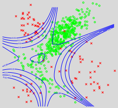

Linear Regression

Lecture *Machine Learning* vom 29-31.3.2023

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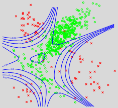
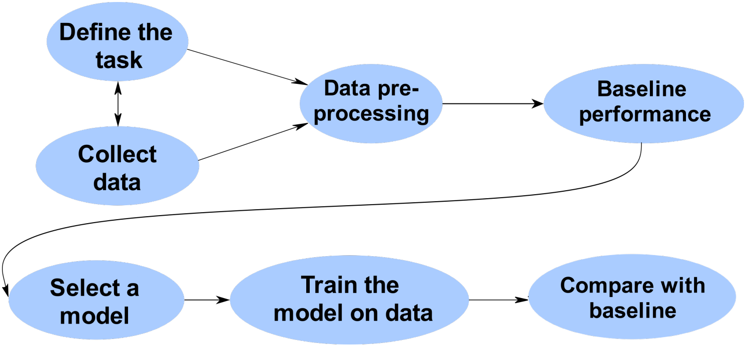
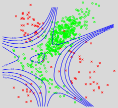


Workflow


Define the task
Collect data
Data pre-processing
Baseline performance
Select a model
Train the model on data
Compare with baseline



Bike Sharing Demand

Data set

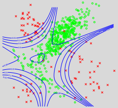
- hourly rental data for Washington bike sharing system
- data fields we will use:
  - *temp* - temperature in Celsius
  - *count* - number of total rents
- source:
  `www.kaggle.com/c/bike-sharing-demand`

First steps

- read data from input file
- visualize data
- summarize data

Task

Predict the demand (count) of bikes based on the temperature



Choosing a model

Supervised learning

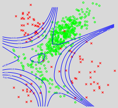
The parameters of a machine learning model are learned from a training set $x^{(1)}, x^{(2)}, \cdots, x^{(m)}$ with known target variables (labels) $y^{(1)}, y^{(2)}, \cdots, y^{(m)}$.

Classification: The target variable is categorical, i.e. an output is a discrete class label.

Regression: The target variable is continuous, i.e. an output is a numeric value.

Unsupervised learning

The parameter of a machine learning model are learned from a training set $x^{(1)}, x^{(2)}, \cdots, x^{(n)}$ without known target variables.



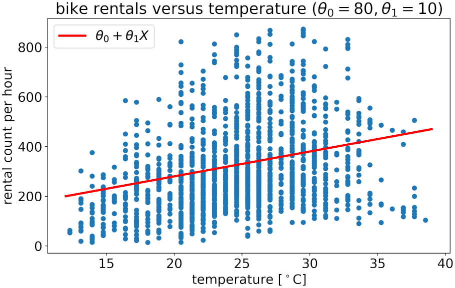
Linear regression

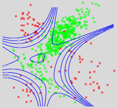
- input variables $x_1, ..., x_n$
- output variable y
- linearity assumption:

$$y = \theta_0 + \theta_1 x_1 + ... + \theta_n x_n$$

Bike rental data set

- only one input variable x_1 : temperature
- y: number of rented bikes
- $y = \theta_0 + \theta_1 x_1$





Hypothesis function

Data set

m training examples (input variables and output variable) with:

$$x^{(i)} = (x_1^{(i)}, \cdots, x_n^{(i)})^T,\ y^{(i)},\ (i = 1, ..., m)$$

Hypothesis function

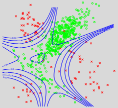
The task is to find $\theta = (\theta_0, \cdots, \theta_n)^T$, such that:

$$y^{(i)} \approx \theta_0 + \theta_1 x_1^{(i)} + \cdots + \theta_n x_n^{(i)} = \theta^T \begin{pmatrix} 1 \\ x^{(i)} \end{pmatrix} =: h_\theta(x^{(i)})$$

The function $h_\theta(x^{(i)})$ is called the hypothesis.

Bike rental data set

$$h_\theta(x^{(i)}) = (\theta_0, \theta_1) \begin{pmatrix} 1 \\ x_1^{(i)} \end{pmatrix}$$



Data matrix

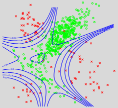
Data matrix

$$X := \begin{pmatrix} 1 & x_1^{(1)} & x_2^{(1)} & \cdots & x_n^{(1)} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_1^{(m)} & x_2^{(m)} & \cdots & x_n^{(m)} \end{pmatrix}$$

Hypothesis

The hypothesis for each training example can be computed with matrix multiplication:

$$\begin{pmatrix} h_\theta(x^{(1)}) \\ \vdots \\ h_\theta(x^{(m)}) \end{pmatrix} = \begin{pmatrix} 1 & x_1^{(1)} & x_2^{(1)} & \cdots & x_n^{(1)} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_1^{(m)} & x_2^{(2)} & \cdots & x_n^{(m)} \end{pmatrix} \begin{pmatrix} \theta_0 \\ \vdots \\ \theta_n \end{pmatrix} = X\theta$$

