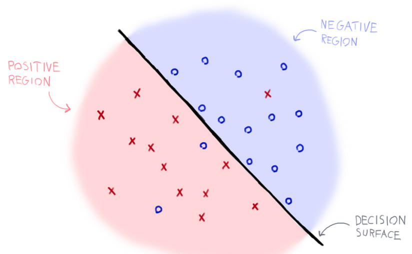
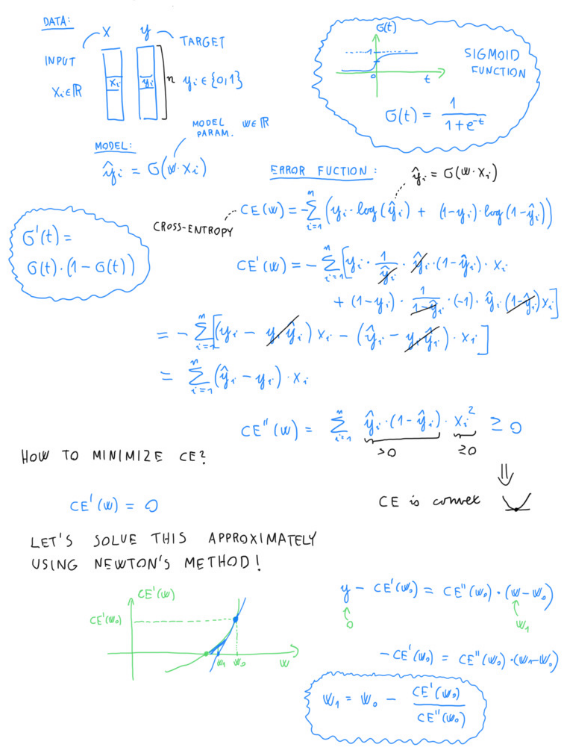
Univariate [Logistic Regression (https://en.wikipedia.org/wiki/Logistic_regression)](https://en.wikipedia.org/wiki/Logistic_regression)

- Logistic regression is an algorithm for **classification**.
- Logistic regression builds a **linear model** that separates the two classes by a hyperplane.



For simplicity, let' discuss first the **univariate** case, with a **binary target** variable and **no bias** term.


G(t)
t
0
1
CE'(w)
CE'(w₀)
w₁
w₀
w

DATA:

INPUT X, $x_i \in \mathbb{R}$

TARGET y, $y_i \in \{0,1\}$, n

MODEL:

$$\hat{y}_i = \sigma(w \cdot x_i)$$

MODEL PARAM. $w \in \mathbb{R}$

SIGMOID FUNCTION

$$\sigma(t) = \frac{1}{1+e^{-t}}$$

$$\sigma'(t) = \sigma(t)\cdot(1-\sigma(t))$$

ERROR FUCTION:

$\hat{y}_i = \sigma(w \cdot x_i)$

CROSS-ENTROPY

$$CE(w) = -\sum_{i=1}^{m}\left(y_i \cdot \log(\hat{y}_i) + (1-y_i)\cdot \log(1-\hat{y}_i)\right)$$

$$CE'(w) = -\sum_{i=1}^{m}\Big[y_i \cdot \frac{1}{\cancel{\hat{y}_i}} \cdot \cancel{\hat{y}_i}\cdot(1-\hat{y}_i)\cdot x_i + (1-y_i)\cdot\frac{1}{\cancel{1-\hat{y}_i}}\cdot(-1)\cdot\hat{y}_i\cancel{(1-\hat{y}_i)}x_i\Big]$$

$$= -\sum_{i=1}^{m}\Big[(y_i - \cancel{y_i\hat{y}_i})x_i - (\hat{y}_i - \cancel{y_i\hat{y}_i})\cdot x_i\Big]$$

$$= \sum_{i=1}^{m}(\hat{y}_i - y_i)\cdot x_i$$

$$CE''(w) = \sum_{i=1}^{m}\underbrace{\hat{y}_i\cdot(1-\hat{y}_i)}_{>0}\cdot\underbrace{x_i^2}_{\geq 0} \geq 0$$

$$\Downarrow$$

CE is convex

HOW TO MINIMIZE CE?

$$CE'(w) = 0$$

LET'S SOLVE THIS APPROXIMATELY USING NEWTON'S METHOD!

