Machine learning

Inleiding & Regressie

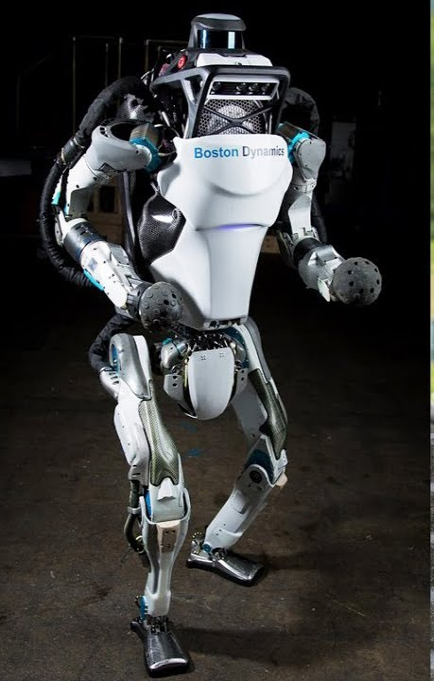
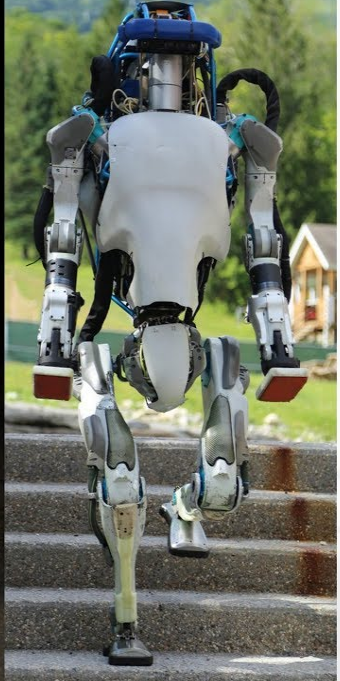
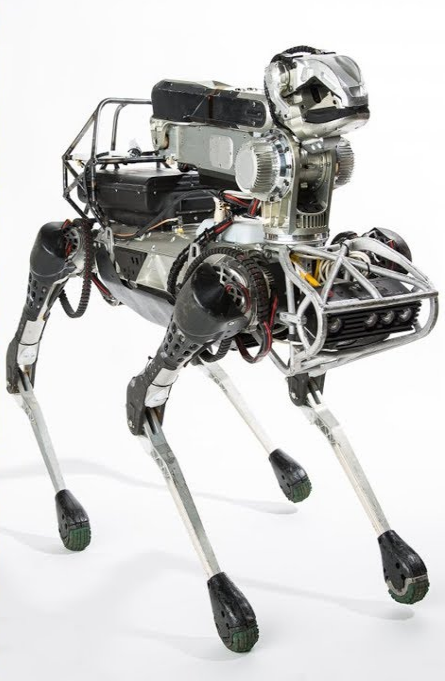
Wouter Gevaert

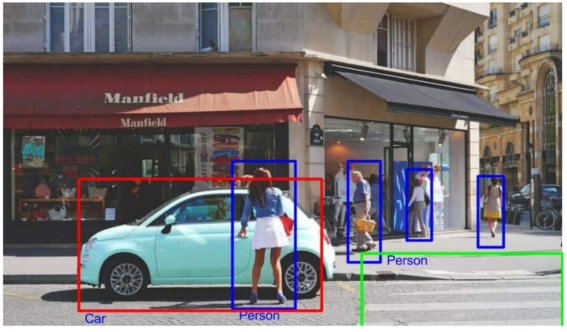
Inhoud

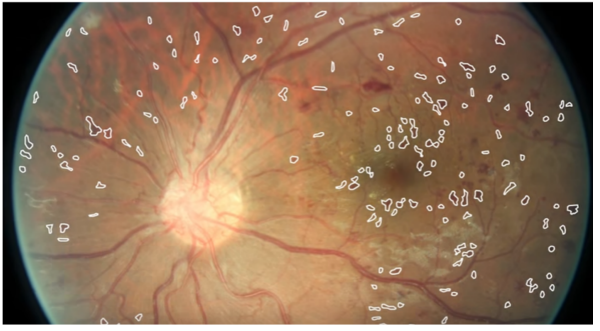
AI in context

Facebook legt experiment rond artificiële intelligentie stil nadat robots eigen geheime taal ontwikkelen

Koen Van De Sype | 01 augustus 2017 | 11u39 | Bron: Next Web, The New York Post, Gizmodo, The Sun

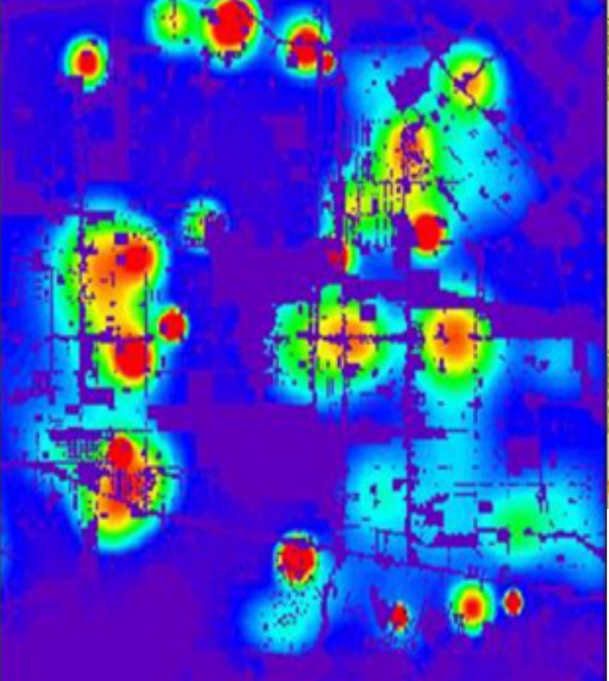

Boston Dynamics



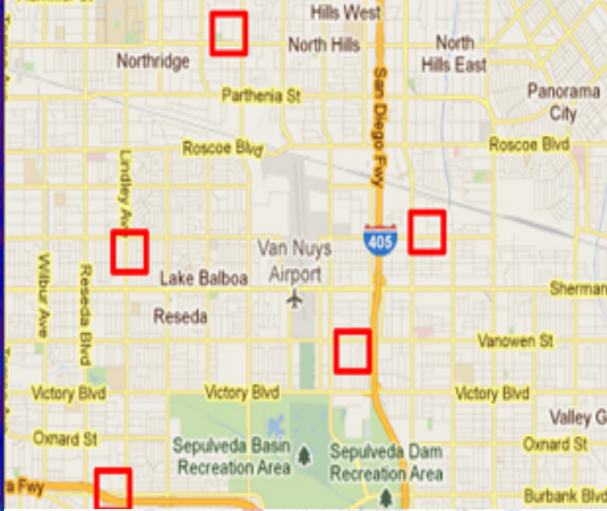




"girl in pink dress is jumping in air."

"black and white dog jumps over bar."



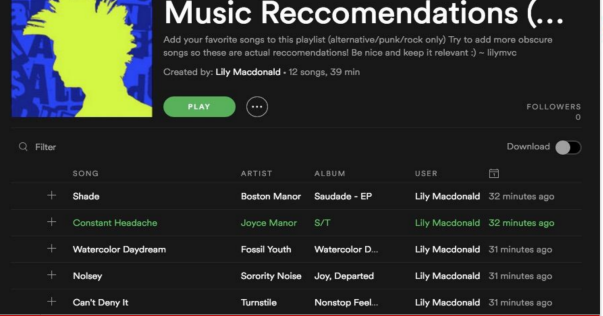


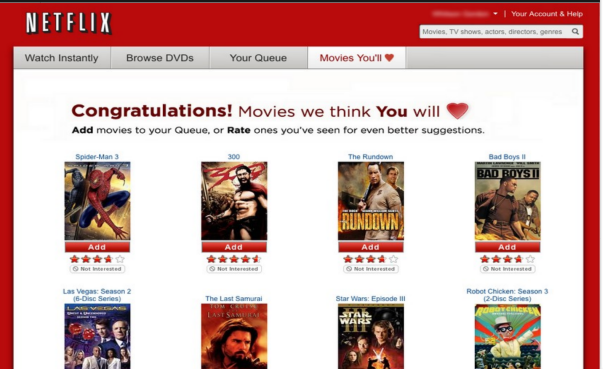
PredPol

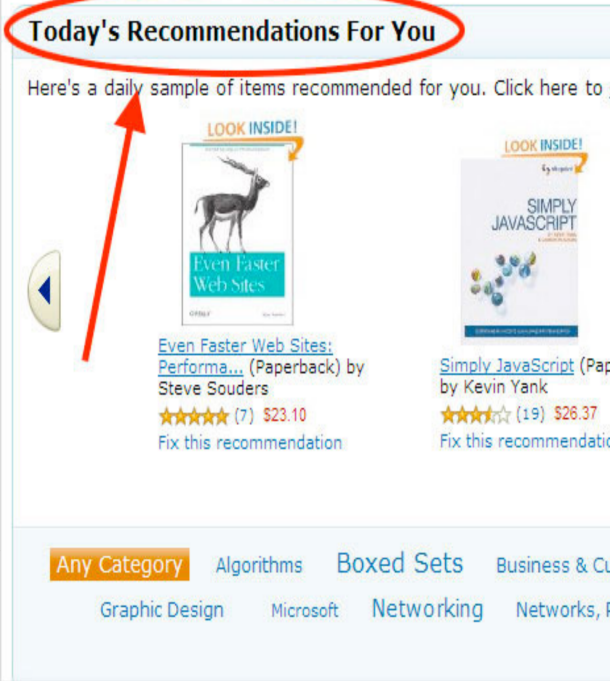
Predict Crime in **Real Time**™

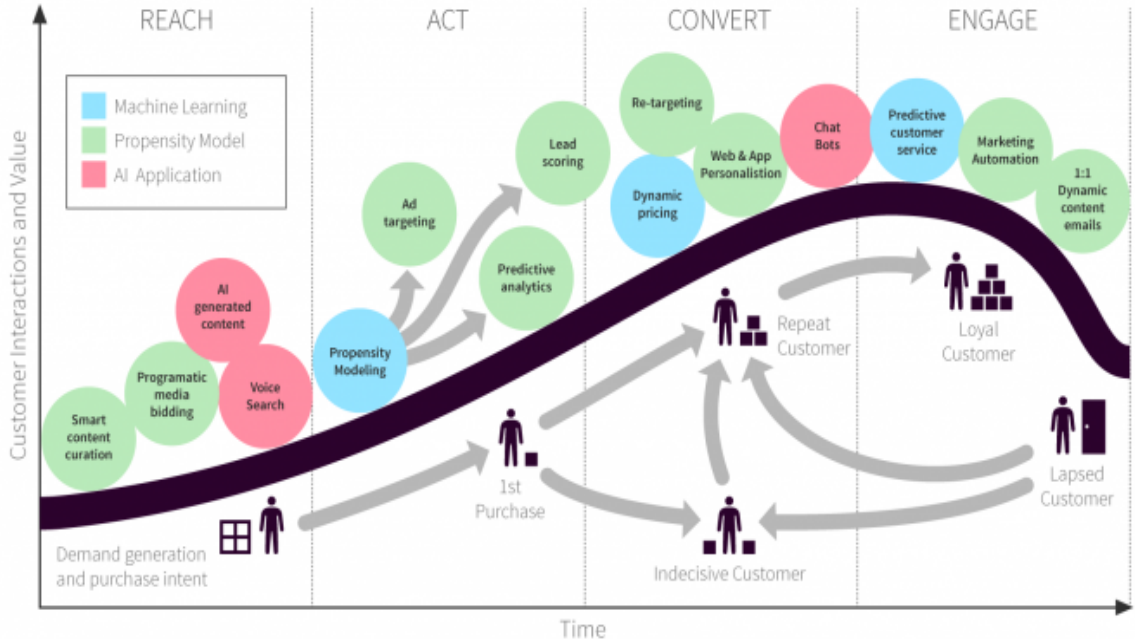
PredPol provides targeted, real-time crime prediction designed for and successfully tested by officers in the field.