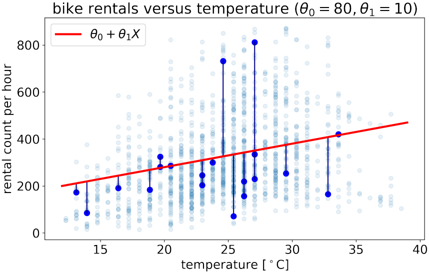


Loss Function

Mean squared error

Define the mean squared error function

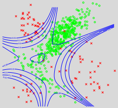
$$E(\theta) := \frac{1}{m}\sum_{i=1}^{m}\left(h_\theta(x^{(i)}) - y^{(i)}\right)^2 = \frac{1}{m}(X\theta - y)^2.$$



Machine learning task

Find θ with minimal loss:

$$E(\theta) \rightarrow min$$



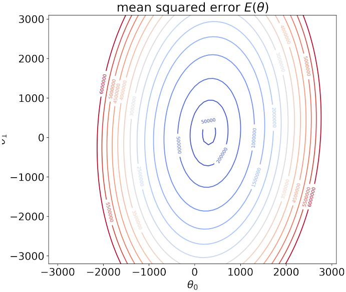
Gradient Descend

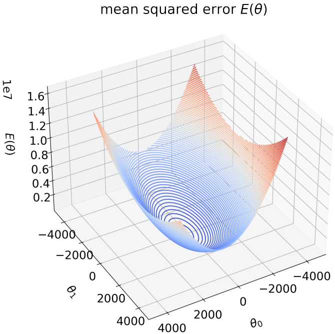
Parameter space

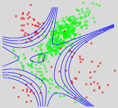
The space of all possible parameters values for the model.

Loss landscape

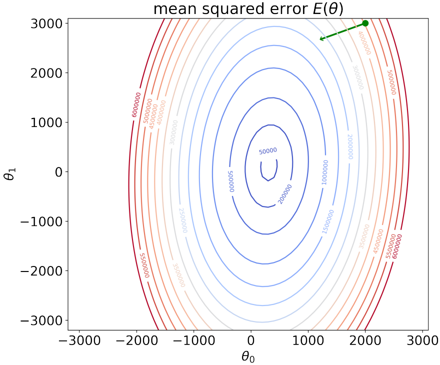
The loss function plotted against the parameter space.





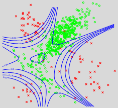


Gradient descend

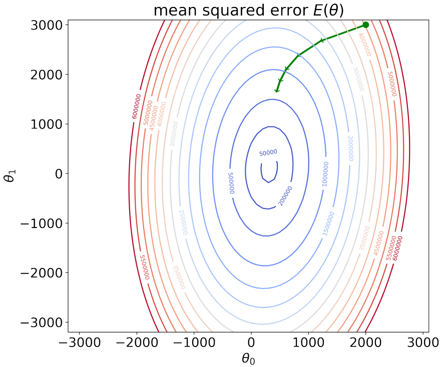


Input

- $\hat{\theta}$: starting parameter
- α : learning rate



Gradient Descend



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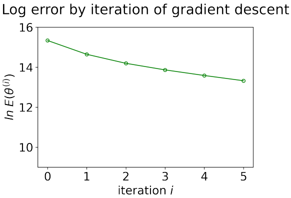
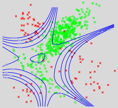
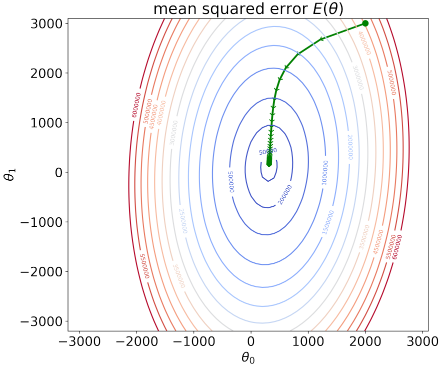




Gradient Descend



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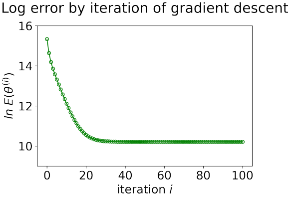
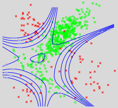




Gradient Descend

Parameter update

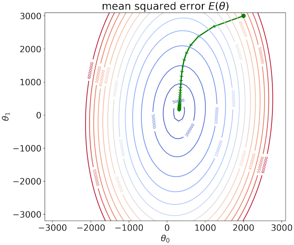
Parameters are iteratively updated, by moving each time a (small) step into the direction of the steepest descend of the target function to be minimized:

