# foundations of data science for everyone

VI: Logistic Regression

AUTHOR AND LECTURER: Farid Qamar

this slide deck: https://slides.com/faridqamar/fdfse\_6



recall:

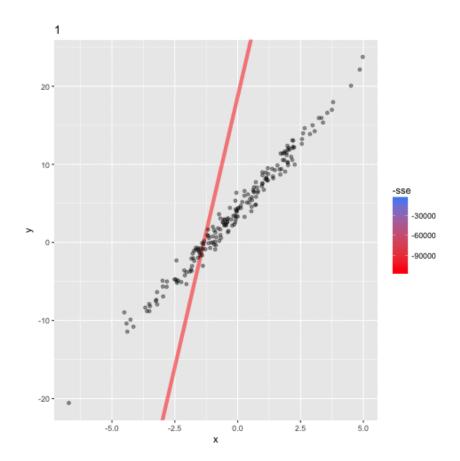
what is a model?

in the ML context:

a model is a low dimensional representation of a higher dimensionality dataset

## what is a machine learning?

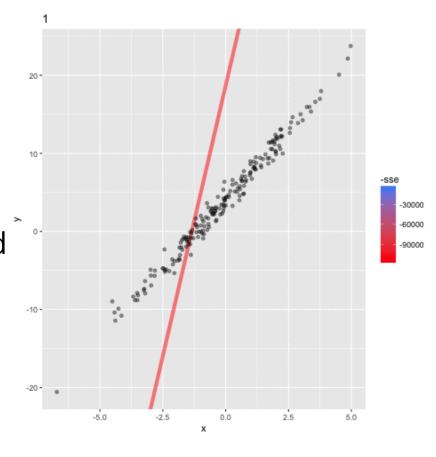
ML: Any model with parameters learned from the data



### what is a machine learning?

ML: Any model with parameters learned from the data

ML models are a parameterized representation of "reality" where the parameters are learned from finite sets (samples) of realizations of that reality (population)



### how do we model?

Choose the model:

a mathematical formula to represent the behavior in the data

parameters

example: line model y = ax + b

### how do we model?

Choose the model:

a mathematical formula to represent the behavior in the data

### **Choose the hyperparameters:**

parameters chosen **before** the learning process, which govern the model and training process

parameters

example: line model y = ax + b

example: the *degree N* of the polynomial  $y = \sum_{i=0}^N c_i x^i$ 

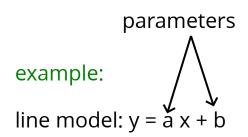
### how do we model?

# **Choose an objective function:**

in order to find the "best" parameters of the model: we need to "optimize" a function.

We need something to be either

**MINIMIZED** or **MAXIMIZED** 



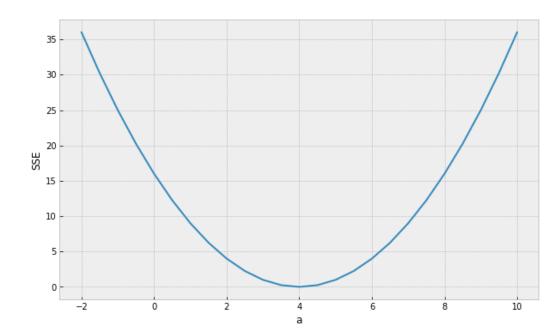
objective function: sum of residual squared (least square fit method)

$$SSE = \sum (y_{i,observed} - y_{i,predicted})^2 \ SSE = \sum (y_{i,observed} - (ax_i + b))^2$$

we want to **minimize** *SSE* as much as possible

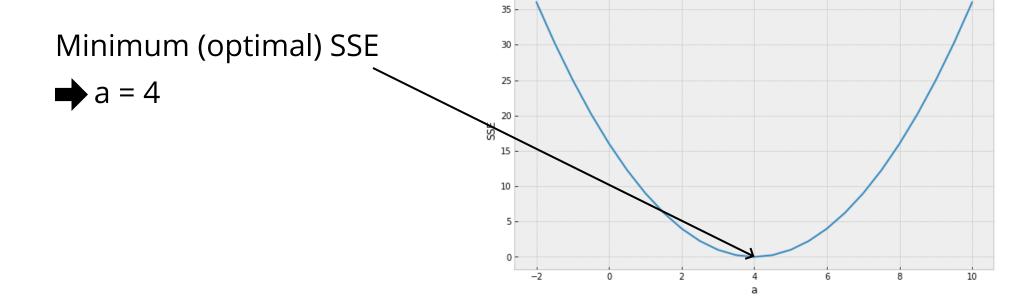
### Optimizing the Objective Function

assume a simpler line model y = ax(b = 0) so we only need to find the "best" parameter a



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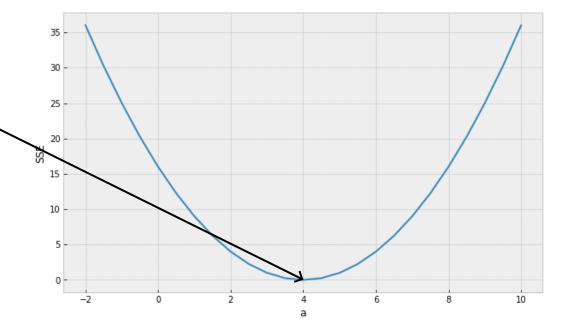
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Minimum (optimal) SSE

a = 4

ow do we find the

How do we find the minimum if we do not know beforehand how the SSE curve looks like?





# General purpose for ML

- to understand the structure of feature space
- regression: to predict unknown values based on known examples
- classification: to identify unknown classes based on known examples
- feature importance: to understand which features are important for the success of the model

# **Linear Regression**

find the optimal parameters
(slope/coefficients and intercept)
of a linear model that best
combine the features
(independent variables) to
describe the target (dependent
variable)

# **Linear Regression**

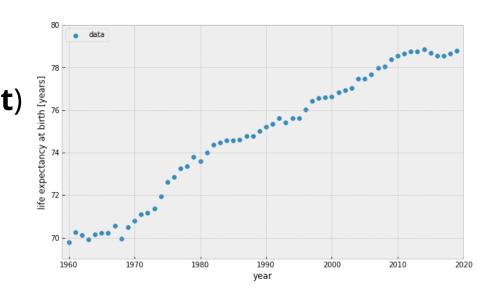
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**World Bank:** Life expectancy at birth in the US

	year	leb
0	1960	69.770732
1	1961	70.270732
2	1962	70.119512
3	1963	69.917073
4	1964	70.165854
5	1965	70.214634
6	1966	70.212195
		•
54	2014	78.841463
55	2015	78.690244
56	2016	78.539024
57	2017	78.539024
58	2018	78.639024
59	2019	78.787805

# **Linear Regression**

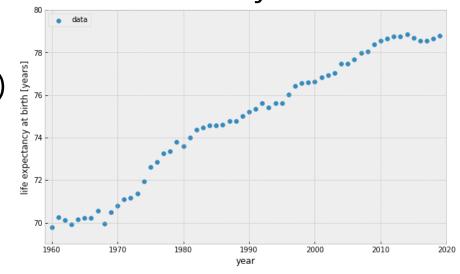
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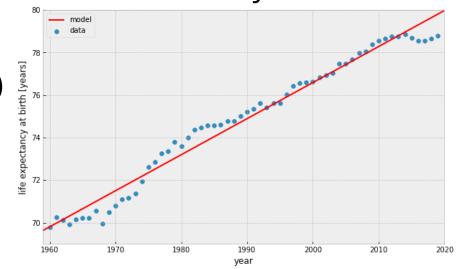
line model y = ax + b