High PUE
ML Control On
ML Control Off
Low PUE


Music Reccomendations (...
Add your favorite songs to this playlist (alternative/punk/rock only) Try to add more obscure songs so these are actual reccomendations! Be nice and keep it relevant :) ~ lilymvc
Created by: Lily Macdonald - 12 songs, 39 min
PLAY
FOLLOWERS 0
Filter
Download
SONG ARTIST ALBUM USER
Shade Boston Manor Saudade - EP Lily Macdonald 32 minutes ago
Constant Headache Joyce Manor S/T Lily Macdonald 32 minutes ago
Watercolor Daydream Fossil Youth Watercolor D... Lily Macdonald 31 minutes ago
Nolsey Sorority Noise Joy, Departed Lily Macdonald 31 minutes ago
Can't Deny It Turnstile Nonstop Feel... Lily Macdonald 31 minutes ago


NETFLIX
Your Account & Help
Movies, TV shows, actors, directors, genres
Watch Instantly
Browse DVDs
Your Queue
Movies You'll ♥
Congratulations! Movies we think You will
Add movies to your Queue, or Rate ones you've seen for even better suggestions.
Spider-Man 3
300
The Rundown
Bad Boys II
Add
Not Interested
Las Vegas: Season 2 (6-Disc Series)
The Last Samurai
Star Wars: Episode III
Robot Chicken: Season 3 (2-Disc Series)


Today's Recommendations For You
Here's a daily sample of items recommended for you. Click here to
LOOK INSIDE!
Even Faster Web Sites
Even Faster Web Sites: Performa... (Paperback) by Steve Souders
(7) $23.10
Fix this recommendation
LOOK INSIDE!
SIMPLY JAVASCRIPT
Simply JavaScript (Pap
by Kevin Yank
(19) $26.37
Fix this recommendatio
Any Category
Algorithms
Boxed Sets
Business & Cu
Graphic Design
Microsoft
Networking
Networks, P


REACH
ACT
CONVERT
ENGAGE
Machine Learning
Propensity Model
AI Application
Customer Interactions and Value
Time
Smart content curation
Programatic media bidding
AI generated content
Voice Search
Propensity Modeling
Ad targeting
Lead scoring
Predictive analytics
Re-targeting
Dynamic pricing
Web & App Personalistion
Chat Bots
Predictive customer service
Marketing Automation
1:1 Dynamic content emails
Demand generation and purchase intent
1st Purchase
Repeat Customer
Loyal Customer
Indecisive Customer
Lapsed Customer

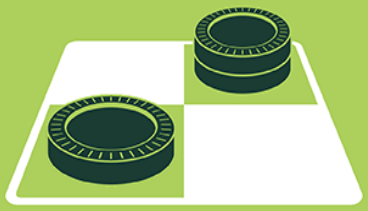




INPUT
OUTPUT
pix2pix
process

ARTIFICIAL INTELLIGENCE

Early artificial intelligence stirs excitement.



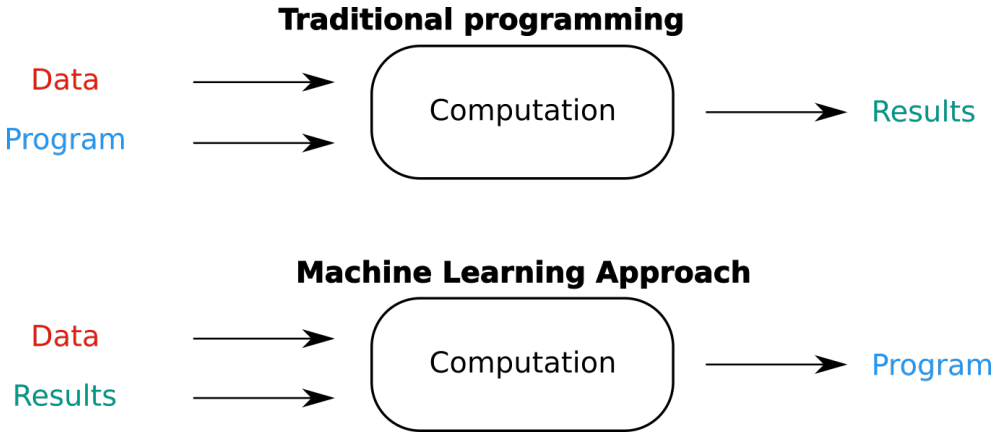
MACHINE LEARNING

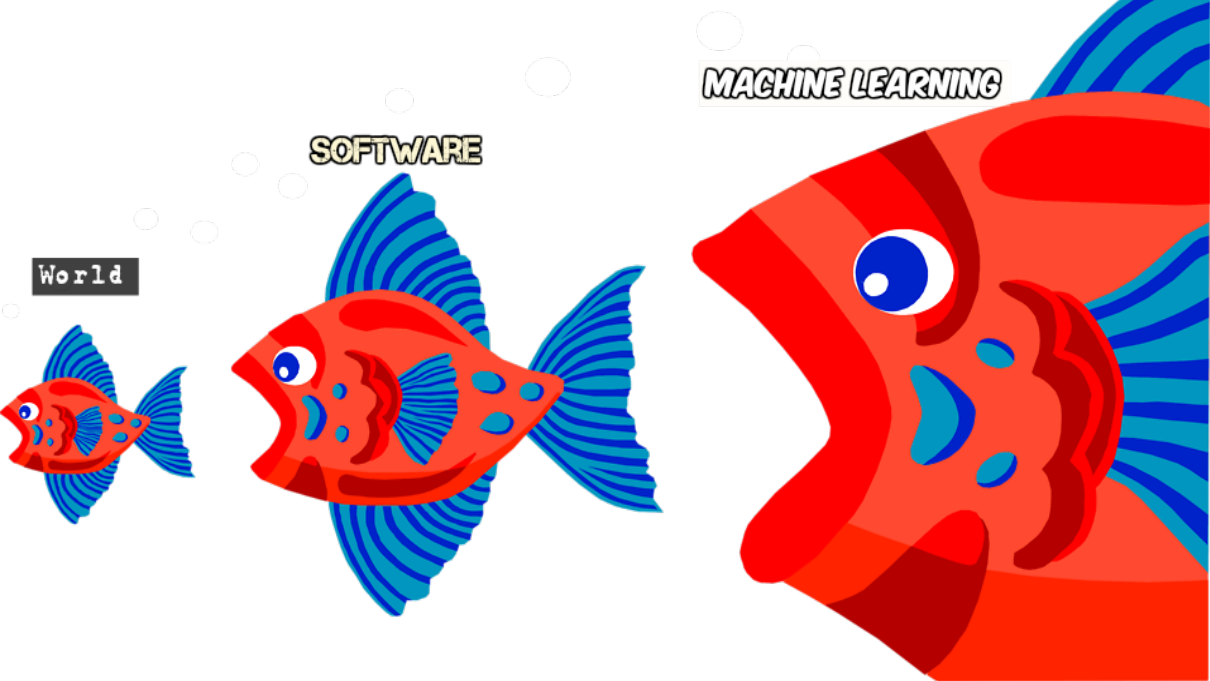
Machine learning begins to flourish.

DEEP LEARNING

Deep learning breakthroughs drive AI boom.

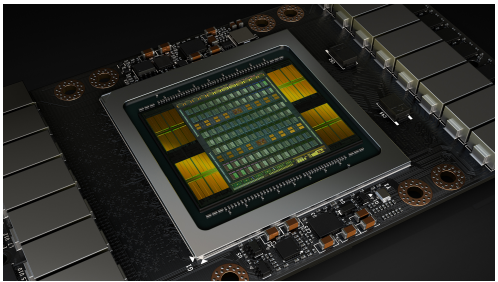
1950's 1960's 1970's 1980's 1990's 2000's 2010's


Traditional programming
Data
Program
Computation
Results
Machine Learning Approach
Data
Results
Computation
Program


World
SOFTWARE
MACHINE LEARNING

Waarom nu?

1. Snellere hardware
2. Betere algoritmes
3. Meer data
4. (Open source) frameworks



Tesla V100 - NVIDIA

15,3 miljard transistoren

5120 CUDA cores

672 tensor cores

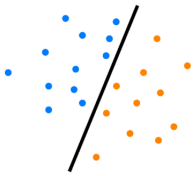
120 TFLOPS peak performance

Hoe leren uit data?

Leeralgoritmes

Supervised

- Inputs met gewenste outputs zijn gegeven.
- Task driven.

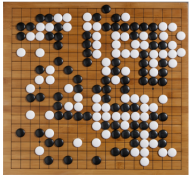


Unsupervised

- De gewenste outputs zijn niet gegeven.
- Data driven (clustering).

Reinforcement

- Beslissingsproces op basis van beloningen.
- Algoritme leert te reageren op zijn omgeving.

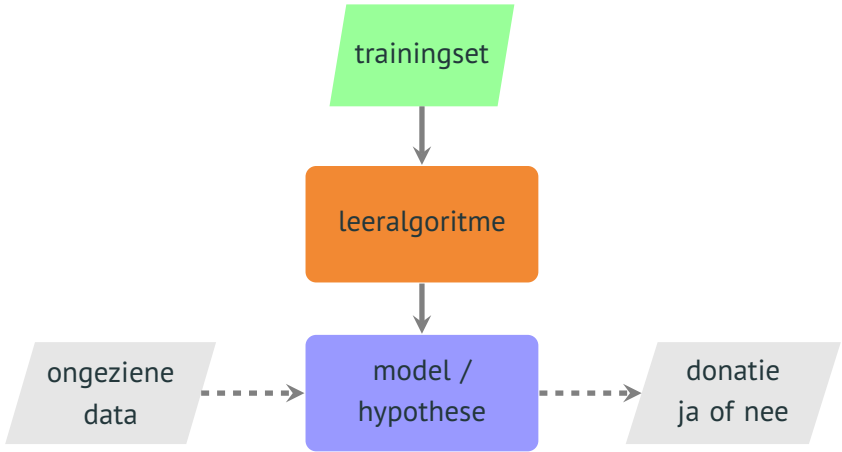


Supervised learning

Is het leren op basis van een gelabelde trainingset. Het algoritme krijgt een **dataset voorzien van de juiste antwoorden**. Na training probeert het algoritme het juiste antwoord te vinden.

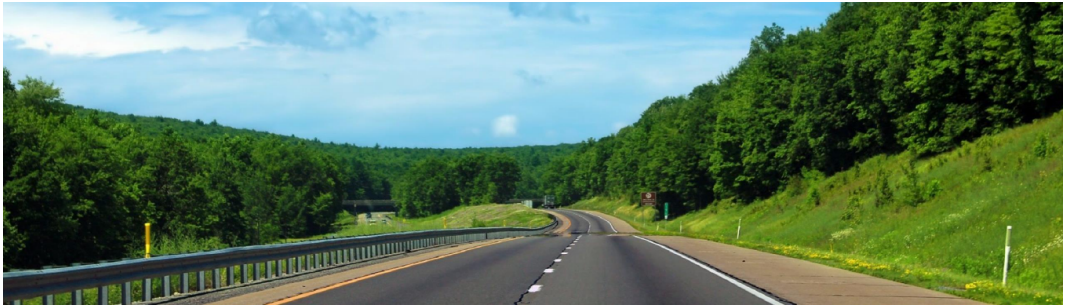
	Person ID	Months since Last Donation	Number of Donations	Total Volume Donated (c.c.)	Months since First Donation	Donated the next month
0	619	2	50	12500	98	1
1	664	0	13	3250	28	1
2	441	1	16	4000	35	1
3	160	2	20	5000	45	1
4	358	1	24	6000	77	0
5	335	4	4	1000	4	0
6	47	2	7	1750	14	1
7	164	1	12	3000	35	0
8	736	5	46	11500	98	1
9	436	0	3	750	4	0

Supervised learning



Supervised learning - voorbeeld

Hoe stuurhoek bepalen bij een self-driving car?