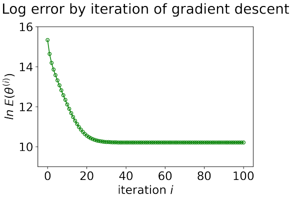
$$\theta \leftarrow \theta - \alpha \cdot \nabla E(\theta)$$

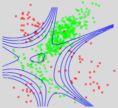
Here,

$$\nabla E(\theta) = \left(\frac{\partial E(\theta)}{\partial \theta_0}, \cdots, \frac{\partial E(\theta)}{\partial \theta_n}\right)^T$$

is the gradient of the mean squared error function in the point θ and α is called the learning rate.



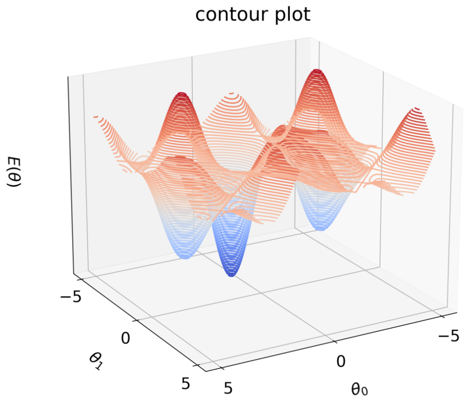


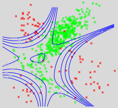


Gradient Descend

Disadvantages

- may converge to a local optimum
- can diverge, if the learning rate is too high
- X is used to compute the gradient in each step





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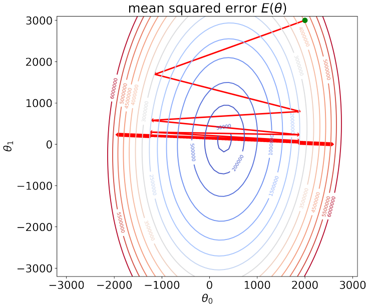
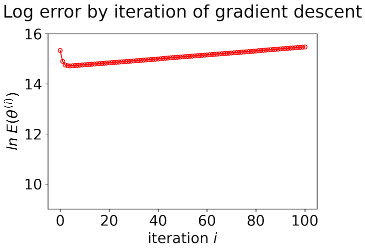
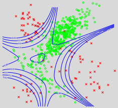






Stochastic Gradient Descend

Stochastic Gradient Descend

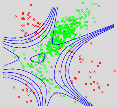
- minimizes the loss function $E(\theta; (X, y))$ by iteratively updating θ based on the gradient ∇E
- uses only a randomly sampled subset (X_{batch}, y_{batch}) (called **batch**) of the test data (X, y) for each update
- the **learning rate** α plays a similar role as in regular gradient descent
- $0 \leq \mu \leq 1$ is called the **momentum**

Algorithm

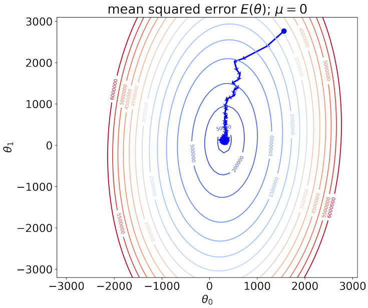
$v \leftarrow 0$

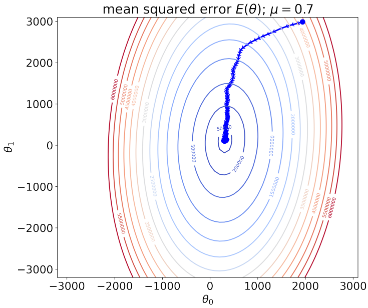
While the *termination condition* is not satisfied

> Sample a random batch (X_{batch}, y_{batch}) from the training data (X, y)
>
> $v \leftarrow \mu \cdot v - \alpha \cdot \nabla E(\theta; (X_{batch}, y_{batch}))$
>
> $\theta \leftarrow \theta + v$



Stochastic Gradient Descend





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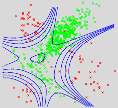

Stochastic Gradient Descend

Termination condition

- a fixed number of iterations has been done
- the accuracy/error on a separate validation set satisfies some condition (e.g. it is plateauing)
- user interruption

Algorithm

$v \leftarrow 0$

While the *termination condition* is not satisfied

> Sample a random batch (X_{batch}, y_{batch}) from the training data (X, y)
>
> $v \leftarrow \mu \cdot v - \alpha \cdot \nabla E(\theta; (X_{batch}, y_{batch}))$
>
> $\theta \leftarrow \theta + v$