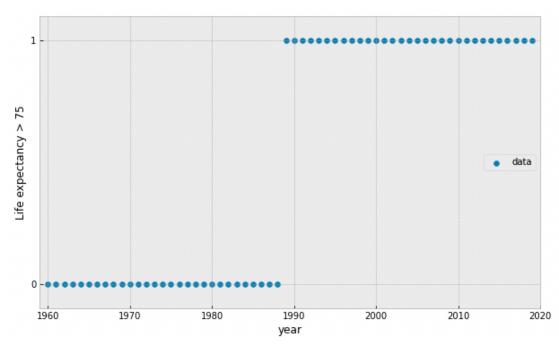
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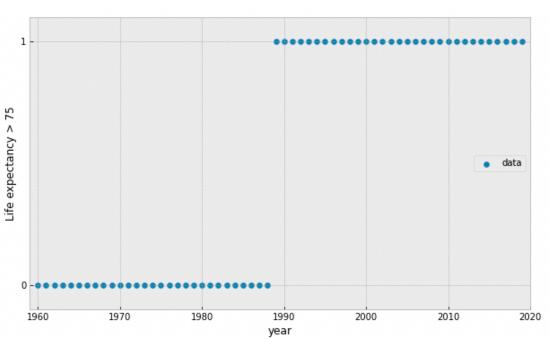
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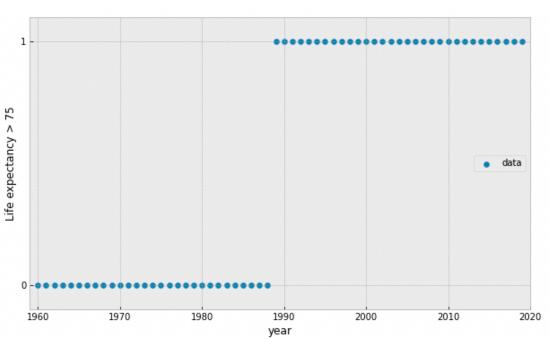
### line model y = ax + b

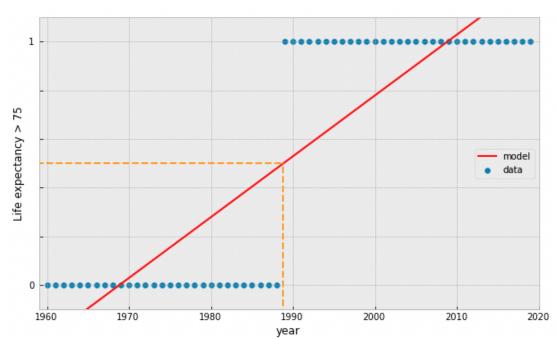


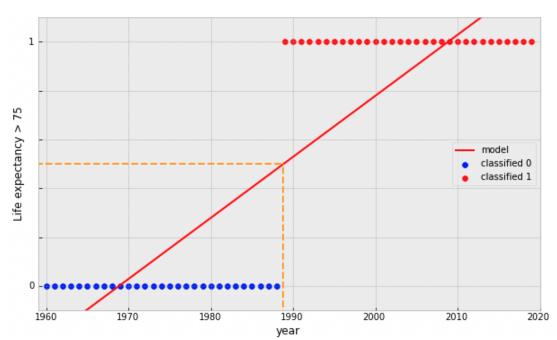
	year	75+
0	1960	0
1	1961	0
2	1962	0
3	1963	0
4	1964	0
5	1965	0
6	1966	0
	•	
54	2014	1
55	2015	1
56	2016	1
57	2017	1
58	2018	1
59	2019	1



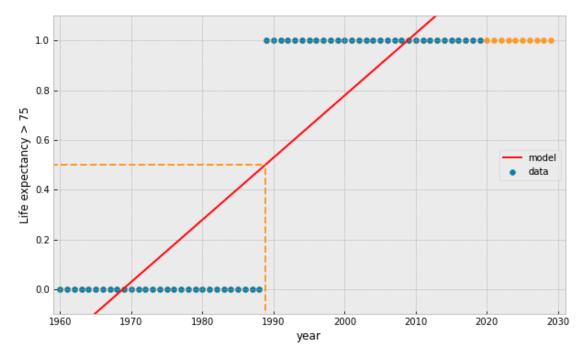




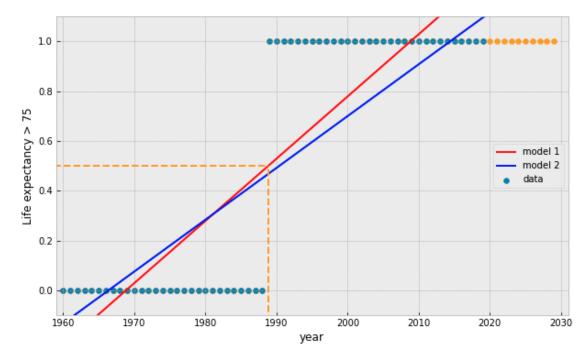




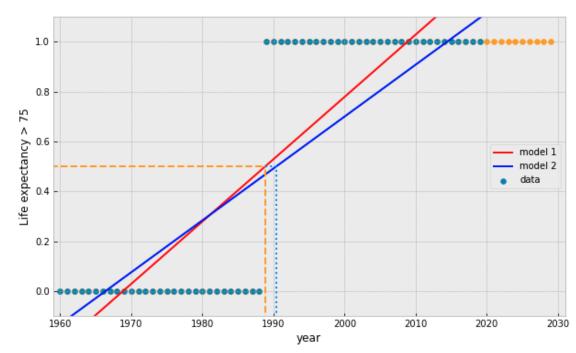
try fitting a linear model...



try fitting a linear model...



try fitting a linear model...





$$f(x)=rac{1}{1+e^{-z}}$$
 ;  $z=ax+b$ 

interpreted as the probability that the target is True (= 1)

### **Objective Function:**

Log-likelihood  $\log(\mathscr{L}) = \sum (y_i \log(f) + (1-y_i) \log(1-f))$ 

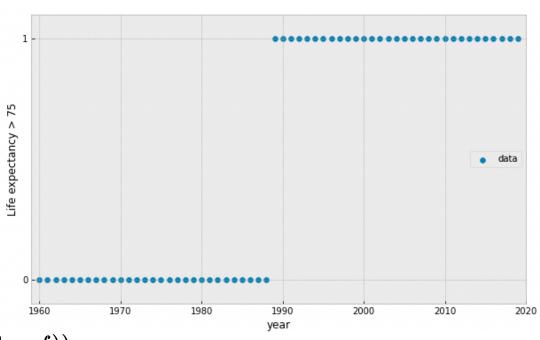
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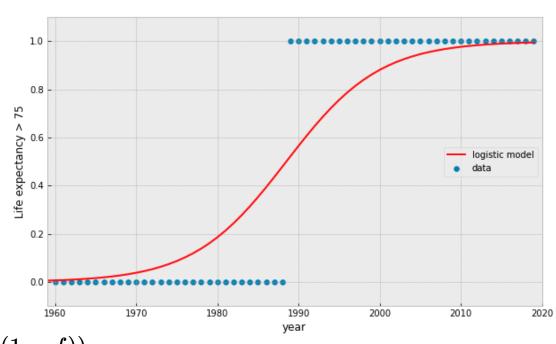
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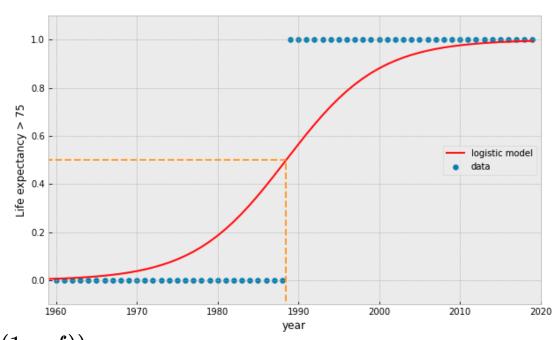
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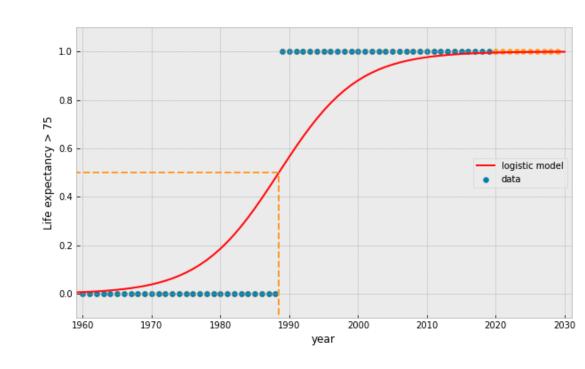
Log-likelihood

