Regression and Gradient Descent

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Weight-Height dataset

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

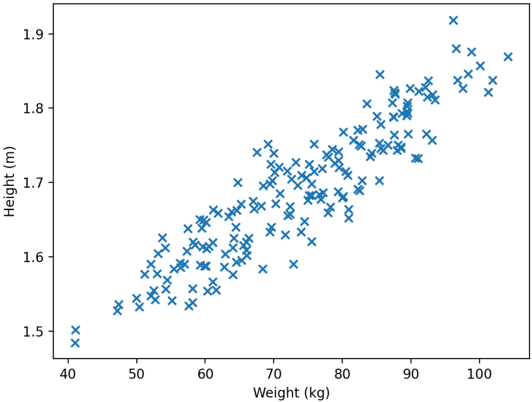


Figure: Plot of the dataset

A solution - Linear Regression model

Remarks:

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

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

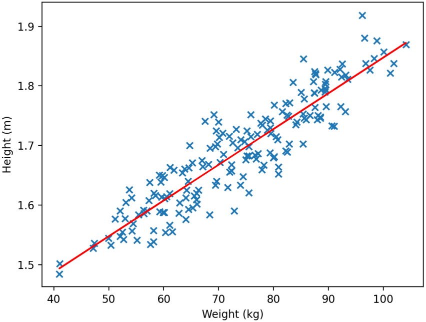


Figure: Linear regression model.

Linear Regression: main ingredients

Notation:

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

Model/hypothesis:

$$h_{\boldsymbol{w}}(x^{(i)}) = w_1 x^{(i)} + w_0$$

where $\boldsymbol{w} = [w_0, w_1]^T$ is the vector of parameters to be learned.

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 **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 “best” set of parameters, we minimize the MSE:

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

Multiple-feature Linear Regression

- Dataset: $\boldsymbol{x}^{(i)} \in \mathbb{R}^n, y^{(i)} \in \mathbb{R}$, where $x_j^{(i)}$ is the j-th feature of the i-th sample and n is the number of features.
- Hypothesis:

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

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

Multiple-feature Linear Regression - MSE

MSE:

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

where

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

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

Coefficient of determination

Idea: X and $\boldsymbol{y}$ can be thought as two random variables.

Let $\boldsymbol{\epsilon} := \boldsymbol{y} - \mathrm{X}\boldsymbol{w}$ the vector of the residuals and $\sigma_{\boldsymbol{y}} := \sqrt{\mathrm{Var}(\boldsymbol{y})}$ the standard deviation of the targets. The quantity

$$R^2 := 1 - \frac{||\boldsymbol{\epsilon}||^2}{\sigma_{\boldsymbol{y}}^2}$$

is called the *coefficient of determination*.

Best case scenario: $\sigma_{\boldsymbol{\epsilon}} = 0$, hence $R^2 = 1$.

Finding 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 allows to decrease the value of the function, *i.e.*

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

Formally:

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

$$\boldsymbol{d}^{j} = -\alpha \nabla E(\boldsymbol{w}^{j})$$

  where $\alpha > 0$ is the **learning rate**.

Gradient Descent - 3D visualization

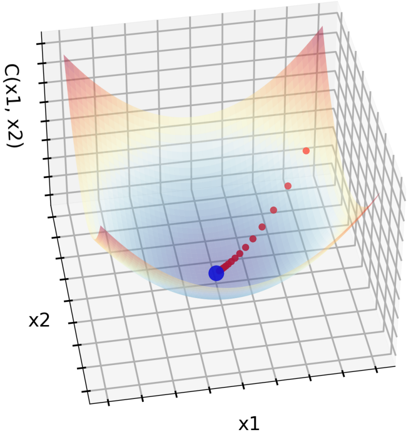


Figure: n blue the global minimum, in red the iteration points.