Supervised learning - voorbeeld

Hoe stuurhoek bepalen bij een self-driving car?

(infrarood) Camera's

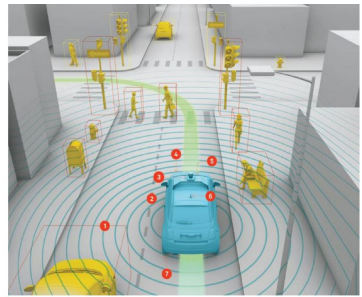
Stereo vision

Radar

LIDAR

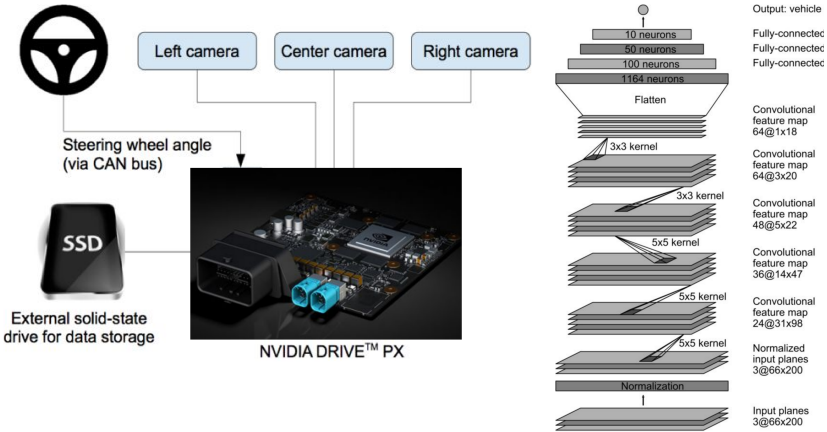
GPS

Audio



Supervised learning - voorbeeld

Hoe stuurhoek bepalen bij een self-driving car?

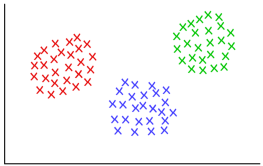


https://selfdrivingcars.mit.edu/deeptesla/

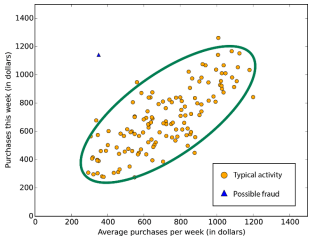
Unsupervised learning

Unsupervised learning toepassingen

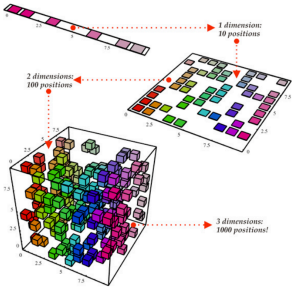
Clustering



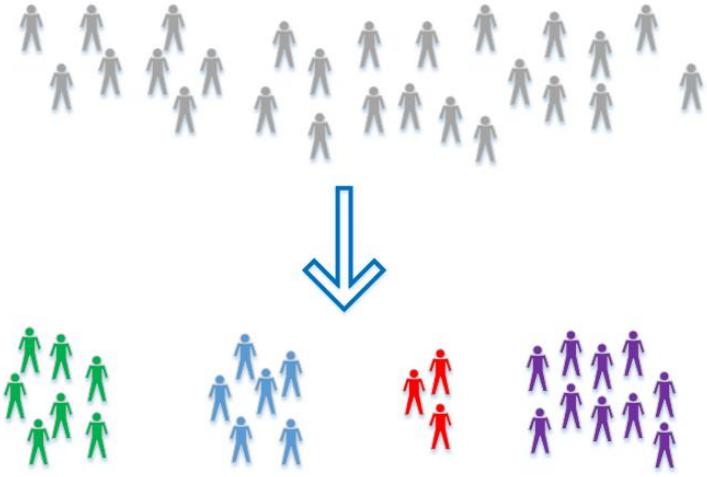
Anomaly detection



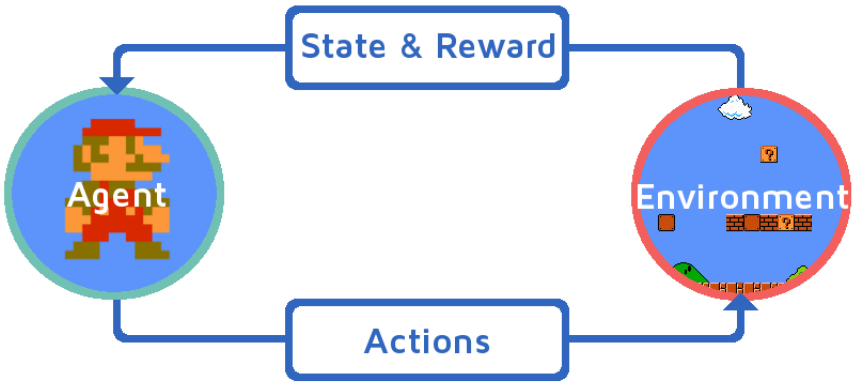
Dimensionality reduction



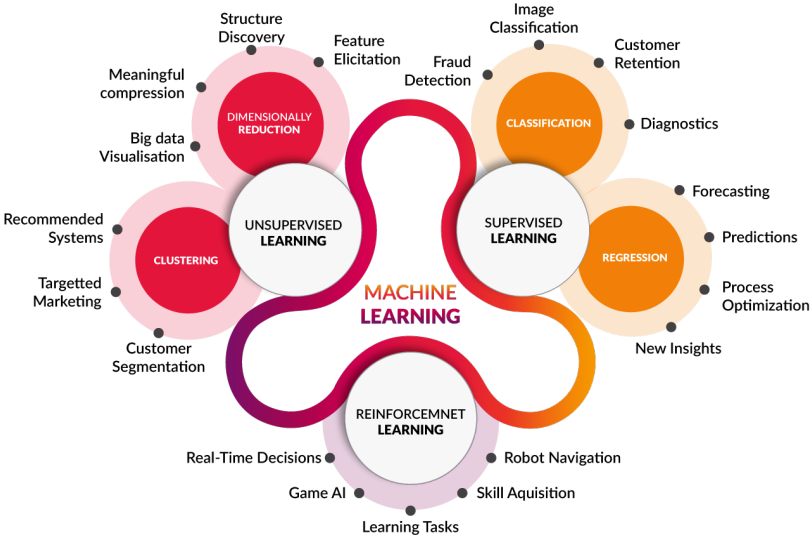
Unsupervised learning



Reinforcement learning

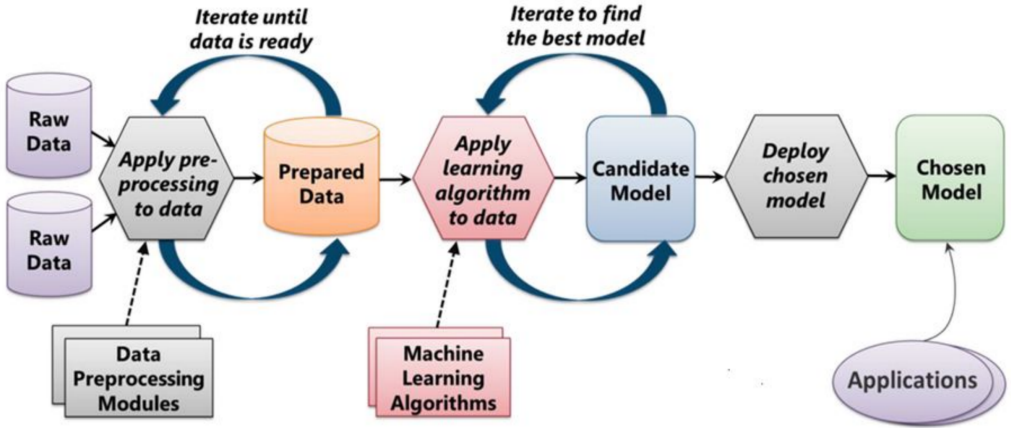


Overzicht leeralgoritmes

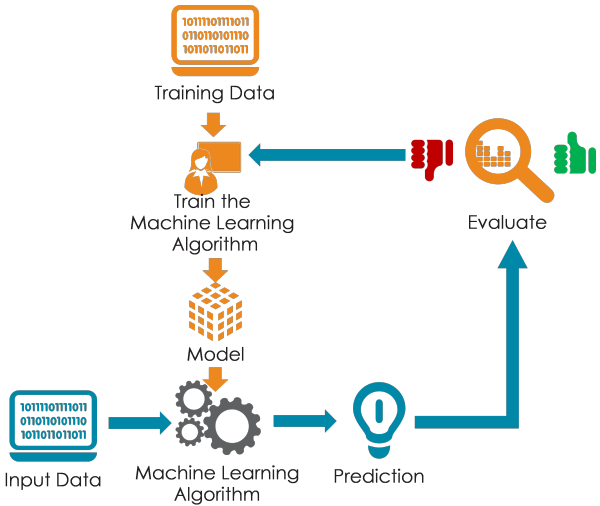


Overzicht leeralgoritmes

Aanpak van een machine learning project

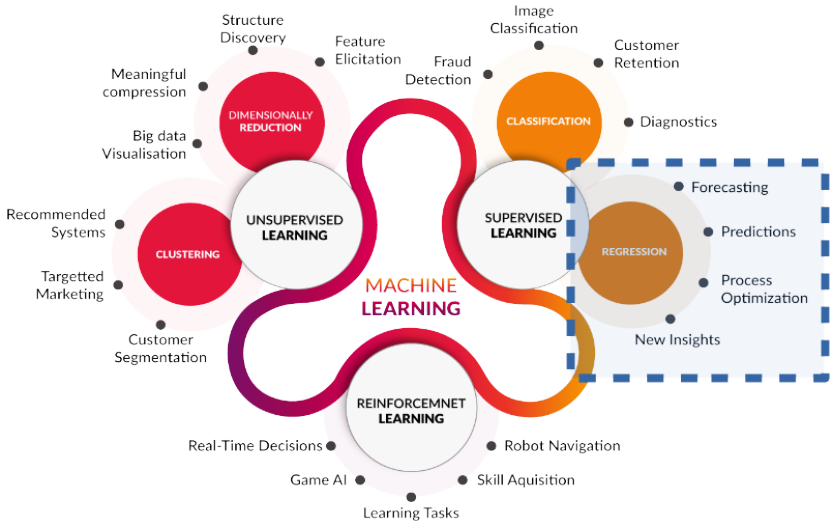


Aanpak van een machine learning project



Enkelvoudige lineaire regressie

Lineaire regressie



Lineaire regressie

	leeftijd	gewicht	bloeddruk
0	52	78	132
1	59	83	143
2	67	88	153
3	73	96	162
4	64	89	154
5	74	100	168
6	54	85	137
7	61	85	149
8	65	94	159
9	46	76	128
10	72	98	166

Voorspel de bloeddruk op basis van leeftijd en gewicht.

features: leeftijd en gewicht.

target: bloeddruk.

