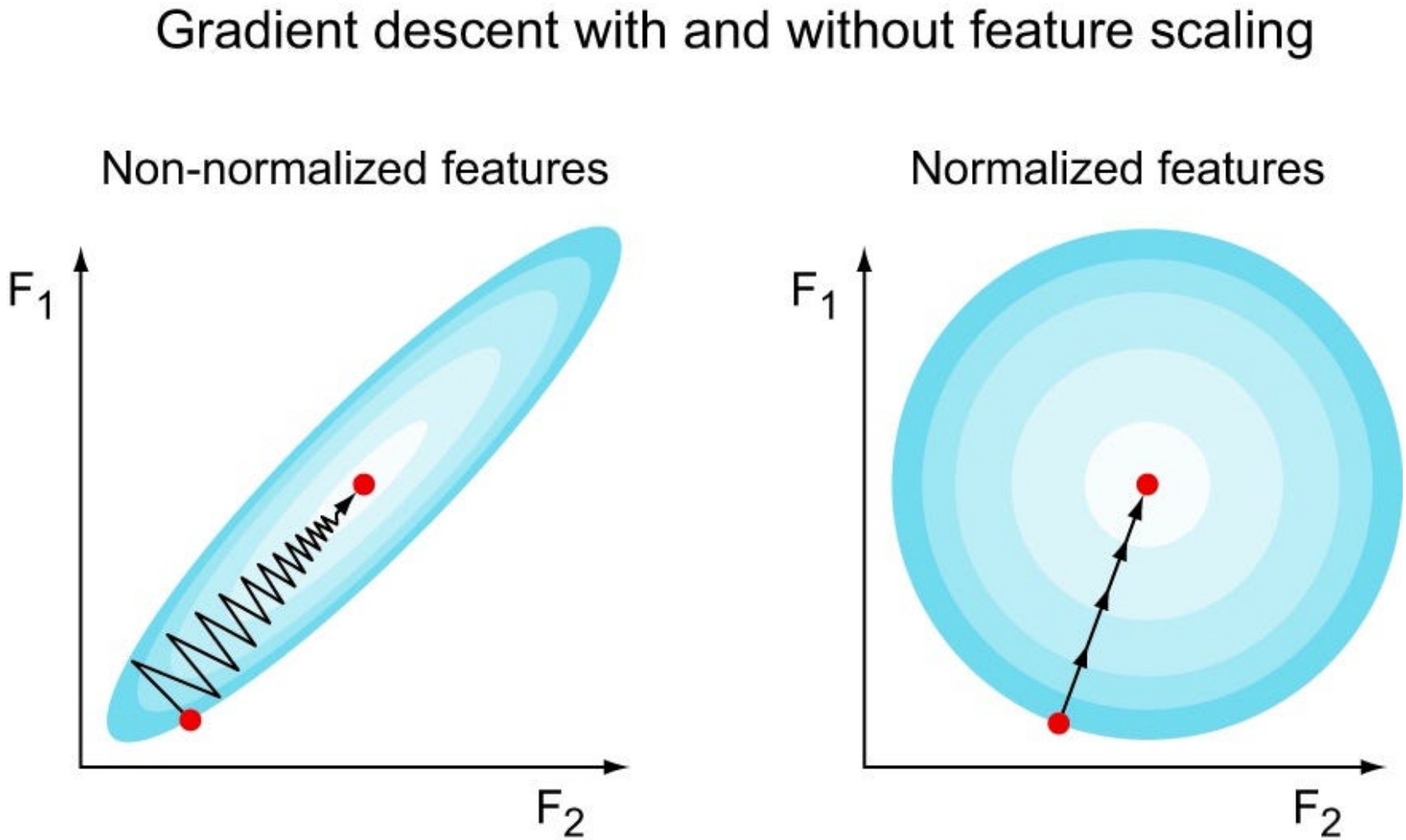
- **Feature scaling**. Compute the max $\boldsymbol{M} := [\max_i x_j^{(i)}]_j$ and the min $\boldsymbol{m} := [\min_i x_j^{(i)}]_j$ data value. Then normalize each feature as follows

$$\boldsymbol{x}^i_{\text{norm}} = \frac{\boldsymbol{x}^{(i)} - \boldsymbol{m}}{\boldsymbol{M} - \boldsymbol{m}}$$

- **Mean normalization**. Compute mean $\boldsymbol{\mu}$ ($\mu_j := \mathbb{E}[[x_j^{(i)}]_i]$) and standard deviation $\boldsymbol{\sigma}$ ($\sigma_j := \sqrt{\text{Var}[[x_j^{(i)}]_i]}$) of the data. Then normalize each feature as follows

$$\boldsymbol{x}^{(i)}_{\text{norm}} = \frac{\boldsymbol{x}^{(i)} - \boldsymbol{\mu}}{\boldsymbol{\sigma}}$$

Tips and Tricks - Standardization



Polynomial regression (PR)

PR corresponds to polynomial hypothesis, i.e. of the form

$$h_{\boldsymbol{w}}(\boldsymbol{x}) = \sum_{j=0}^{n} w_j x_j^j.$$

More in general: linear basis expansion (LBE)

$$h_{\boldsymbol{w}}(\boldsymbol{x}) = \sum_{j=0}^{n} w_j \phi_j(\boldsymbol{x}),$$

where $\phi_j : \mathbb{R}^n \to \mathbb{R}$.