Gradient Descent: Effect of the learning rate/1

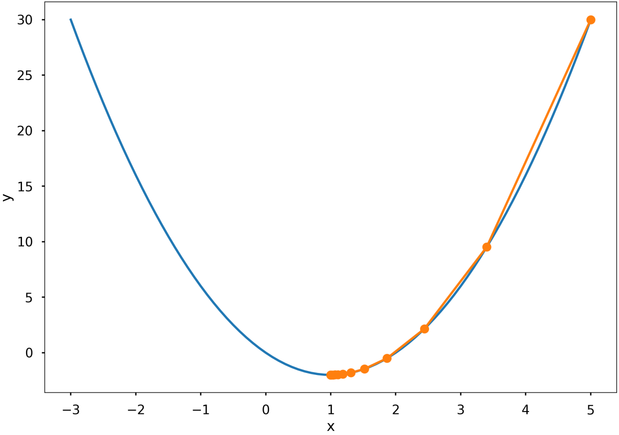


Figure: Learning rate = 0.1

Gradient Descent: Effect of the learning rate/2

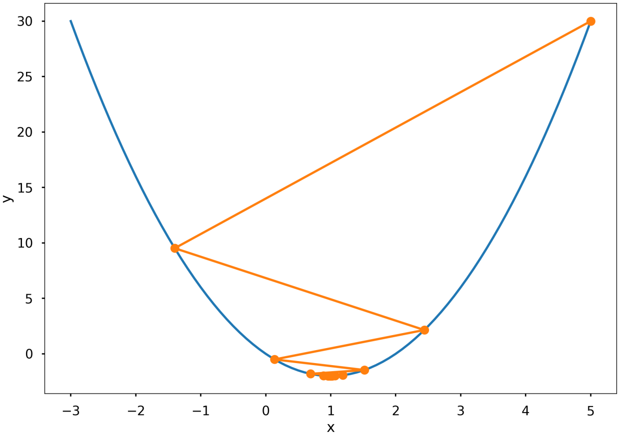


Figure: Learning rate $= 0.4$

Gradient Descent: Effect of the learning rate/3

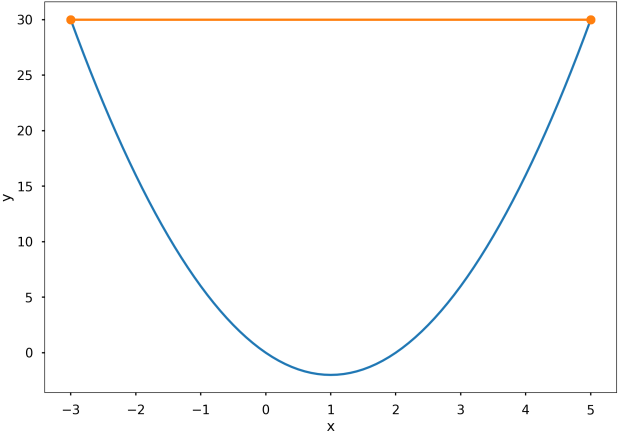


Figure: Learning rate = 0.5

Batch GD, SGD and Mini-Batch GD - 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 computing the gradient of the entire cost (error) 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 batch GD and SGD is called the **mini-batch** GD.

Batch GD, SGD and Mini-Batch GD - Algorithms

Batch GD

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

SGD (online)

- Start with an initial guess $\boldsymbol{w}^0$.
- For each epoch $j \geq 0$:
  - draw a random sample i from the dataset;
  - for each $1 \leq i \leq N$ update $\boldsymbol{w} = \boldsymbol{w} - \alpha \nabla E_i(\boldsymbol{w})$.

Mini-Batch GD

- Fix an integer $1 \leq \mathrm{mb} \leq N$ (mini-batch size).
- Start with an initial guess $\boldsymbol{w}^0$.
- For each epoch $j \geq 0$:
  - draw a random batch from the dataset;
  - for each $0 \leq i < \frac{N}{\mathrm{mb}}$ update

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

Tips and Tricks - How to choose?

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

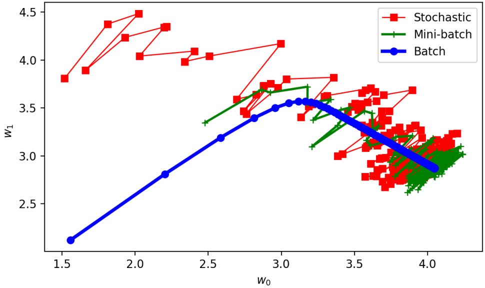


Figure: Batch GD vs SGD vs Mini-Batch GD

Normal Equation for LR and Gradient Descent

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):

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

- 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.

What if $X^T X$ 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 hyperparameters (explicit solution).
- No iterations.
- $\mathcal{O}(N^3)$, 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 have similar magnitudes!

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

Common techniques:

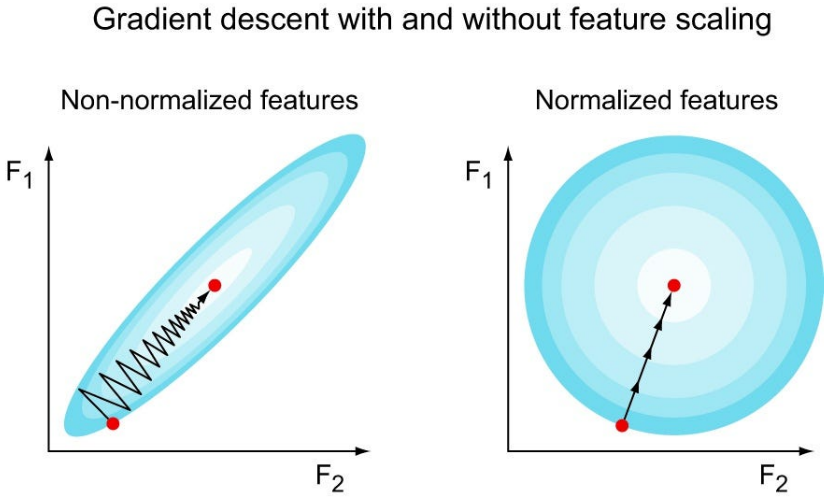
- **Feature scaling**. Compute the feature max $\boldsymbol{M} := [\max_i x_j^{(i)}]$ and the feature min $\boldsymbol{m} := [\min_i x_j^{(i)}]$ vectors. Then normalize features as follows

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

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

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

Tips and Tricks - Standardization



Polynomial Regression

Polynomial Regression $\rightarrow$ polynomial hypothesis.

Example: quadratic hypothesis (single feature):

$$h_{\boldsymbol{w}}(x_1) = w_0 + w_1 x_1 + w_2 x_1^2$$

(in case of two features, there is also the term $x_1 x_2$)

To fit this model, use Linear Regression with features $x_1 = x_1$ and $x_2 = x_1^2$.