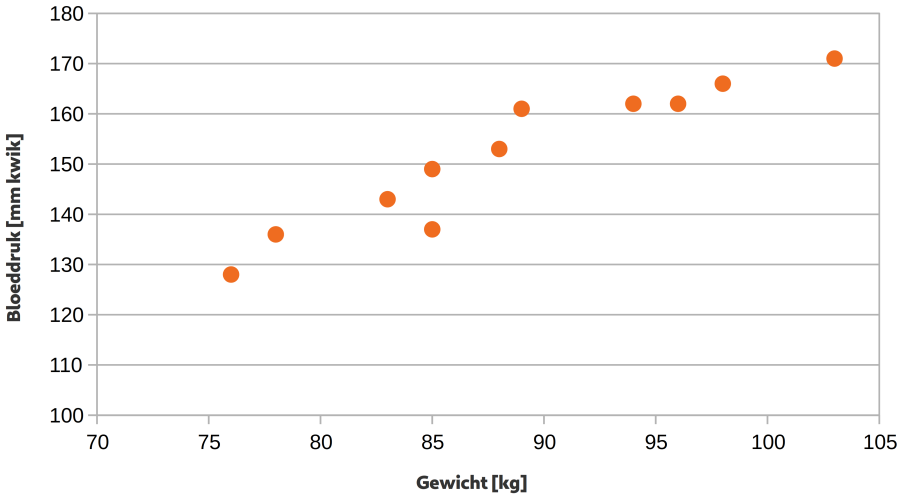
trainingset met 11 training examples.

Regressie

Bij regressie is de output/target een (continue) variabele.

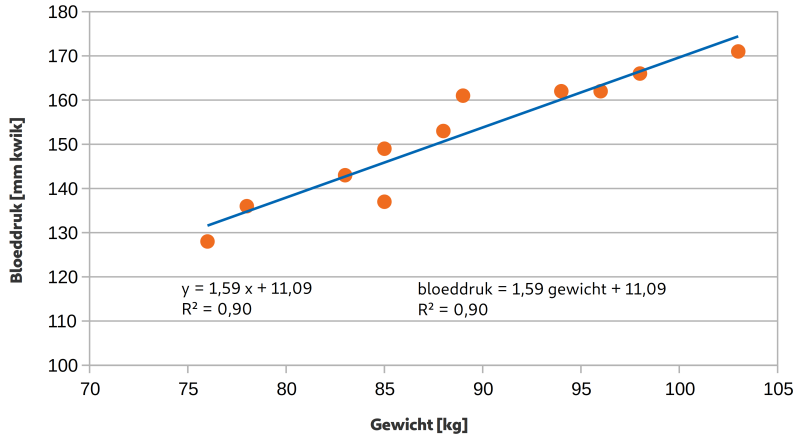
Enkelvoudige lineaire regressie

Scatterplot



Enkelvoudige lineaire regressie

Op zoek naar het verband tussen gewicht en bloeddruk



Lineaire trendlijn als model $h_\theta(x)$ (= hypothese)

Enkelvoudige lineaire regressie

Op zoek naar het verband tussen gewicht en bloeddruk

Het verband (model of hypothese) $h_\theta(x)$ is van de vorm:

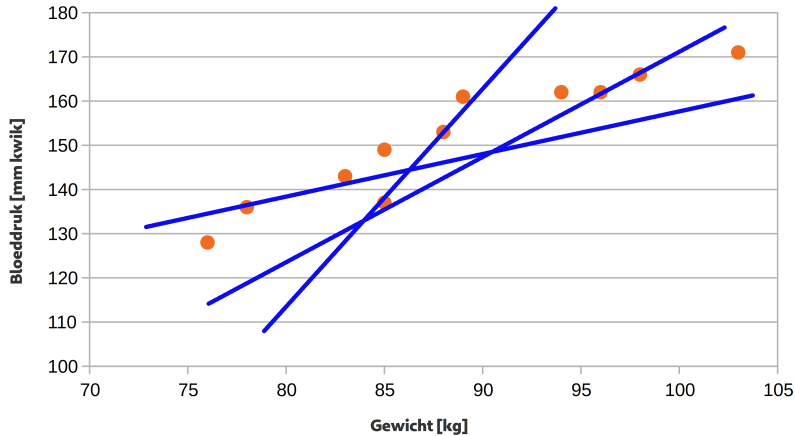
$$h_\theta(x) = \theta_0 + \theta_1 x$$

- Bepalen van de optimale waarden voor θ_0 en θ_1.
  - θ_0 = snijpunt met de y-as.
  - θ_1 = helling van de rechte.
- De parameters θ_i = **weights**.
- Het zoeken van het model / hypothese = **training / learning**.

Enkelvoudige lineaire regressie

Op zoek naar het verband tussen gewicht en bloeddruk

Welke zijn de optimale waarden voor θ_0 en θ_1?

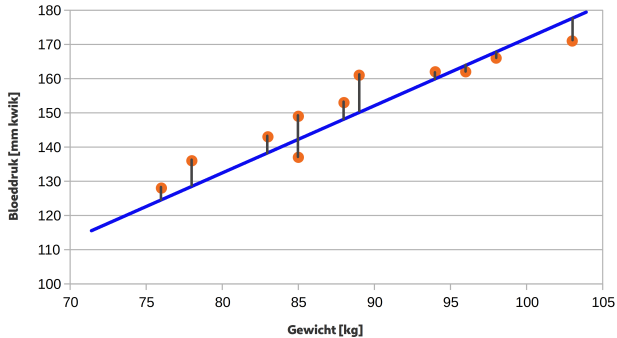


Enkelvoudige lineaire regressie

Op zoek naar het verband tussen gewicht en bloeddruk

Minimaliseer de kostenfunctie $J(\theta)$ via Least Mean Squares methode (LMS).

$$J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$$

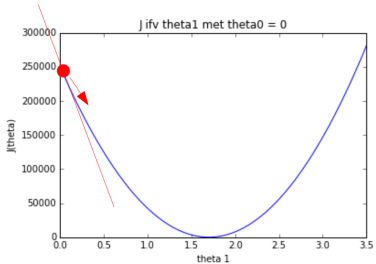


Enkelvoudige lineaire regressie

Gradient Descent (GDS)

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} \left((\theta_1 x^{(i)} + \theta_0) - y^{(i)} \right)^2$$

Stel de parameters θ_0 en θ_1 voortdurend bij in een iteratief proces tot je de waarden voor θ_0 en θ_1 hebt gevonden die de kleinst mogelijke waarde voor J(θ_0 ,θ_1) opleveren.



$$J(\theta_0 = 0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} \left((\theta_1 x^{(i)}) - y^{(i)} \right)^2$$

Enkelvoudige lineaire regressie

Gradient Descent (GDS) - algoritmisch

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^{m} \left((\theta_1 x^{(i)} + \theta_0) - y^{(i)} \right)^2$$

Bepaal de gradient naar θ_0 en θ_1

$$\frac{dJ(\theta)}{d\theta_0} = \frac{2}{2m} \sum_{i=1}^{m} \left((\theta_1 x^{(i)} + \theta_0) - y^{(i)} \right)$$

$$\frac{dJ(\theta)}{d\theta_1} = \frac{2}{2m} \sum_{i=1}^{m} \left((\theta_1 x^{(i)} + \theta_0) - y^{(i)} \right) x^{(i)}$$

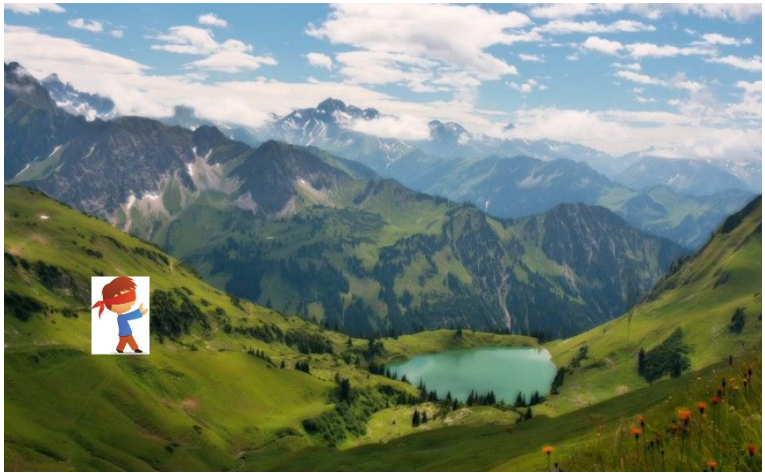
Update de parameters θ_0 en θ_1 volgens:

$$\theta_0 := \theta_0 - \eta \frac{dJ(\theta)}{d\theta_0} \text{ en } \theta_1 := \theta_1 - \eta \frac{dJ(\theta)}{d\theta_1}$$

μ is de learning rate

Enkelvoudige lineaire regressie

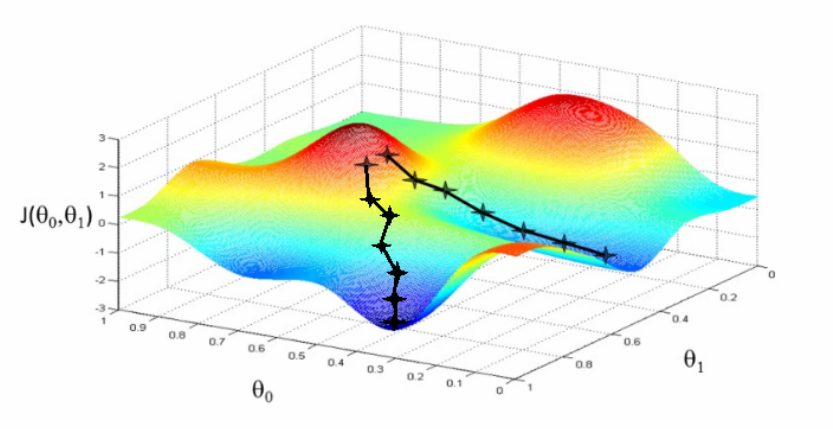
Gradient Descent (GDS)



Enkelvoudige lineaire regressie

Gradient Descent (GDS)

Lokaal versus globaal optimum

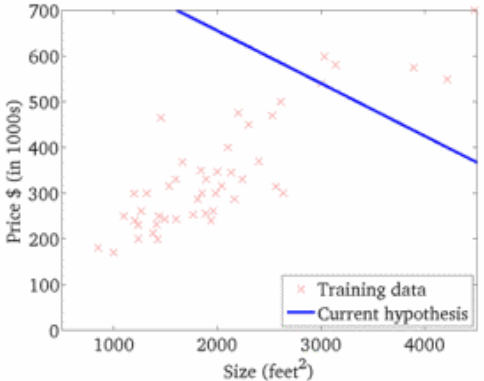


Enkelvoudige lineaire regressie

Gradient Descent (GDS)

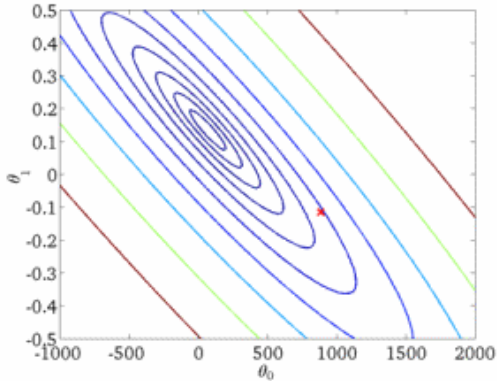
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)

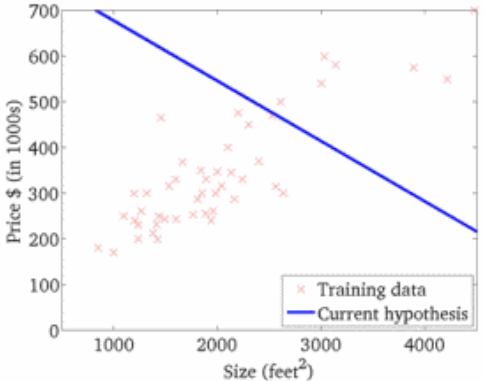


Enkelvoudige lineaire regressie

Gradient Descent (GDS)