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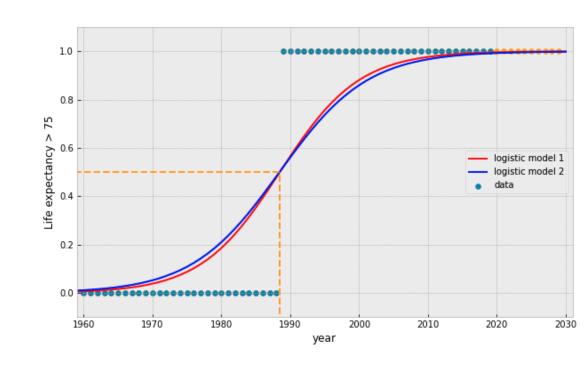
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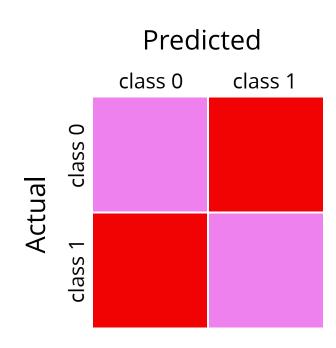
#### **Confusion Matrix**

indicates the model's "confusion" between classification outcomes

smaller off-diagonal elements & larger diagonal elements

=

model more effective at correctly labeling classes

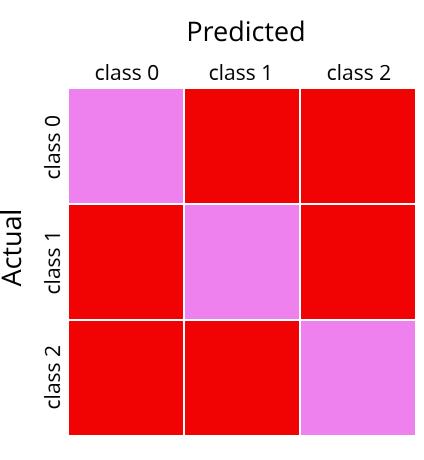


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#### **Confusion Matrix**

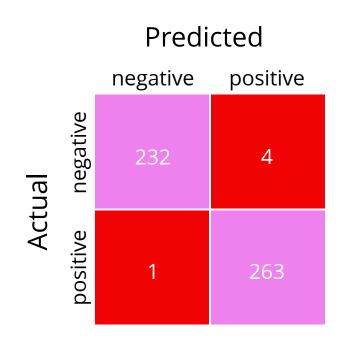
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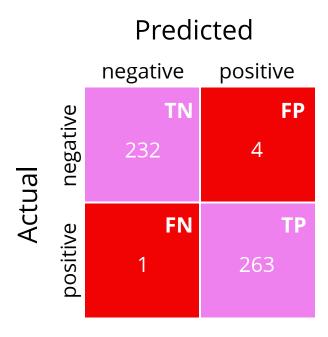
for example...
model predicting 500 objects:



### True/False Positives/Negatives

#### Classification outcomes:

```
true positives (TP): "+" correctly labeled as "+"
true negatives (TN): "-" correctly labeled as "-"
false positives (FP): "-" incorrectly labeled as "+"
false negatives (FN): "+" incorrectly labeled as "-"
```



#### Accuracy

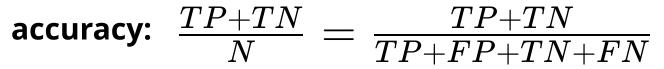
#### Classification outcomes:

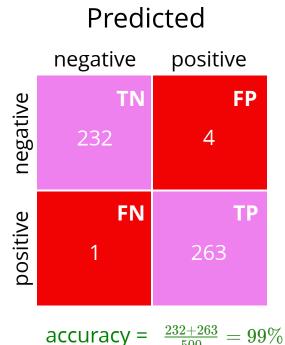
true positives (TP): "+" correctly labeled as "+"

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false positives (FP): "-" incorrectly labeled as "+"

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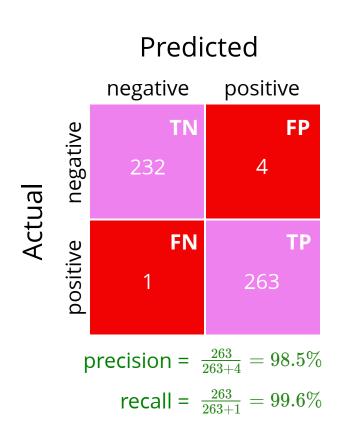
#### **Precision and Recall**

#### Classification outcomes:

```
true positives (TP): "+" correctly labeled as "+"
```

## precision: $\frac{TP}{TP+FP}$

recall: 
$$\frac{TP}{TP+FN}$$



#### **Precision and Recall**

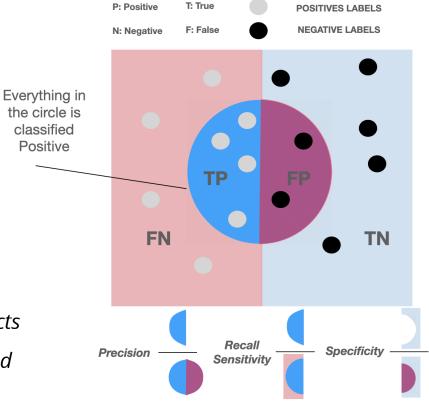
precision: (or specificity)

$$rac{TP}{TP+FP}$$
 Fraction of objects you think are positive that actually are positive

recall: (or sensitivity)

$$rac{TP}{TP{+}FN}$$
 Fraction of positive objects

F1-score:  $\frac{2 \times \text{precision} \times \text{recall}}{\text{precision} + \text{recall}}$ 



https://en.wikipedia.org/wiki/Precision\_and\_recall

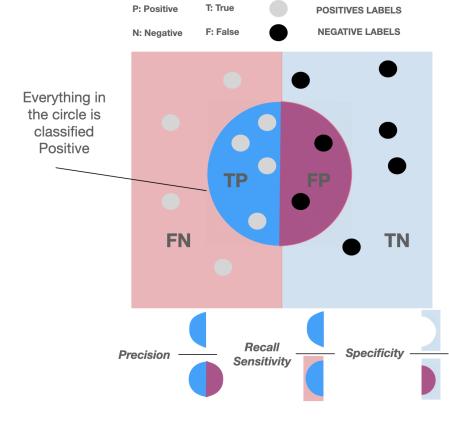
Current classifier accuracy: 50%

Precision?

Recall?

Specificity?

Sensitivity?



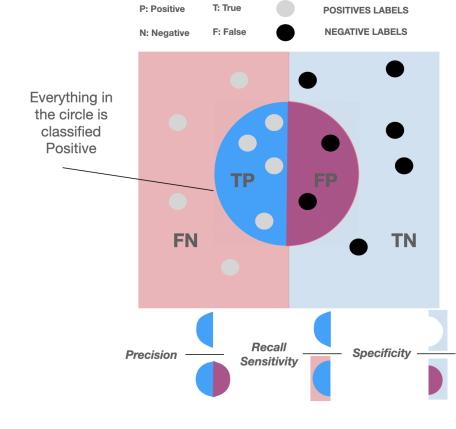
https://en.wikipedia.org/wiki/Precision\_and\_recall

#### Current classifier accuracy: 50%

Precision = 
$$4/6 = 0.7$$

Recall = 
$$4/8 = 0.5$$

Sensitivity = 0.5



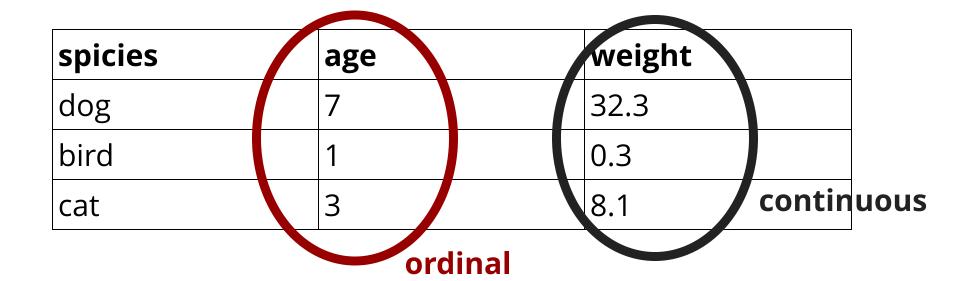
https://en.wikipedia.org/wiki/Precision\_and\_recall