$$\underset{0}{y} - CE'(w_0) = CE''(w_0)\cdot(\underset{w_1}{w} - w_0)$$

$$-CE'(w_0) = CE''(w_0)\cdot(w_1 - w_0)$$

$$\boxed{w_1 = w_0 - \frac{CE'(w_0)}{CE''(w_0)}}$$

The Programming Exam Problem

In [1]:

```
import pandas as pd
data = [
    {'name': 'David Beckham',    'study_time': 0,   'result': 0},
    {'name': 'Jessica Scott',    'study_time': 7,   'result': 1},
    {'name': 'Jack Johnson',     'study_time': 3.5, 'result': 0},
    {'name': 'Scunner Campbell', 'study_time': 6,   'result': 0},
    {'name': 'Plain Jane ',      'study_time': 3,   'result': 1},
    {'name': 'Archie Gillis',    'study_time': 15,  'result': 1},
]
df = pd.DataFrame(data)
df
```

Out[1]:

	name	study_time	result
0	David Beckham	0.0	0
1	Jessica Scott	7.0	1
2	Jack Johnson	3.5	0
3	Scunner Campbell	6.0	0
4	Plain Jane	3.0	1
5	Archie Gillis	15.0	1

The above toy data set contains 2 attributes of 6 students:

- Hours spent on preparing for the exam.
- Did the student pass the exam? (0=no, 1=yes)

Exercise 1: Train a univariate logistic regression model that estimates the `result` column from the `study_time` column!

In [2]:

```
x = df['study_time'].values # input vector
y = df['result'].values     # target vector

# subtract mean from inpute
xm = x.mean()
x -= xm

print(x,y)
```

```
[-5.75  1.25 -2.25  0.25 -2.75  9.25] [0 1 0 0 1 1]
```

In [3]:

```
import numpy as np
def sigmoid(t):
    return 1/(1+np.exp(-t))
```

In [4]:

```
# sigmoid (x)

w = 0 # initial model parameter

yhat = sigmoid(x*w)
yhat
```

Out[4]:

```
array([0.5, 0.5, 0.5, 0.5, 0.5, 0.5])
```

In [5]:

```
ce_i = ((yhat - y) * x).sum()

ce_ii= (yhat * (1-yhat) * x**2).sum()

ce_i, ce_ii
```

Out[5]:

```
(-7.75, 33.21875)
```

In [6]:

```
# 1st Newton's step

w -= ce_i / ce_ii
w
```

Out[6]:

```
0.2333019755409219
```

In [7]:

```
yhat = sigmoid(x*w)
yhat
```

Out[7]:

```
array([0.20726573, 0.57239452, 0.37170029, 0.51457724, 0.34488937,
       0.896418  ])
```

In [8]:

```
# 2nd Newton's step

w -= ce_i / ce_ii
w
```

Out[8]:

```
0.4666039510818438
```

In [9]:

```
yhat = sigmoid(x*w)
yhat
```

Out[9]:

```
array([0.06398561, 0.64181602, 0.2592522 , 0.52912972, 0.21701265,
       0.98682389])
```

In [10]:

```
# Newton steps in for loop
for it in range(10):
    yhat = sigmoid(x*w)
    ce = -(np.log(yhat)* y + np.log(1-yhat) * (1-y)).sum()
    ce_i = ((yhat - y) * x).sum()
    ce_ii= (yhat * (1-yhat) * x**2).sum()
    w -= ce_i / ce_ii
    print(f'w = {w:.9f} CE(w) = {ce:.9}')
    print(yhat)
```

```
w = 0.333032246 CE(w) = 3.103909
[0.06398561 0.64181602 0.2592522  0.52912972 0.21701265 0.98682389]
w = 0.359110223 CE(w) = 3.06404697
[0.1284274  0.60259521 0.32096893 0.5208025  0.28580655 0.95608321]
w = 0.360846759 CE(w) = 3.06039476
[0.11255707 0.61037476 0.30831727 0.52242933 0.27139565 0.96516813]
w = 0.360853783 CE(w) = 3.06038094
[0.11156354 0.61089086 0.30748466 0.52253764 0.27045238 0.96570413]
w = 0.360853783 CE(w) = 3.06038094
[0.11155953 0.61089295 0.30748129 0.52253808 0.27044857 0.96570628]
w = 0.360853783 CE(w) = 3.06038094
[0.11155953 0.61089295 0.30748129 0.52253808 0.27044857 0.96570628]
w = 0.360853783 CE(w) = 3.06038094
[0.11155953 0.61089295 0.30748129 0.52253808 0.27044857 0.96570628]
w = 0.360853783 CE(w) = 3.06038094
[0.11155953 0.61089295 0.30748129 0.52253808 0.27044857 0.96570628]
w = 0.360853783 CE(w) = 3.06038094
[0.11155953 0.61089295 0.30748129 0.52253808 0.27044857 0.96570628]
w = 0.360853783 CE(w) = 3.06038094
[0.11155953 0.61089295 0.30748129 0.52253808 0.27044857 0.96570628]
```