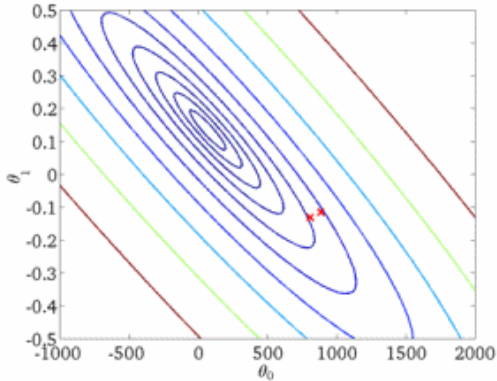
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)

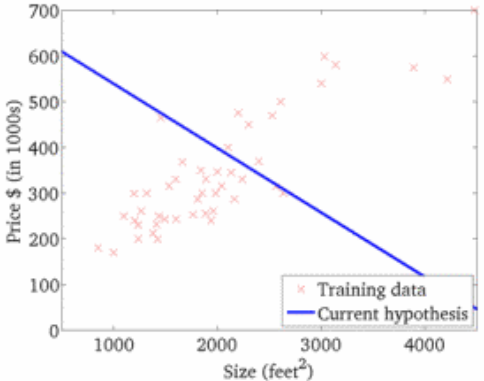


Enkelvoudige lineaire regressie

Gradient Descent (GDS)

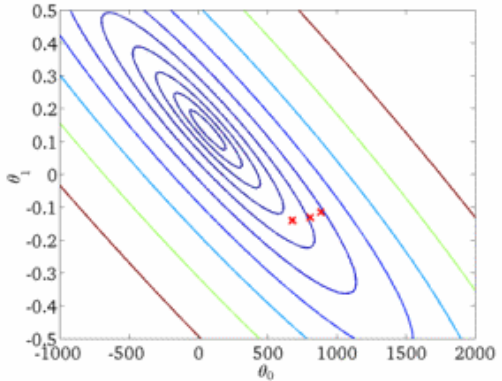
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)

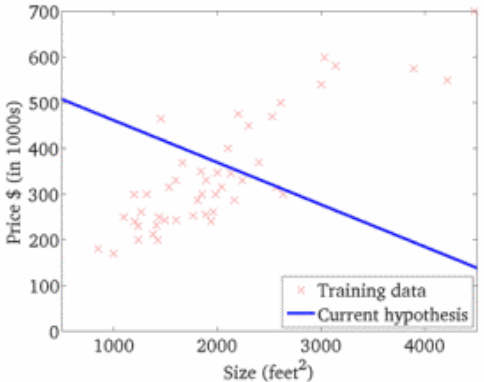


Enkelvoudige lineaire regressie

Gradient Descent (GDS)

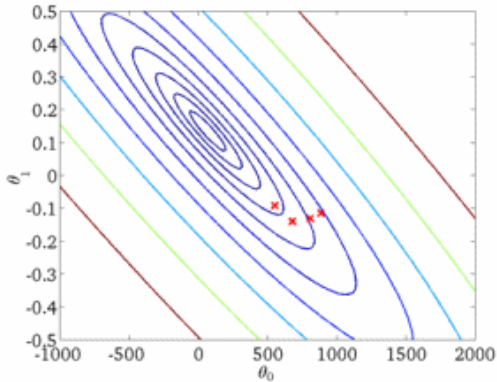
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)

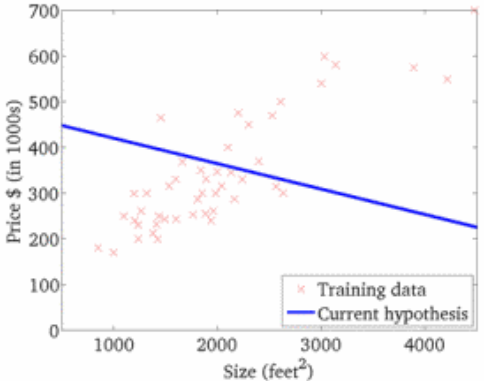


Enkelvoudige lineaire regressie

Gradient Descent (GDS)

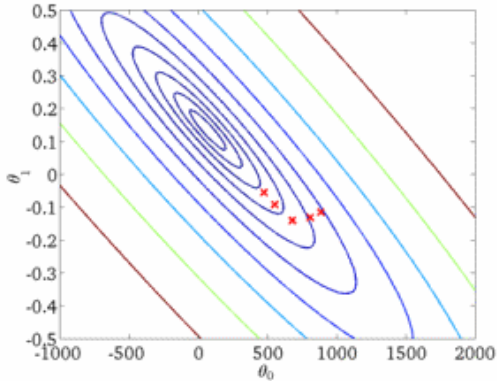
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)

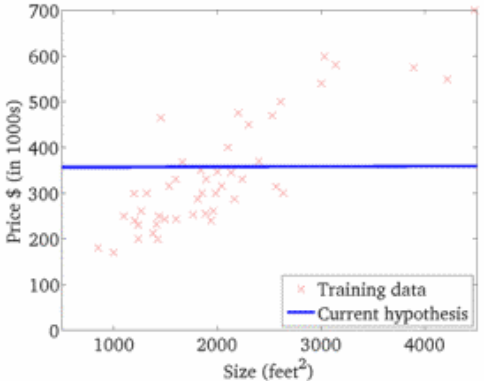


Enkelvoudige lineaire regressie

Gradient Descent (GDS)

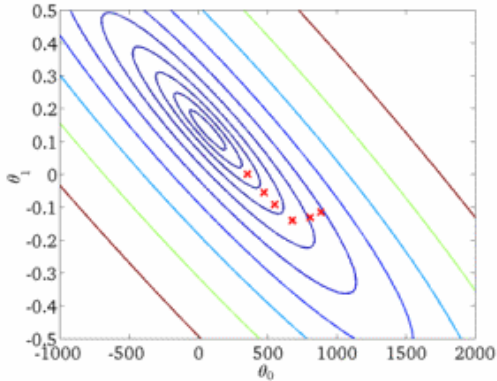
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)

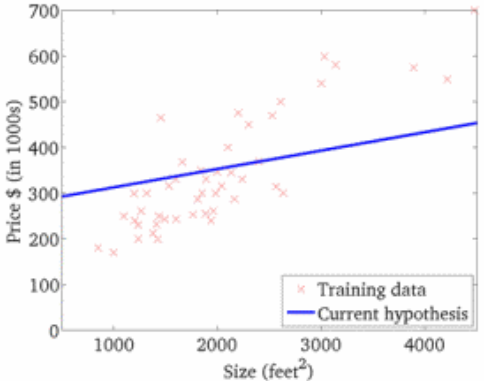


Enkelvoudige lineaire regressie

Gradient Descent (GDS)

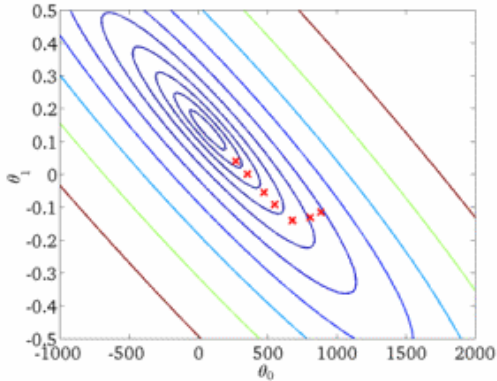
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)

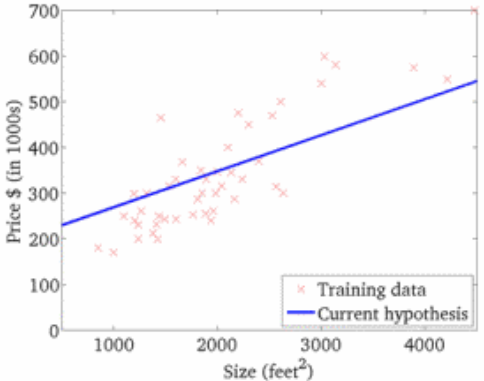


Enkelvoudige lineaire regressie

Gradient Descent (GDS)

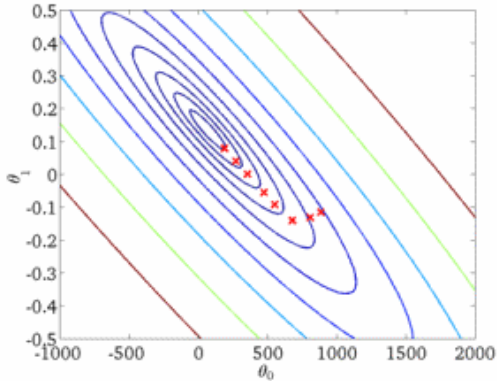
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)

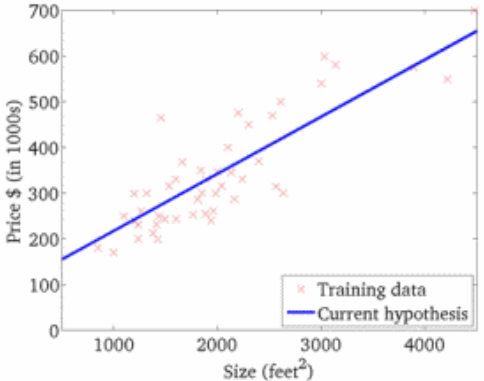


Enkelvoudige lineaire regressie

Gradient Descent (GDS)

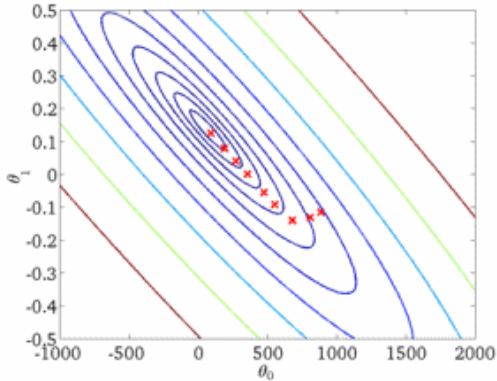
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



$J(\theta_0, \theta_1)$

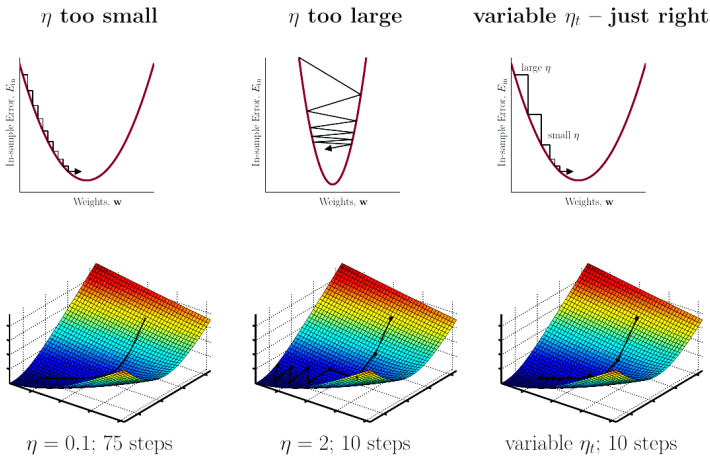
(function of the parameters θ_0, θ_1)



Enkelvoudige lineaire regressie

Gradient Descent (GDS)

Invloed van de learning rate



Meervoudige lineaire regressie

Meervoudige lineaire regressie

Definitie en voorbeelden

Bij meervoudige regressie (multiple regression) wordt het model/hypothese bepaald aan de hand van een trainingset met **meerdere features**.

- Bloeddruk wordt bepaald aan de hand van gewicht en leeftijd.
- Voorspel de kwaliteit van wijn op basis van de zuurtegraad, suikergehalte, chloriden, dichtheid, sulfaten, hoeveelheid alcohol, ...
- Voorspel het warmteverlies van een huis op basis van het type glas, muurisolatie, oriëntatie van het huis,...