# encoding categorical variables

spicies	age	weight
dog	7	32.3
bird	1	0.3
cat	3	8.1

spicies	age	weight	
dog	7	32.3	
bird	1	0.3	
cat	3	8.1	continuous





### numerical encoding

change categorical to (integer) numerical

spicies	age	weight	
1	7	32.3	
2	1	0.3	
3	3	8.1	

### one-hot encoding

change each category to a binary

cat	bird	dog	age	weight
0	0	1	7	32.3
0	1	0	1	0.3
1	0	0	3	8.1

## implies an order that does not exist

## numerical encoding

change categorical to (integer) numerical

spicies	age	weight
1	7	32.3
2	1	0.3
3	3	8.1

dog=1, bird=2, cat=3
...dog < bird < cat... ??</pre>

# ignores covariance between features increases the dimensionality

problematic if you are interested in feature importance

#### one-hot encoding

change each category to a binary

cat	bird	dog	age	weight
0	0	1	7	32.3
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spicies	age	weight
1	7	32.3
2	1	0.3
3	3	8.1

## Definitely Preferred!

ignores covariance between features

increases the dimensionality problematic if you are interested in feature

atic if you are interested in feat ↑ importance

#### one-hot encoding

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cat	bird	dog	age	weight
0	0	1	7	32.3
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1	0	0	3	8.1

# normalization

COVARIANCE = correlation / variance

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02:00	100			UMIDITĂ(%)	VENTO(KM/H)	RAFFICHE(KM/H)
		-	21	57	7)	20
05:00	4	~	20	57	7)	16
08:00	2	-	20	61	(5)	14
11:00	-	-	23	55	7,	16
14:00		50%	26	58	(7)	20
17:00	4	50%	22	62	1 22	50
20:00		10%	18	77	1 16	45
23:00	-	-	17	75	1 12	(32)

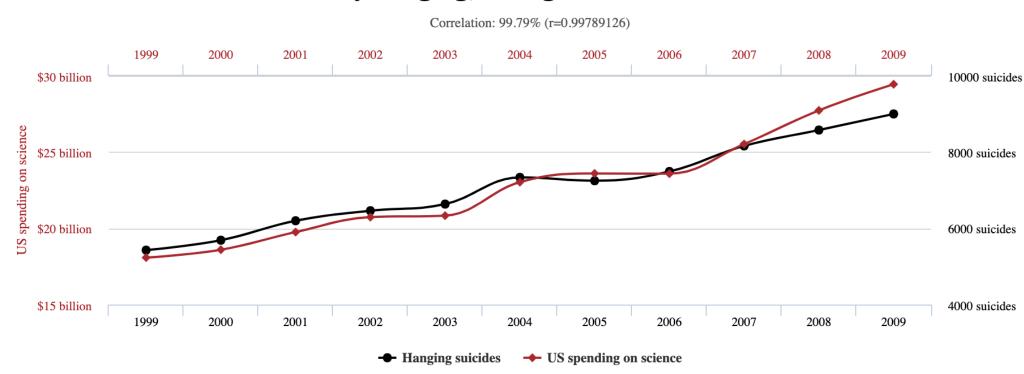
Bacheca – Parma domani mercoledì 18 settembre – meteoweek.com

axis 1 -> features

#### US spending on science, space, and technology

correlates with

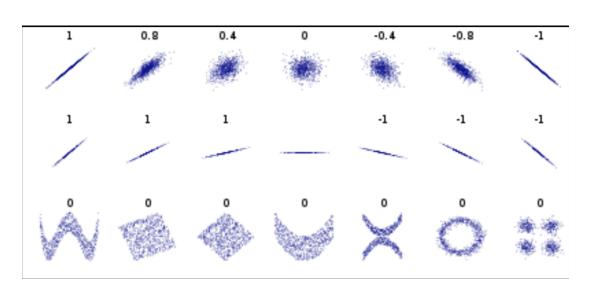
#### Suicides by hanging, strangulation and suffocation

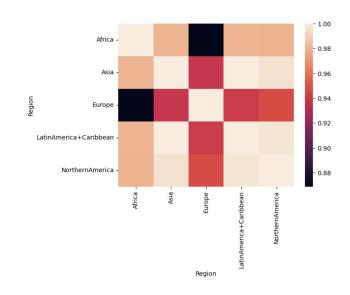


https://www.tylervigen.com/spurious-correlations

Pearson's correlation (linear correlation)

$$r_{xy} = rac{\sum_{i=1}^{n}(x_i - ar{x})(y_i - ar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - ar{x})^2}\sqrt{\sum_{i=1}^{n}(y_i - ar{y})^2}}$$

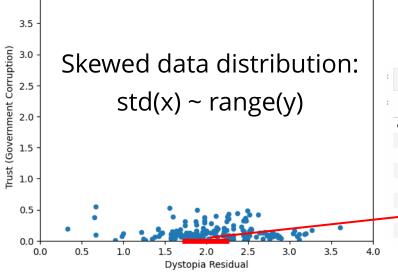




### **Generic preprocessing... WHY??**

Worldbank Happyness Dataset https://github.com/fedhere/MLPNS\_FBianco/blob/main/clustering/happiness\_solution.ipynb

	Country	Region	Happiness Score	Standard Error	Economy (GDP per Capita)	Family	Health (Life Expectancy)	Freedom	Trust (Government Corruption)	Generosity	Dy Re
0	Switzerland	Western Europe	7.587	0.03411	1.39651	1.34951	0.94143	0.66557	0.41978	0.29678	2
1	Iceland	Western Europe	7.561	0.04884	1.30232	1.40223	0.94784	0.62877	0.14145	0.43630	2
2	Denmark	Western Europe	7.527	0.03328	1.32548	1.36058	0.87464	0.64938	0.48357	0.34139	2.

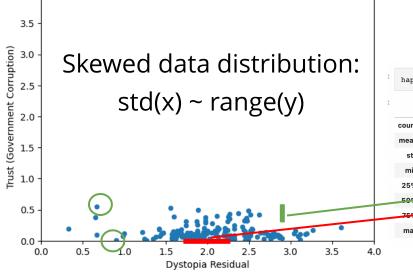


	ness15.descri	De()								
	Happiness Score	Standard Error	Economy (GDP per Capita)	Family	Health (Life Expectancy)	Freedom	Trust (Government Corruption)	Generosity	Dystopia Residual	yea
count	160.000000	158.000000	160.000000	158.000000	160.000000	160.000000	160.000000	160.000000	158.000000	160.00000
mean	5.365756	0.047885	0.842979	0.991046	0.628037	0.428151	0.143023	0.236448	2.098977	2015.05000
std	1.141280	0.017146	0.402840	0.272369	0.246332	0.149803	0.119492	0.126605	0.553550	0.44580
min	2.839000	0.018480	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.328580	2015.00000
25%	4.517750	0.037268	0.539453	0.856823	<del>0.43</del> 7897	0.328630	0.061067	0.148800	1.759410	2015.00000
50%	5.203000	0.043940	0.901085	1.029510	0.695745	0.434635	0.107220	0.216130	2.095415	2015.00000
75%	6.193250	0.052300	1.155523	1.214405	0.809837	0.547057	0.179565	0.307547	2.462415	2015.00000
max	7.587000	0.136930	1.690420	1.402230	1.025250	0.669730	0.551910	0.795880	3.602140	2019.00000

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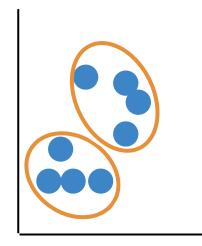


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## unsupervised vs supervised learning

#### **Unsupervised learning**

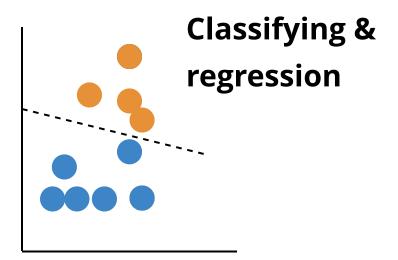
- understanding structure
- anomaly detection
- dimensionality reduction



Clustering

#### Supervised learning

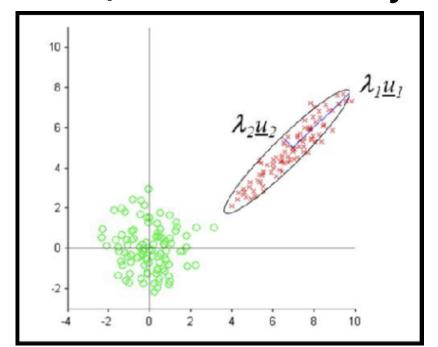
- classification
- prediction
- feature selection



## **Generic preprocessing**

Data can have covariance (and it almost always does!)