Underfitting and overfitting - main intuition

Imagine that you have to prepare an exam.

Doing only a few exercises lead a poor perfomance both on homeworks and on the exam exercises. This is called *underfitting*: you have a bad performance on the exam because you did not trained enough.

Moreover, brutally memorize all the homework lead to a perfect score on homeworks (trivially) but probably a bad score on the exam exercises. This is called *overfitting*: you have a bad performance on the exam because you did not captured the true essence of your homework, you have also memorize their "noise" (homework pecularities).

Underfitting and overfitting - another example

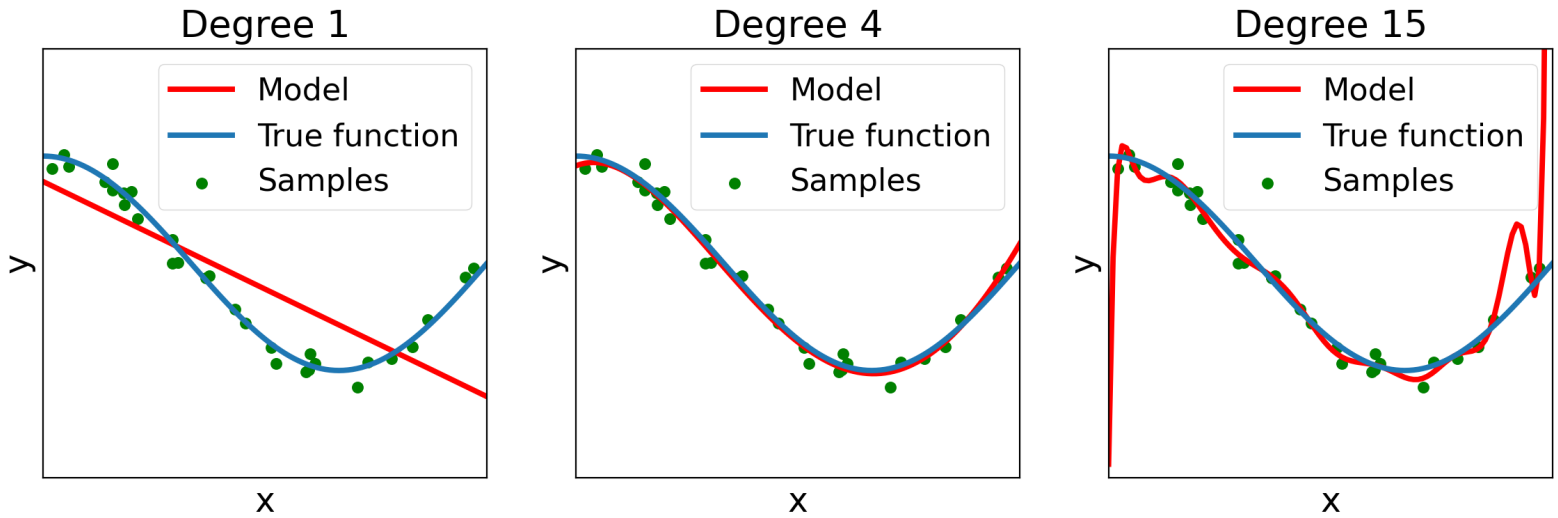


Figure: Underfitting (degree 1), good fitting (degree 4), overfitting (degree 15).

Overfitting can be countered in many ways, including:

- Validation, the true core of Machine Learning;
- Regularization.

Regularization

Overfitting is highly correlated with "complex" models. To avoid "complex" models, the idea is to penalize models with large weights. One way to do it is to consider the following cost function

$$E_r(\boldsymbol{w}) = E(\boldsymbol{w}) + R_\lambda(\boldsymbol{w}).$$

R_λ is called *regularization term*. $\lambda > 0$ is an hyperparameter that must be chosen in the model selection phase.
Most common regularization techniques:

- Tikhonov regularization: $R_\lambda(\boldsymbol{w}) = \lambda||w||_2$. Tends to bring all the weights to small values.
- Lasso: $R_\lambda(\boldsymbol{w}) = \lambda||w||_1$. Tends to bring some weights to 0 (feature selection).

LR with Tikhonov regularization

Cost function (with no regularization):

$$E(\boldsymbol{w}) = \frac{1}{N}||\mathrm{X}\boldsymbol{w} - \boldsymbol{y}||^2.$$

New cost function:

$$E_r(\boldsymbol{w}) = E(\boldsymbol{w}) + \lambda||\boldsymbol{w}||^2.$$

Gradient of the cost function:

$$\nabla E_r(\boldsymbol{w}) = \nabla E(\boldsymbol{w}) + 2\lambda\boldsymbol{w} = 2(\frac{1}{N}\mathrm{X}^T(\mathrm{X}\boldsymbol{w} - \boldsymbol{y}) + \lambda\boldsymbol{w})$$

Normal equation:

$$\boldsymbol{w} = (\mathrm{X}^T\mathrm{X} + \lambda\mathrm{I})^{-1}\mathrm{X}^T\boldsymbol{y}$$

Note that in this case $\mathrm{X}^T\mathrm{X} + \lambda\mathrm{I}$ is *always* invertible (why? :))