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_n x_n$$

Meervoudige lineaire regressie

Voorbeeld - Voorspel de huisprijs op basis van onderstaande features

- CRIM - per capita crime rate by town.
- ZN - proportion of residential land zoned for lots over 25,000 sq.ft.
- INDUS - proportion of non-retail business acres per town.
- CHAS - Charles River dummy variable (1 if tract bounds river; 0 otherwise).
- NOX - nitric oxides concentration (parts per 10 million).
- RM - average number of rooms per dwelling.
- AGE - proportion of owner-occupied units built prior to 1940.
- DIS - weighted distances to five Boston employment centres.
- RAD - index of accessibility to radial highways.
- TAX - full-value property-tax rate per $10000.
- PTRATIO - pupil-teacher ratio by town.
- B - $1000(B_k - 0.63)^2$ where B_k is the proportion of blacks by town.
- **LSTAT** % lower status of the population.
- **Price** - Median value of owner-occupied homes in 1000's.

	CRIM	ZN	INDUS	CHAS	NOX	RM	AGE	DIS	RAD	TAX	PT	B	LSTAT	Price
0	0.00632	18.0	2.31	0	0.538	6.575	65.199997	4.0900	1	296	15.300000	396.899994	4.98	504.000000
1	0.02731	0.0	7.07	0	0.469	6.421	78.900002	4.9671	2	242	17.799999	396.899994	9.14	453.600008
2	0.02729	0.0	7.07	0	0.469	7.185	61.099998	4.9671	2	242	17.799999	392.829987	4.03	728.700016
3	0.03237	0.0	2.18	0	0.458	6.998	45.799999	6.0622	3	222	18.700001	394.630005	2.94	701.400032
4	0.06905	0.0	2.18	0	0.458	7.147	54.200001	6.0622	3	222	18.700001	396.899994	5.33	760.200016

Statistische vooranalyse

Consistentie van de dataset

	CRIM	ZN	INDUS	CHAS	NOX	RM	AGE	DIS	RAD	TAX	PT	B	LSTAT	Price
count	506.000000	506.000000	506.000000	506.000000	506.000000	506.000000	506.000000	506.000000	506.000000	506.000000	506.000000	506.000000	506.000000	506.000000
mean	4.673727	11.363636	11.136779	0.069170	25.892968	87.231275	68.574901	11.445487	9.549407	408.237154	18.455534	356.674030	12.653063	473.188934
std	25.223207	23.322453	6.860353	0.253994	132.093200	747.124382	28.148862	172.108941	8.707259	168.537116	2.164946	91.294863	7.141062	193.139186
min	0.006320	0.000000	0.460000	0.000000	0.385000	3.561000	2.900000	1.129600	1.000000	187.000000	12.600000	0.320000	1.730000	105.000000
25%	0.082045	0.000000	5.190000	0.000000	0.449000	5.888000	45.025000	2.100175	4.000000	279.000000	17.400000	375.377487	6.950000	357.525002
50%	0.256510	0.000000	9.690000	0.000000	0.538000	6.210000	77.500000	3.207450	5.000000	330.000000	19.050000	391.440002	11.360000	445.200016
75%	3.689388	12.500000	18.100000	0.000000	0.624000	6.630750	94.074999	5.213925	24.000000	666.000000	20.200001	396.225006	16.954999	525.000000
max	537.000000	100.000000	27.740000	1.000000	713.000000	8375.000000	100.000000	3875.000000	24.000000	711.000000	22.000000	396.899994	37.970001	1050.000000

- Volledigheid van de dataset.
- Inconsistenties.
- Spreiding van de gegevens.

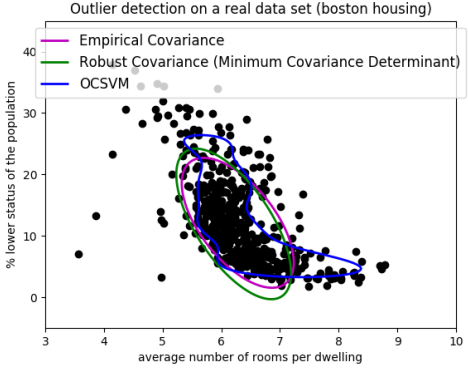
Verwijder de CHAS kolom:

```
dataset.drop('CHAS', axis=1, inplace=True)
```

Statistische vooranalyse

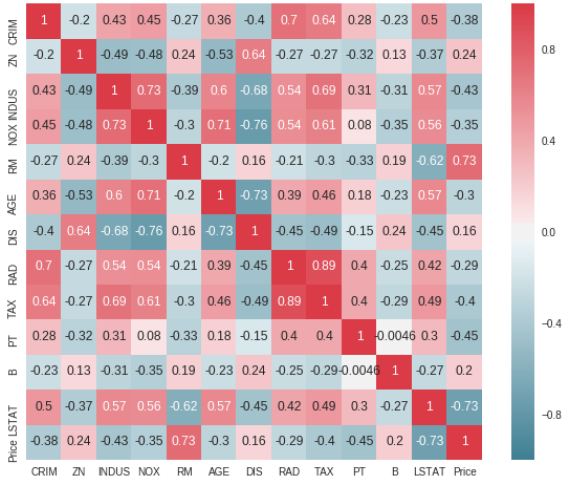
Uitschieters

- Vinden en verwijderen van extreme waarden/samples.
- Geavanceerde technieken (zie later bij clustering).



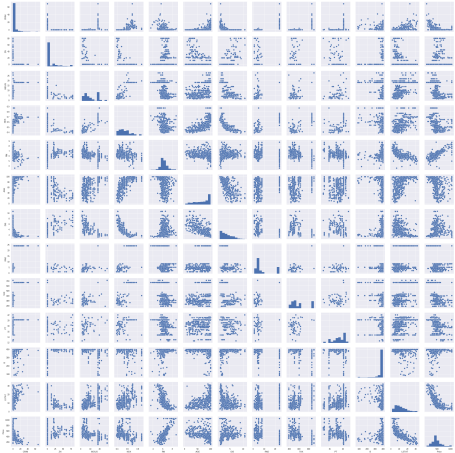
Statistische vooranalyse

Onderlinge correlaties - heatmap



Statistische vooranalyse

Onderlinge correlaties - pairplot



Features en targets

Dataset opsplitsen in features en targets

CRIM	ZN	INDUS	NOX	RM	AGE	DIS	RAD	TAX	PT	B	LSTAT	Price
0.00632	18.0	2.31	0.538	6.575	65.199997	4.0900	1	296	15.300000	396.899994	4.98	504.000000
0.02731	0.0	7.07	0.469	6.421	78.900002	4.9671	2	242	17.799999	396.899994	9.14	453.600008
0.02729	0.0	7.07	0.469	7.185	61.099998	4.9671	2	242	17.799999	392.829987	4.03	728.700016
0.03237	0.0	2.18	0.458	6.998	45.799999	6.0622	3	222	18.700001	394.630005	2.94	701.400032
0.06905	0.0	2.18	0.458	7.147	54.200001	6.0622	3	222	18.700001	396.899994	5.33	760.200016

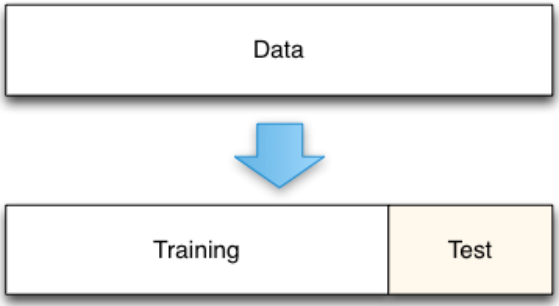
features X

targets y

```
features = list(dataset.columns[:dataset.columns.size-1])
X = dataset[features].values
y= dataset['Price'].values

# Een alternatief voor het opsplitsen in training en test set:
X = dataset.ix[:,0:dataset.columns.size-1].copy()
y = dataset.ix[:,dataset.columns.size-1:dataset.columns.size].copy()
```

Trainen van het model

Dataset opsplitsen in training en test set



Belangrijk om eerst te randomiseren.

```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.33,
random_state=0)
```

Trainen van het model

Initialiseren en trainen van het regressiemodel

```
lregmodel = linear_model.LinearRegression()
lregmodel.fit(X_train,y_train)
```

Model:

```
print('coeffs:␣',lregmodel.coef_)
print('intercept', lregmodel.intercept_)

>> coeffs:  [ -3.56141289e+00   4.05479295e-01   8.14080284e-01  -2.70514977e+02
             8.96450415e+01  -3.02997261e-01  -2.77339444e+01
             7.47151897e+00  -2.92233040e-01  -1.61741146e+01   7.62044683e-02
            -1.17962045e+01]

>> intercept: 650.652022517
```

$$\begin{aligned} Price = &-3.56 \times CRIM + 0.41 \times ZN + 0.81 \times INDUS - 270.51 \times NOX + 89.65 \times RM \\ &- 0.30 \times AGE - 27.74 \times DIS + 7.47 \times RAD - 0.29 \times TAX - 16,17 \times PT \\ &+ 0.08 \times B - 11.80 \times LSTAT + 650.65 \end{aligned}$$

Testen van het model

Voorspellingen maken

Voorspel de prijs van een huis waarbij

CRIM	ZN	INDUS	NOX	RM	AGE	DIS	RAD	TAX	PT	B	LSTAT
0.11	0	12.03	0.57	6.80	89.30	2.39	1	273	21.00	393.45	6.48

```
house = np.array([0.11, 0,12.03, 0.57, 6.80, 89.30, 2.39, 1,
                                    273, 21.00, 393.45, 6.48])

price = lregmodel.predict(house.reshape(1,-1))

print('De prijs van het huis bedraagt: ', price)

>> De prijs van het huis bedraagt:  563.68335073
```

reshape(1,-1) maakt een rijvector

Werkelijke prijs = 562.00

Testen van het model

Performantie en scores van het model: MAE (Mean Absolute Error)

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i|$$

Is het **gemiddelde van de absolute waarden** van het verschil tussen de werkelijke waarden y_i en de voorspelde waarden $\hat{y}_i$.

```
from sklearn.metrics import mean_absolute_error
y_predicted = lregmodel.predict(X_test)
MAE = mean_absolute_error(y_test,y_predicted)
print('MAE = ',MAE)

>> MAE =  64.0090867586
```

Testen van het model

Performantie en scores van het model: MSE (Mean Squared Error)

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

Is het **gemiddelde van de gekwadrateerde waarden** van het verschil tussen de werkelijke waarden y_i en de voorspelde waarden $\hat{y}_i$.

```
from sklearn.metrics import mean_squared_error
y_predicted = lregmodel.predict(X_test)
MSE = mean_squared_error(y_test,y_predicted)
print('MSE = ',MSE)

>> MSE =  7803.89332739
```

Testen van het model

Performantie en scores van het model: Determinatiecoëfficiënt (R^2)

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2}$$

Zegt hoeveel van de variabiliteit verklaard wordt door het model.
Bij perfecte voorspellingen is $R^2 = 1$

Een negatieve waarde voor R^2 betekent dat het model slechter scoort dan een horizontale lijn ($y_i = \bar{y}$).

```
from sklearn.metrics import r2_score
y_predicted = lregmodel.predict(X_test)
r2 = r2_score(y_test,y_predicted)
print('r2 score = ',r2)
### alternatieve manier voor het bepalen van de r2 score
    r2 = lregmodel.score(X_test,y_test)

>> r2 score =  0.754254234917
```

Feature engineering

Normalisatie

Doel van normalisatie

Normalisatie zorgt ervoor dat de features op **dezelfde schaalverdeling** staan.