ORIGINAL DATA



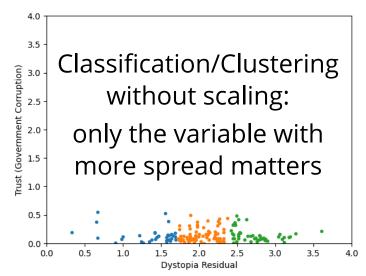
STANDARDIZED DATA

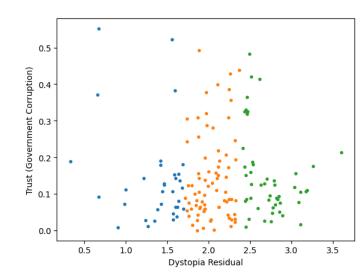
Data that is not correlated appear as a sphere in the Ndimensional feature space

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0	Switzerland	Western Europe	7.587	0.03411	1.39651	1.34951	0.94143	0.66557	0.41978	0.29678	
1	Iceland	Western Europe	7.561	0.04884	1.30232	1.40223	0.94784	0.62877	0.14145	0.43630	
2	Denmark	Western Europe	7.527	0.03328	1.32548	1.36058	0.87464	0.64938	0.48357	0.34139	

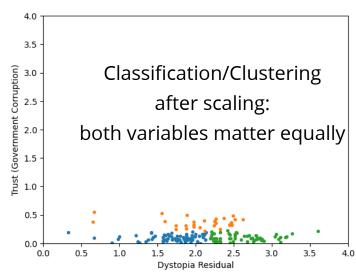


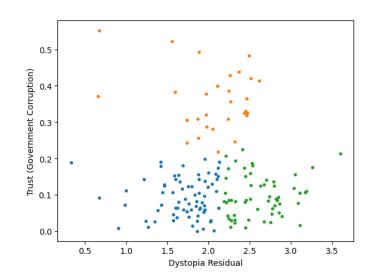


## **Generic preprocessing... WHY??**

#### Worldbank Happyness Dataset

	Country	Region	Happiness Score	Standard Error	Economy (GDP per Capita)	Family	Health (Life Expectancy)	Freedom	Trust (Government Corruption)	Generosity	[
0	Switzerland	Western Europe	7.587	0.03411	1.39651	1.34951	0.94143	0.66557	0.41978	0.29678	
1	Iceland	Western Europe	7.561	0.04884	1.30232	1.40223	0.94784	0.62877	0.14145	0.43630	
2	Denmark	Western Europe	7.527	0.03328	1.32548	1.36058	0.87464	0.64938	0.48357	0.34139	

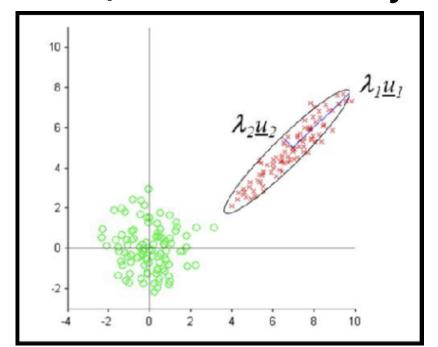




## **Generic preprocessing**

Data can have covariance (and it almost always does!)

ORIGINAL DATA



STANDARDIZED DATA

Data that is not correlated appear as a sphere in the Ndimensional feature space

## Generic preprocessing: most commo will just correct for the spread and c

for each feature: divide by standard deviation and subtract mean

```
X = preprocessing.scale(X, axis=0)
Last executed 2018-12-12 09:35:39 in 46ms
 X.mean(axis=0)
Last executed 2018-12-12 09:35:40 in 13ms
array([ 3.85590369e-16, -6.93196168e-17, -5.90549813e-16, -5.95882091e-16,
       -8.49165306e-16, -1.57568821e-15, -8.00508267e-16,
                                                             5.55890004e-16,
       -5.16564452e-16, 1.09378357e-15, 3.46598084e-16, 2.31954102e-16,
        2.78611537e-16, -2.51283611e-16, 8.66495210e-18, 3.03939858e-16,
       -3.66594127e-17, -9.27149875e-16, -6.39873386e-16,
                                                             2.93275302e-17,
        9.19817992e-17, 6.33208038e-18, -1.99960433e-17,
                                                             9.55144336e-16,
       -2.20623011e-16, 6.93196168e-17, -9.46479383e-17, 2.26621824e-16,
        6.93196168e-17, 2.32953905e-161)
 X.std(axis=0)
Last executed 2018-12-12 09:36:28 in 19ms
```

# whitening

The term "whitening" refers to white noise, i.e. noise with the same power at all frequencies"

PLUTO Manhattan data (42,000 x 15) correlation matrix

$$\Sigma = \begin{bmatrix} \mathrm{E}[(X_1 - \mu_1)(X_1 - \mu_1)] & \mathrm{E}[(X_1 - \mu_1)(X_2 - \mu_2)] & \cdots & \mathrm{E}[(X_1 - \mu_1)(X_n - \mu_n)] \\ \mathrm{E}[(X_2 - \mu_2)(X_1 - \mu_1)] & \mathrm{E}[(X_2 - \mu_2)(X_2 - \mu_2)] & \cdots & \mathrm{E}[(X_2 - \mu_2)(X_n - \mu_n)] \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{E}[(X_n - \mu_n)(X_1 - \mu_1)] & \mathrm{E}[(X_n - \mu_n)(X_2 - \mu_2)] & \cdots & \mathrm{E}[(X_n - \mu_n)(X_n - \mu_n)] \end{bmatrix}.$$

axis 1 -> features

PLUTO Manhattan data (42,000 x 15) correlation matrix

A covariance matrix is diagonal if the data has no correlation

## Full On Whitening

: remove covariance by dia transforming the data with diagonalizes the covaria

## find the matrix W that diagonalized $\Sigma$

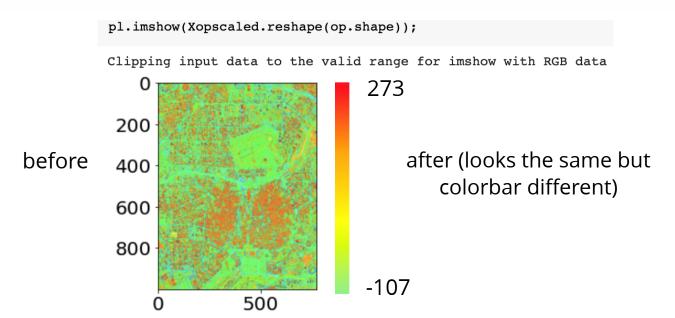
```
from zca import ZCA
import numpy as np
X = np.random.random((10000, 15)) # data
array
trf = ZCA().fit(X)
X whitened = trf.transform(X)
X reconstructed =
trf.inverse transform(X whitened)
```

## Generic preprocessing: other common

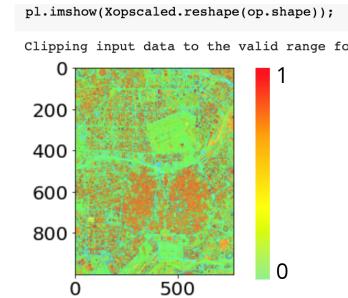
for image processing (e.g. segmentation) often you need to mimmax preprocess

```
from sklearn import preprocessing

Nopscaled = preprocessing.minmax_scale(image_pixels.astype(float), axis=1)
```



Xopscaled.reshape(op.shape)[200, 700]



#### https://www.nature.com/articles/nmeth.3812.pdf

#### POINTS OF SIGNIFICANCE

# Analyzing outliers: influential or nuisance?

Some outliers influence the regression fit more than others.