In ons voorbeeld van de huizenprijs:

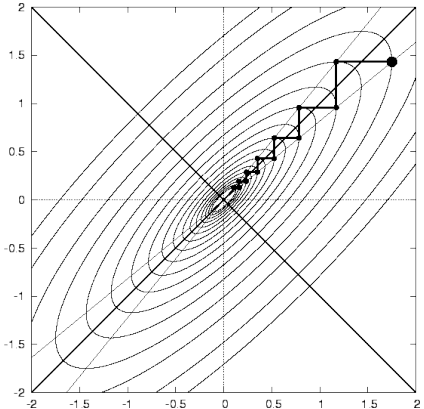
	CRIM	ZN	INDUS	NOX	RM	AGE	DIS	RAD	TAX	PT	B	LSTAT
count	441.000000	441.000000	441.000000	441.000000	441.000000	441.000000	441.000000	441.000000	441.000000	441.000000	441.000000	441.000000
mean	2.649013	9.988662	10.759479	0.547575	6.265785	67.632200	3.851895	8.478458	389.045351	18.387302	375.393853	12.165329
std	6.273766	19.941189	6.749778	0.112896	0.685393	27.997824	2.054524	8.000859	158.293650	2.164533	49.296266	6.632866
min	0.006320	0.000000	1.250000	0.385000	3.561000	2.900000	1.169100	1.000000	188.000000	12.600000	83.449997	1.730000
25%	0.081870	0.000000	5.190000	0.449000	5.877000	45.000000	2.122200	4.000000	277.000000	17.000000	377.730011	6.920000
50%	0.217190	0.000000	8.140000	0.524000	6.172000	74.500000	3.375100	5.000000	311.000000	18.700001	392.200012	10.740000
75%	1.656600	12.500000	18.100000	0.609000	6.590000	93.599998	5.231100	8.000000	432.000000	20.200001	396.899994	15.940000
max	67.920799	80.000000	27.740000	0.871000	8.780000	100.000000	10.710300	24.000000	711.000000	22.000000	396.899994	31.990000

NOX: $0.385 \longmapsto 0.871$ terwijl TAX: $188 \longmapsto 711$

Normalisatie

Doel van normalisatie

Gradient Descent convergeert minder snel als features op een verschillende schaalgrootte staan.

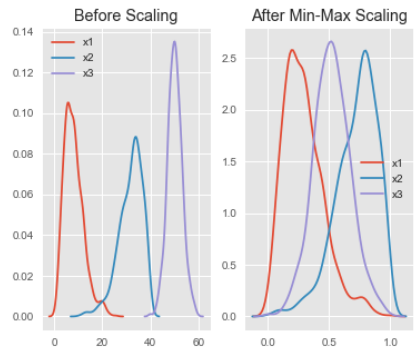


Normalisatie

MIN-MAX scaling

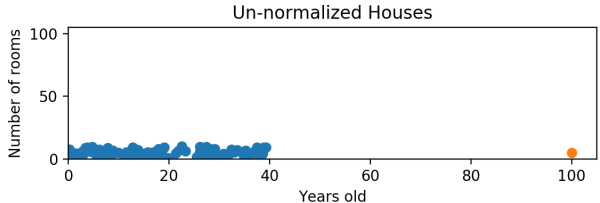
$$x_{s_i} = \frac{x_i - Min(x)}{Max(x) - Min(x)}$$

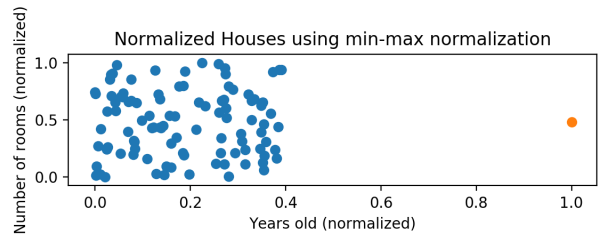
- Schaalt alle features tussen 0 en 1.
- Werkt goed bij niet Gaussiaanse distributies en bij kleine variantie.
- De scheefheid (skew) blijft bewaard.
- Gevoelig voor uitschieters.



Normalisatie

MIN-MAX scaling





Normalisatie

MIN-MAX scaling

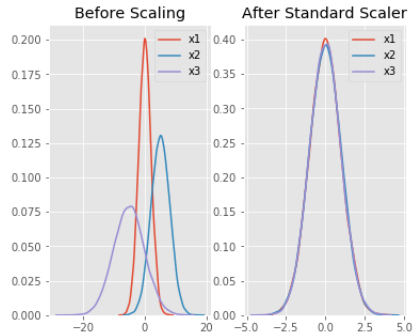
```
from sklearn.preprocessing import MinMaxScaler

scaler = MinMaxScaler.fit(X_train)
X_train = scaler.transform(X_train)
X_test = scaler.transform(X_test)

# alternatief
scaler = MinMaxScaler()
X_train = scaler.fit_transform(X_train)
X_test = scaler.transform(X_test)
```

Normalisatie

Standard scaling

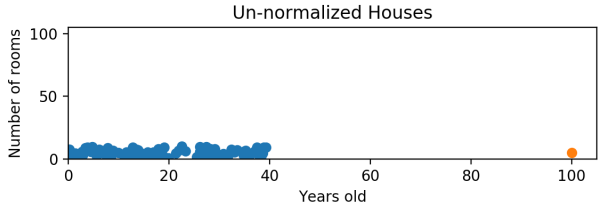
$$x_{s_i} = \frac{x_i - mean(x)}{stdev(x)}$$

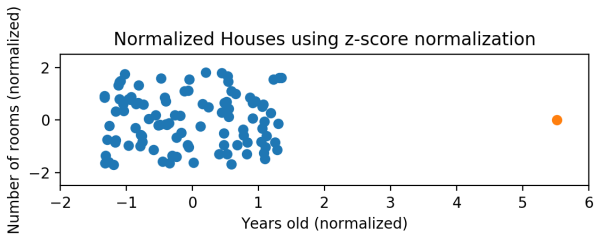
- Geschaalde features:gemiddelde = 0 en standaardafwijking = 1.
- Geschaalde features schommelen rond 0 (soms nodig bij deep learning).
- Vervormt geen relatieve afstanden tussen de feature waarden.
- Kan beter overweg met uitschieters.
- Garandeert geen genormaliseerde data op exact dezelfde schaal.



Normalisatie

Standard scaling





Normalisatie

Standard scaling

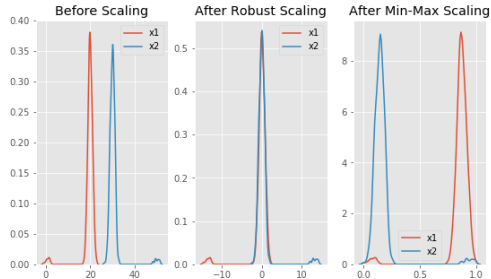
```
from sklearn.preprocessing import StandardScaler

scaler = StandardScaler.fit(X_train)
X_train = scaler.transform(X_train)
X_test = scaler.transform(X_test)

# alternatief
scaler = StandardScaler()
X_train = scaler.fit_transform(X_train)
X_test = scaler.transform(X_test)
```

Normalisatie

Robust scaling

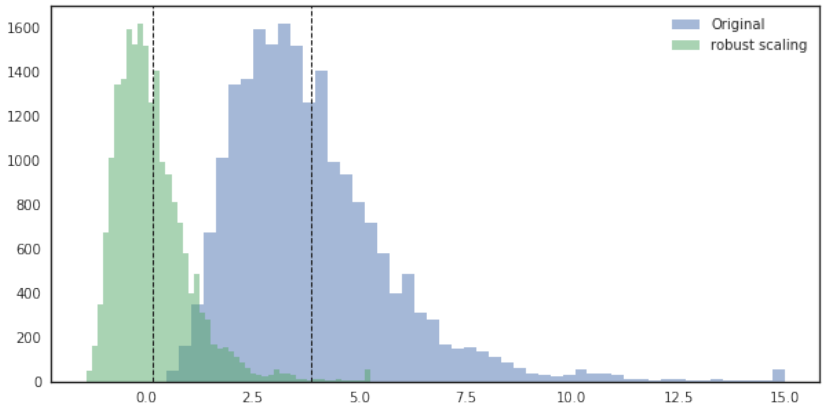
$$x_{s_i} = \frac{x_i - Q_2(x)}{Q_3(x) - Q_1(x)}$$

- Lijkt op MIN-MAX scaler maar gebruikt de interkwartielafstand ipv range.
- Houdt geen rekening met uitschieters.
- Gebruikt minder data bij het bepalen van de schaal.
- Range van de genormaliseerde data is groter dan bij MIN-MAX scaling.
- Garandeert geen genormaliseerde data op exact dezelfde schaal.



Normalisatie

Robust scaling



Normalisatie

Robust scaling

```
from sklearn.preprocessing import RobustScaler

scaler = RobustScaler.fit(X_train)
X_train = scaler.transform(X_train)
X_test = scaler.transform(X_test)

# alternatief
scaler = RobustScaler()
X_train = scaler.fit_transform(X_train)
X_test = scaler.transform(X_test)
```

Feature expansion

Nieuwe features

Bedenken van nieuwe features

Voorbeelden:

- Uit de lengte en breedte van een huis de oppervlakte halen als nieuwe feature.
- Uit een start en eindpunt de afstand halen als nieuwe feature.
- Uit een datum afleiden welke dag van de week het is.
- Veranderingen in de features.
- Nieuwe opgemeten parameters.

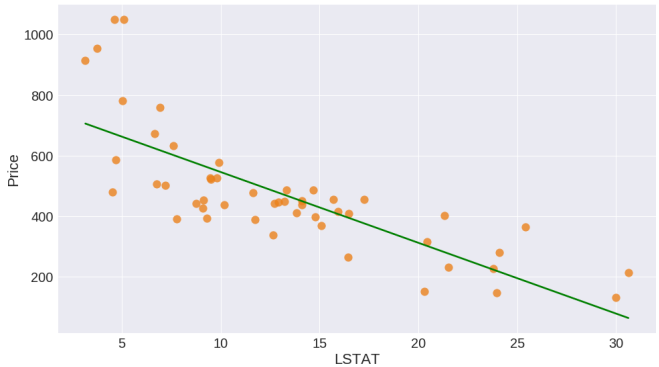
Feature expansion

Hogere-orde features

Het verband tussen features en de target(s) is niet altijd linear.

Voorbeeld: samenhang tussen LSTAT (x_1) en de huizenprijs (P).