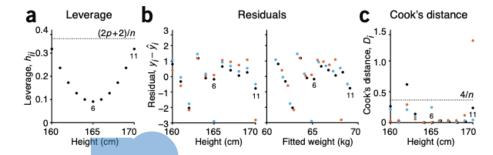
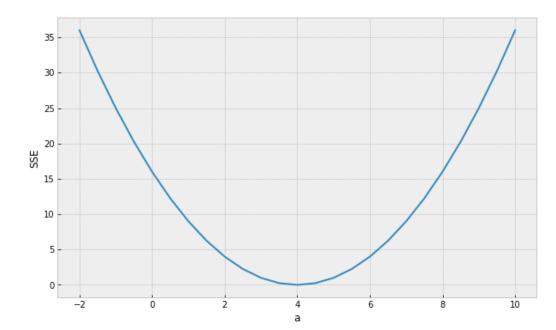


Figure 2 | The leverage, residual and Cook's distance of an observation are used to assess the robustness of the fit. (a) The leverage of an observation tells us about its potential to influence the fit and increases as the square

# https://github.com/fedhere/FDSFE\_FBianco/blob/main/HW5/Multiple\_Linear\_Regression.ipynb

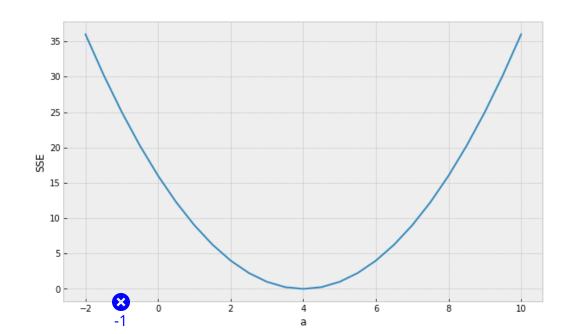




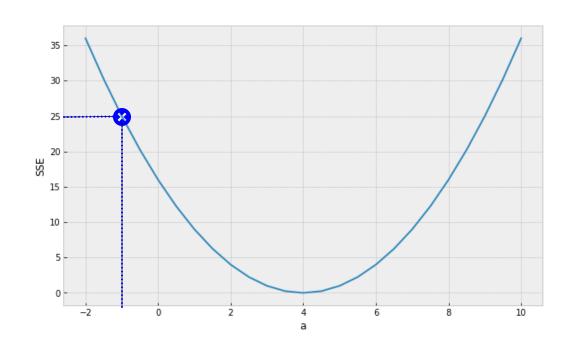


assume a simpler line model y = ax(b = 0) so we only need to find the "best" parameter a

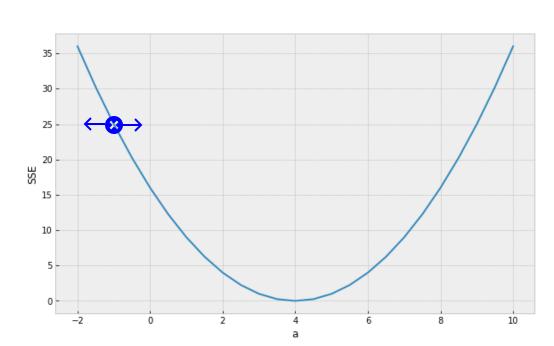
1. choose initial value for a



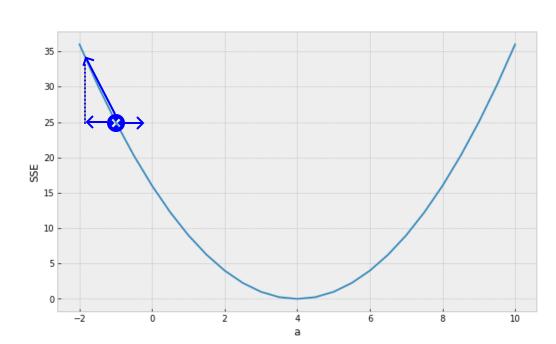
- 1. choose initial value for *a*
- 2. calculate the SSE



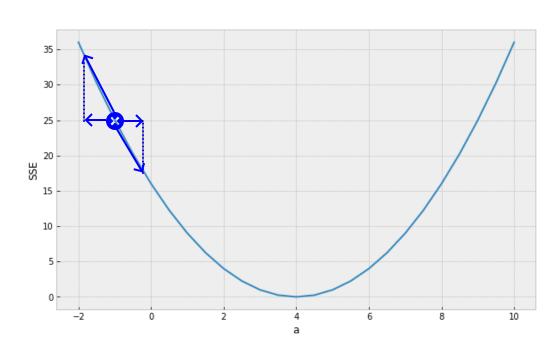
- 1. choose initial value for *a*
- 2. calculate the SSE
- 3. calculate best direction to go to decrease the SSE



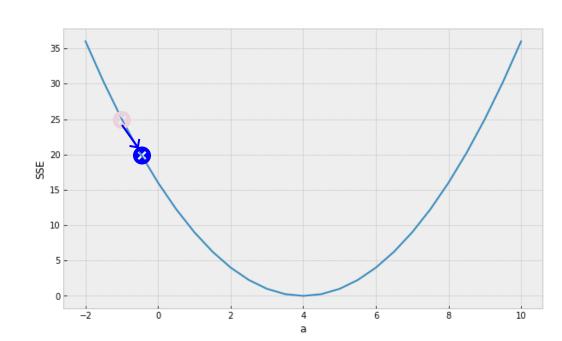
- 1. choose initial value for *a*
- 2. calculate the SSE
- 3. calculate best direction to go to decrease the SSE



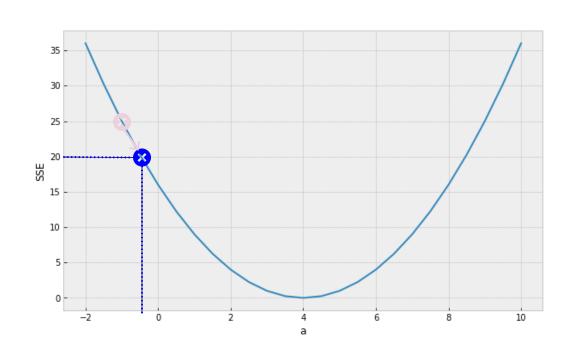
- 1. choose initial value for *a*
- 2. calculate the SSE
- 3. calculate best direction to go to decrease the SSE



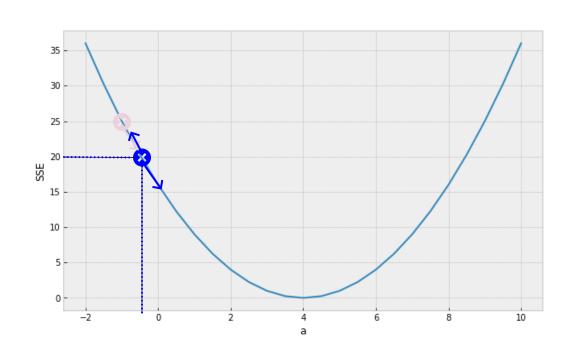
- 1. choose initial value for  $\alpha$
- 2. calculate the SSE
- 3. calculate best direction to go to decrease the SSE
- 4. step in that direction



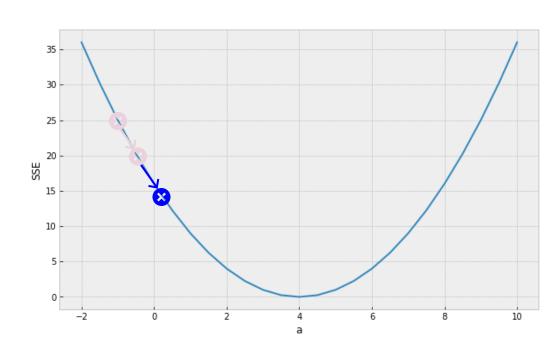
- 1. choose initial value for *a*
- 2. calculate the SSE
- 3. calculate best direction to go to decrease the SSE
- 4. step in that direction
- 5. go back to step 2 and repeat



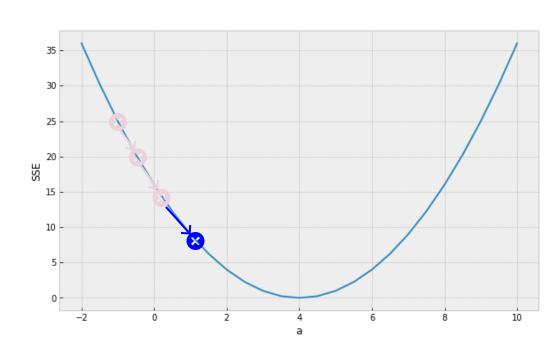
- 1. choose initial value for *a*
- 2. calculate the SSE
- 3. calculate best direction to go to decrease the SSE
- 4. step in that direction
- 5. go back to step 2 and repeat



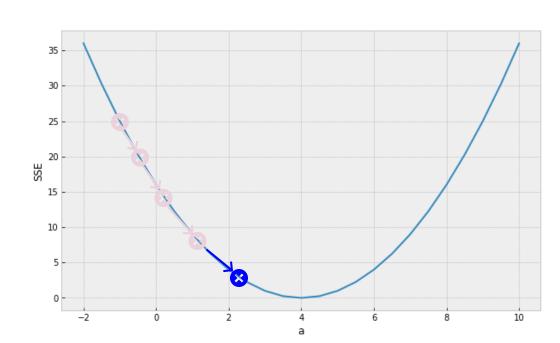
- 1. choose initial value for  $\alpha$
- 2. calculate the SSE
- 3. calculate best direction to go to decrease the SSE
- 4. step in that direction
- 5. go back to step 2 and repeat



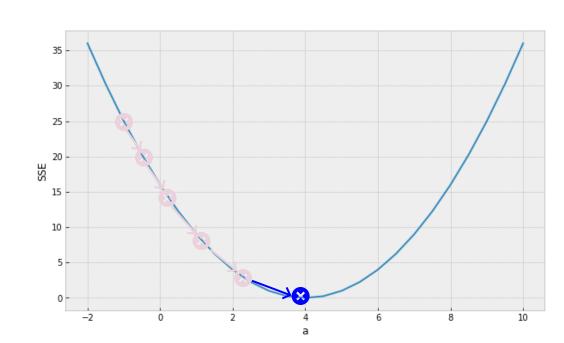
- 1. choose initial value for *a*
- 2. calculate the SSE
- 3. calculate best direction to go to decrease the SSE
- 4. step in that direction
- 5. go back to step 2 and repeat



- 1. choose initial value for *a*
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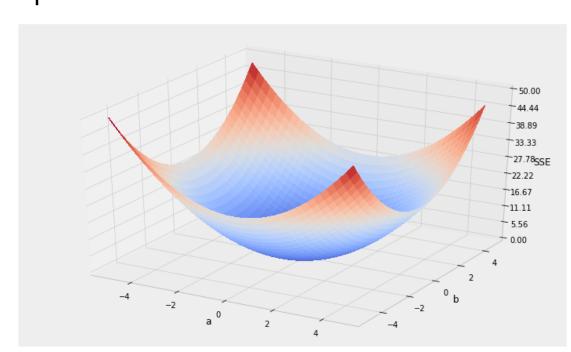


- 1. choose initial value for *a*
- 2. calculate the SSE
- 3. calculate best direction to go to decrease the SSE
- 4. step in that direction
- 5. go back to step 2 and repeat



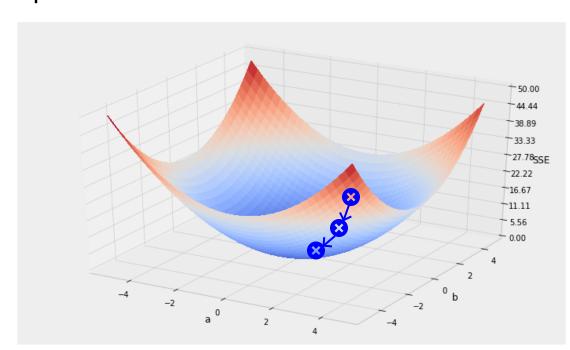
for a line model y = ax + bwe need to find the "best" parameters a and b

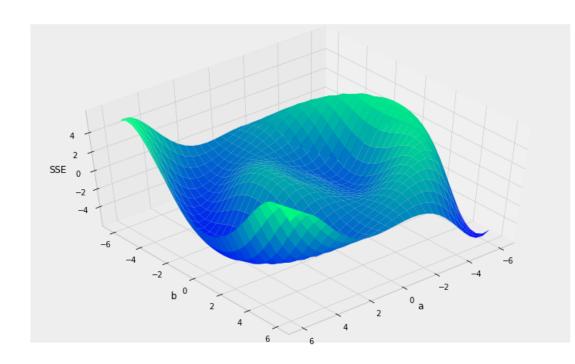
- 1. choose initial value for a & b
- 2. calculate the SSE
- 3. calculate best direction to go to decrease the SSE
- 4. step in that direction
- 5. go back to step 2 and repeat



for a line model y = ax + bwe need to find the "best" parameters a and b

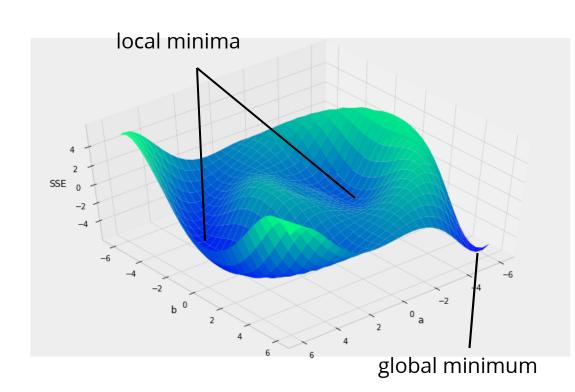
- 1. choose initial value for a & b
- 2. calculate the SSE
- 3. calculate best direction to go to decrease the SSE
- 4. step in that direction
- 5. go back to step 2 and repeat



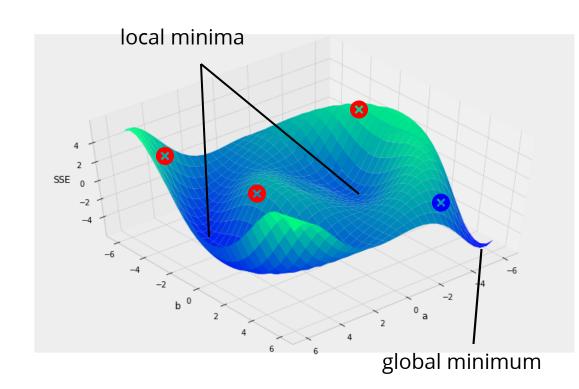


#### Things to consider:

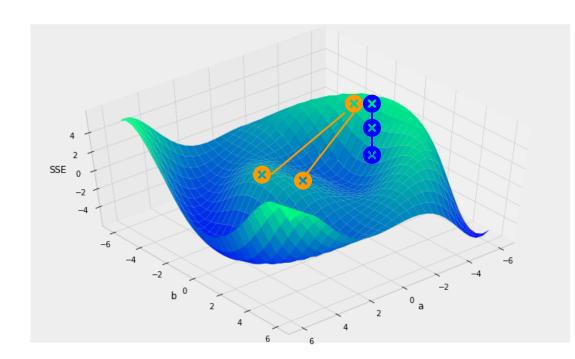
- local vs. global minima



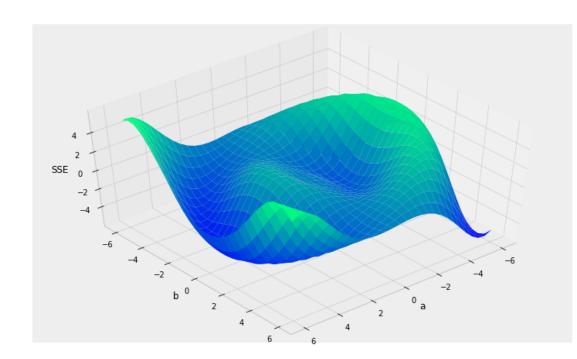
- local vs. global minima
- initialization: choosing starting spot?



- local vs. global minima
- initialization: choosing starting spot?
- learning rate: how far to step?

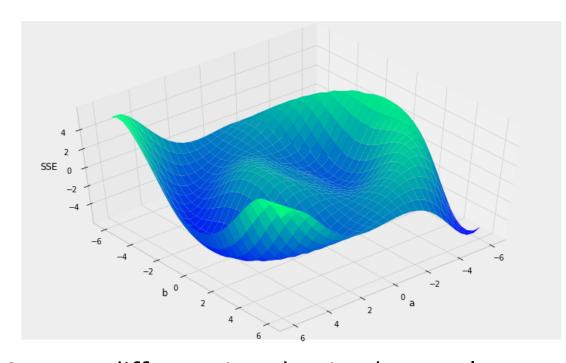


- local vs. global minima
- initialization: choosing starting spot?
- learning rate: how far to step?
- stopping criterion: when to stop?



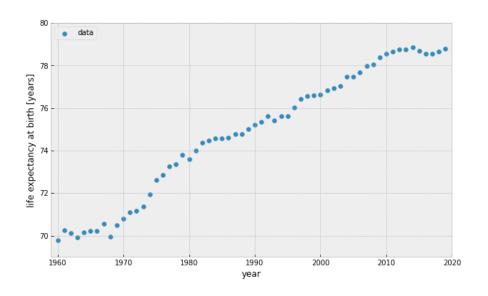
#### Things to consider:

- local vs. global minima
- initialization: choosing starting spot?
- learning rate: how far to step?
- stopping criterion: when to stop?