$$P = \theta_0 + \theta_1 x_1$$

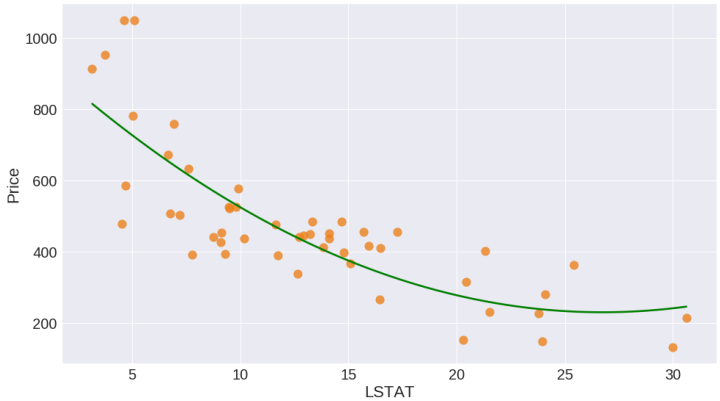


Feature expansion

Hogere-orde features

Toevoegen van een extra hogere-orde feature $x_2 = x_1^2$

$$P = \theta_0 + \theta_1 x_1 + \theta_2 x_2$$

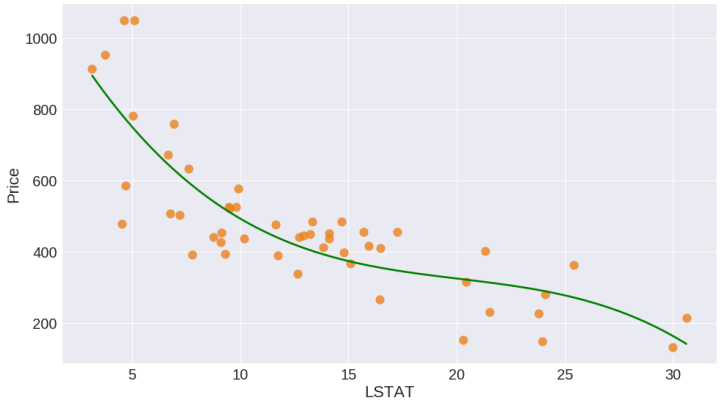


Feature expansion

Hogere-orde features

Toevoegen van een extra hogere-orde feature $x_3 = x_1^3$

$$P = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3$$

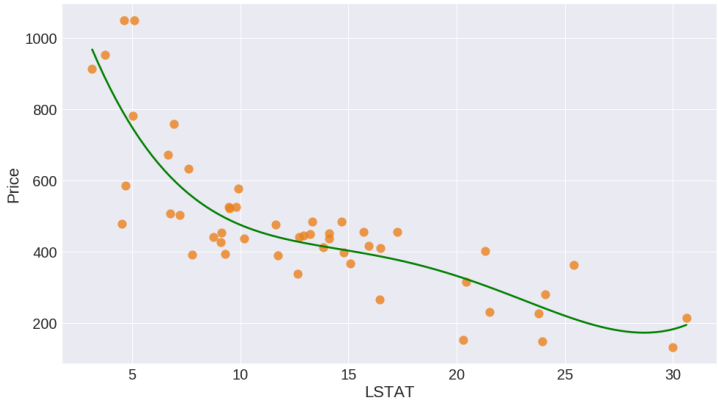


Feature expansion

Hogere-orde features

Toevoegen van een extra hogere-orde feature $x_4 = x_1^4$

$$P = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + \theta_4 x_4$$



Feature expansion

Hogere-orde features

```
# toevoegen van extra feature: LSTAT^2 LSTAT^3
dataset.insert(dataset.columns.size-1,'LSTAT^2',dataset.LSTAT**2)
dataset.insert(dataset.columns.size-1,'LSTAT^3',dataset.LSTAT**3)
```

	CRIM	ZN	INDUS	NOX	RM	AGE	DIS	RAD	TAX	PT	B	LSTAT	LSTAT^2	LSTAT^3	Price
0	0.00632	18.0	2.31	0.538	6.575	65.199997	4.0900	1	296	15.300000	396.899994	4.98	24.800400	123.505993	504.000000
1	0.02731	0.0	7.07	0.469	6.421	78.900002	4.9671	2	242	17.799999	396.899994	9.14	83.539606	763.552030	453.600008
2	0.02729	0.0	7.07	0.469	7.185	61.099998	4.9671	2	242	17.799999	392.829987	4.03	16.240902	65.450837	728.700016
3	0.03237	0.0	2.18	0.458	6.998	45.799999	6.0622	3	222	18.700001	394.630005	2.94	8.643600	25.412185	701.400032
4	0.06905	0.0	2.18	0.458	7.147	54.200001	6.0622	3	222	18.700001	396.899994	5.33	28.408899	151.419431	760.200016

Model met extra features trainen en nadien evalueren op test set.

Opgepast: bij de test set moet je ook dezelfde features toevoegen.

One-hot encoding

Doel van one-hot encoding

Omzetten van categorische variabelen naar meerde aparte features.

Label Encoding

Food Name	Categorical #	Calories
Apple	1	95
Chicken	2	231
Broccoli	3	50

One Hot Encoding

Apple	Chicken	Broccoli	Calories
1	0	0	95
0	1	0	231
0	0	1	50

One-hot encoding

One-hot encoding in Sklearn

```
dataset = pd.concat([dataset,pd.get_dummies(dataset['food_name'], prefix='food')],axis=1)
dataset.drop(['food_name'],axis=1, inplace=True)
dataset.head()
```

	food_name	Calories
0	Apple	95
1	Chicken	231
2	Broccoli	50
3	Chocolat	549

	Calories	food_Apple	food_Broccoli	food_Chicken	food_Chocolat
0	95	1	0	0	0
1	231	0	0	1	0
2	50	0	1	0	0
3	549	0	0	0	1

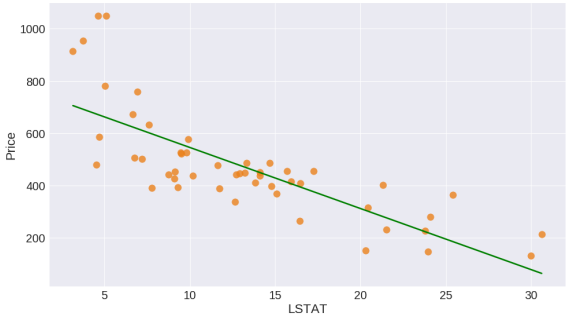
Underfitting en overfitting

Underfitting en overfitting

Underfitting

Underfitting treedt op wanneer een model de training data niet kan modelleren en ook niet kan generaliseren op nieuwe data.

- Het model is te 'simpel'.
- Model met een hoge bias.

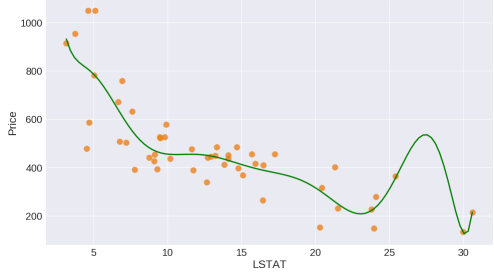


Underfitting en overfitting

Overfitting

Overfitting treedt op wanneer een model de training data te goed modelleert en niet kan generaliseren op nieuwe data.

- Het model is te 'complex'.
- De ruis van willekeurige fluctuaties in de data wordt opgepikt.
- Model met een hoge variance.



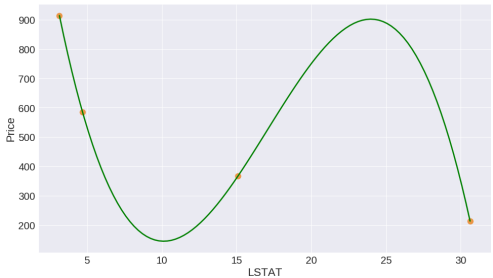
Underfitting en overfitting

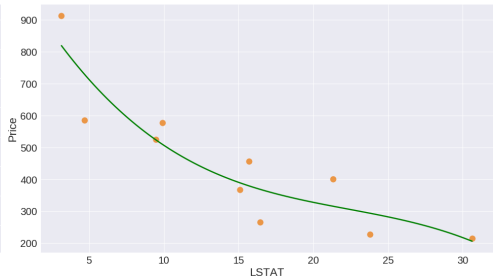
Overfitting

Afhanklijkheid van grootte van de trainingset (aantal observaties m).

- Bij weinig observaties: snel overfitting bij complexer model.
- Bij veel observaties: minder snel overfitting bij complexer model.

Voorbeeld: Derde orde polynoom





Underfitting en overfitting

Regularisatie (regularization)

Methode om de mate van bias van een hypothese te regelen en een goed evenwicht te vinden tussen underfitting en overfitting.

$$J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right)^2 + R(\theta)$$

$R(\theta)$ is de regularisatie-term. Dit is een extra kostenterm die het gebruik van hogere orde features afstraft tenzij ze de globale kostenfunctie doen dalen.

Underfitting en overfitting

Regularisatie (regularization)

Voorbeeld van een regularisatie

$$J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right)^2 + \lambda \theta \theta^T$$

λ is een tuning parameter (hyper parameter)

- $\lambda = 0 \Rightarrow$ geen regularisatie.
- $\lambda = \infty \Rightarrow \theta = 0$.
- λ tussenin regelt de mate van regularisatie.

$\theta = \{\theta_1, \ldots, \theta_n\}$

intercept θ_0 wordt meestal niet geregulariseerd.

Underfitting en overfitting

Regularisatie (regularization)

Voorbeeld van een regularisatie

$$J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} \left(h_\theta(x^{(i)}) - y^{(i)} \right)^2 + \lambda \theta \theta^T$$

De tuningparameter λ regelt de complexiteit van de hypothese

- Kleine waarde voor λ: lage bias, hoge variantie (overfitting).
- Grote waarde voor λ: hoge bias, lage variantie (underfitting).

Afhankelijk van hoe R gedefiniëerd wordt is er andere benaming voor de regularisatie:

- Ridge regression (L2 regularisatie) .
- Lasso regression (L1 regularisatie).

Underfitting en overfitting

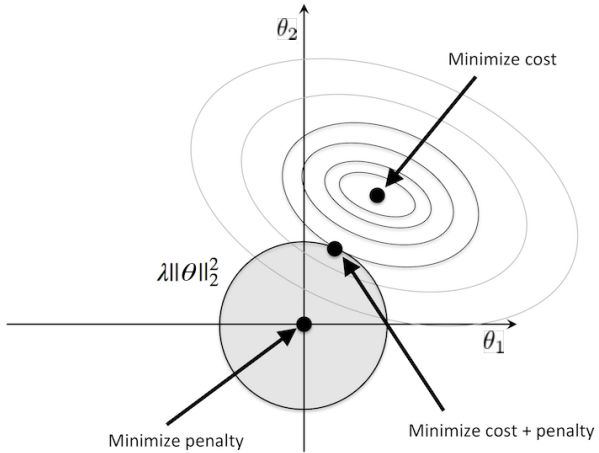
Regularisatie via L2 norm

$$J_{L2} = J + \lambda_2 \sum_{j=1}^{m} \theta_j^2$$

$$J_{L2} = \sum_{i=1}^{n} (\text{target}^{(i)} - \text{output}^{(i)}) + \lambda_2 \sum_{j=1}^{m} \theta_j^2$$

Underfitting en overfitting

Regularisatie via L2 norm



Underfitting en overfitting

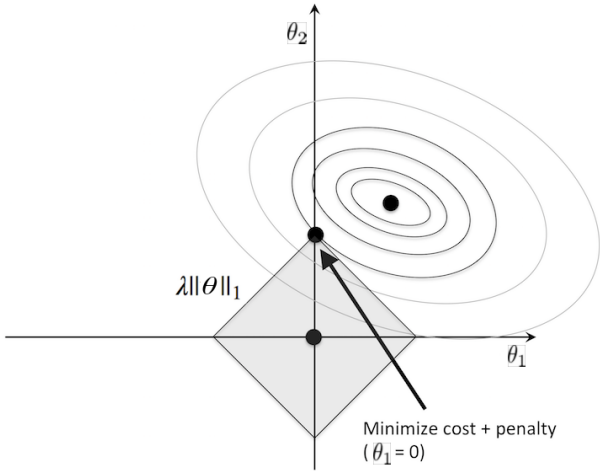
Regularisatie via L1 norm

$$J_{L1} = J + \lambda_1 \sum_{j=1}^{m} |\theta_j|$$

$$J_{L1} = \sum_{i=1}^{n} (\text{target}^{(i)} - \text{output}^{(i)}) + \lambda_1 \sum_{j=1}^{m} |\theta_j|$$

Underfitting en overfitting

Regularisatie via L1 norm



Underfitting en overfitting

Voorbeeld regularisatie op huizenprijzen

Via Ridge of Lasso regressie met regularisatieparameter α.

- hoe groter α, hoe sterker de regularisatie en dus hoe minder complex het model.
- hoe kleiner α, hoe zwakker de regularisatie en dus hoe complexer het model.

```
regmodel = Ridge(alpha=0.14,tol=0.0001,fit_intercept=True)
regmodel.fit(X_train,y_train)
regmodel.score(X_test,y_test)
>> 0.79834480089914472

lregmodel = Lasso(alpha=0.5,tol=0.0001,fit_intercept=True)
lregmodel.fit(X_train,y_train)
lregmodel.score(X_test,y_test)
>> 0.8437113338085345
```