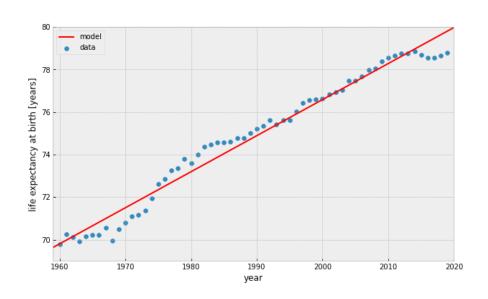


<u>Stochastic</u> Gradient Descent (SGD): use a different (random) sub-sample of the data at each iteration

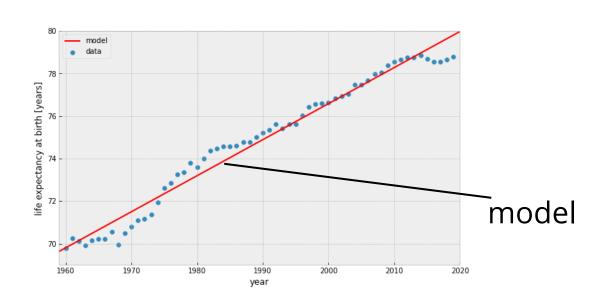




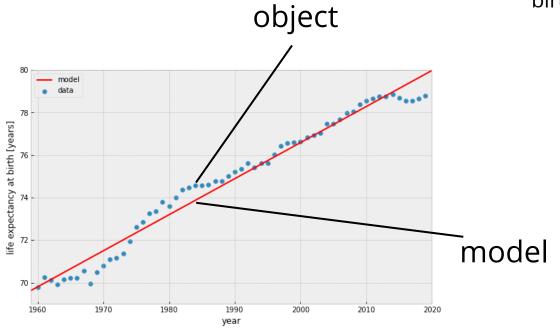
	year	leb		
0	1960	69.770732		
1	1961	70.270732 70.119512		
2	1962			
3	1963	69.917073		
4	1964	70.165854		
5	1965	70.214634		
6	1966	70.212195		
		•		
54	2014	78.841463		
55	2015	78.690244		
56	2016	78.539024		
57	2017	78.539024		
58	2018	78.639024		
59	2019	78.787805		



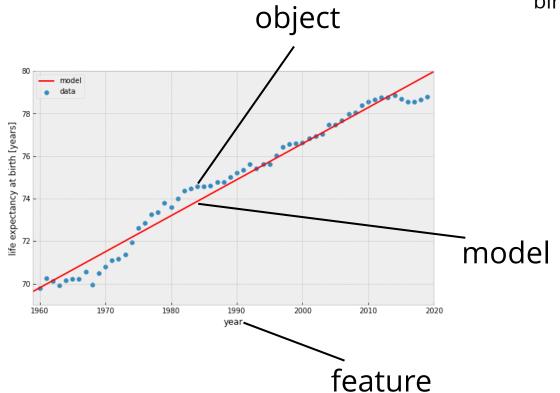
year	leb		
1960	69.770732		
1961	70.270732 70.119512		
1962			
1963	69.917073		
1964	70.165854		
1965	70.214634		
1966	70.212195		
	•		
2014	78.841463		
2015	78.690244		
2016	78.539024		
2017	78.539024		
2018	78.639024		
2019	78.787805		
	1960 1961 1962 1963 1964 1965 1966 2014 2015 2016 2017 2018		



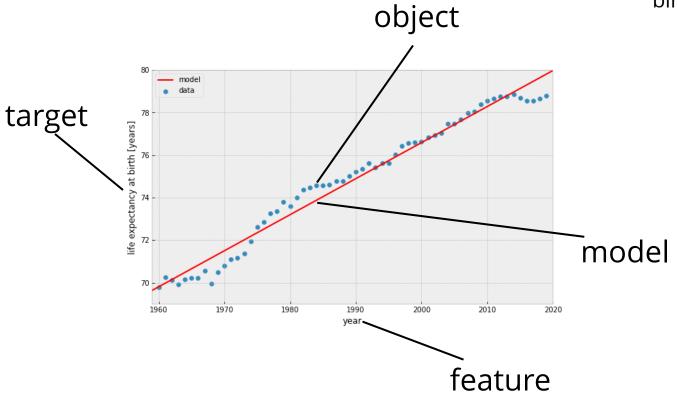
	year	leb		
0	1960	69.770732		
1	1961	70.270732		
2	1962	70.119512		
3	1963	69.917073		
4	1964	70.165854		
5	1965 70.21	70.214634		
6	1966	70.212195		
		•		
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57	2017	78.539024		
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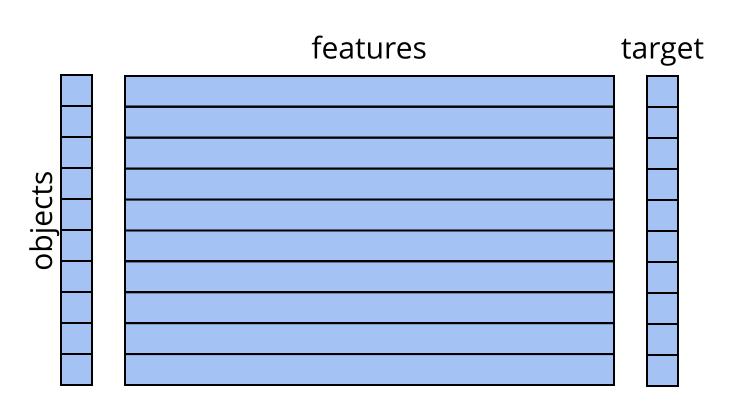
	year	leb		
0	1960	69.770732		
1	1961	70.270732		
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5	1965	70.214634		
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	year	leb		
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1	1961	70.270732		
2	1962	70.119512		
3	1963	69.917073		
4	1964	70.165854		
5	1965	70.214634		
6	1966	70.212195		
		•		
54	2014	78.841463		
55	2015	78.690244 78.539024		
56	2016			
57	2017	78.539024		
58	2018	78.639024 78.787805		
59	2019			



	year	leb		
0	1960	69.770732 70.270732		
1	1961			
2	1962	70.119512		
3	1963	69.917073		
4	1964	70.165854		
5	1965	70.214634		
6	1966	70.212195		
		•		
54	2014	78.841463		
55	2015	78.690244		
56	2016	78.539024		
57	2017	78.539024		
58	2018	78.639024		
59	2019	78.787805		



	Ī	features			target	
bjects		transaction_date	house_age	distance_nearest_MRT_station	convenience_stores	house_price_unit_area
	0	2012.917	32.0	84.87882	10	37.9
	1	2012.917	19.5	306.59470	9	42.2
	2	2013.583	13.3	561.98450	5	47.3
	3	2013.500	13.3	561.98450	5	54.8
	4	2012.833	5.0	390.56840	5	43.1
0	409	2013.000	13.7	4082.01500	0	15.4
	410	2012.667	5.6	90.45606	9	50.0
	411	2013.250	18.8	390.96960	7	40.6
	412	2013.000	8.1	104.81010	5	52.5
	413	2013.500	6.5	90.45606	9	63.9

1 feature

$$y = ax + b$$

- 1 target
- 2 parameters

- 1 feature
- 1 target
- 2 parameters

- y = ax + b
- $y=\beta_0+\beta_1x_1$

- 1 feature
- y = ax + b

- 1 target
- 2 parameters

 $y=eta_0+eta_1x_1$ 

# Multiple Linear Regression

- *n* features
- 1 target

- 1 feature
- 1 target
- 2 parameters

$$y = ax + b$$

 $y=\beta_0+\beta_1x_1$ 

# Multiple Linear Regression

- *n* features
- 1 target
- *n*+1 parameters
- $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + ... + \beta_n x_n$

- 1 feature
- 1 target
- 2 parameters

$$y = ax + b$$

 $y=eta_0+eta_1x_1$ 

# Multiple Linear Regression

- *n* features
- 1 target
- *n*+1 parameters

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + ... + \beta_n x_n$$

$$y=\sum_{i=0}^n eta_i x_i$$
 ;  $x_0=ec{1}$