In [11]:

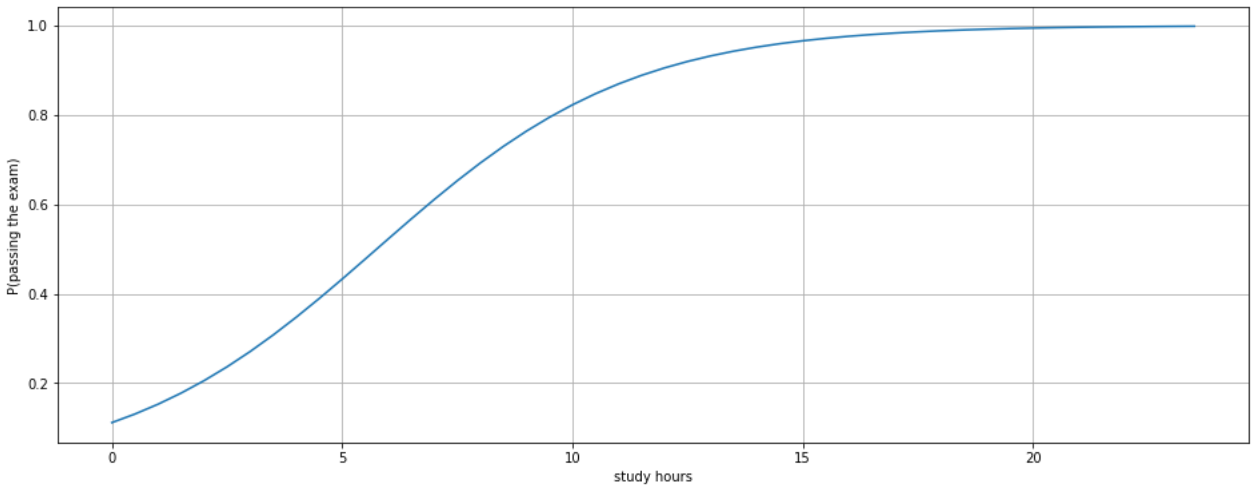
```
ce = -(np.log(yhat)* y + np.log(1-yhat) * (1-y)).sum()
```

In [12]:

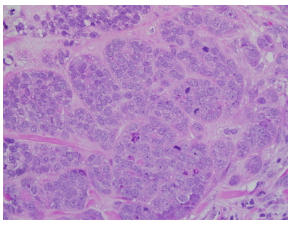
```
# Display the probability of passing the exam (according to the model)
# as a function of the study hours!
import matplotlib.pyplot as plt
x2 = np.arange(0, 24, 0.5)
yhat2 = sigmoid((x2 - xm) * w)
plt.figure(figsize=(16,6))
plt.plot(x2, yhat2)
plt.grid(True)
plt.xlabel('study hours')
plt.ylabel('P(passing the exam)')
```

Out[12]:

```
Text(0, 0.5, 'P(passing the exam)')
```



The Wisconsin Breast Cancer Problem



The Wisconsin Breast Cancer data set contains the attributes of 699 suspicious lesions in tissue microscopy images. The raw data is contained in wisconsin_data.txt (../_data/wisconsin_data.txt), the description can be read in wisconsin_names.txt (../_data/wisconsin_names.txt). The task is to estimate if the lesion is malicious (4) or benign (2), based on the image attributes of the lesion. Therefore the task is a binary classification problem.

Exercise 2: Train a univariate logistic regression model for each input feature separately, and measure the *average* cross-entropy of the models! Use the full data set both for training and evaluation!

In [13]:

```
# Column names.
names = [
    'Sample_code_number',
    'Clump_Thickness',
    'Uniformity_of_Cell_Size',
    'Uniformity_of_Cell_Shape',
    'Marginal_Adhesion',
    'Single_Epithelial_Cell_Size',
    'Bare_Nuclei',
    'Bland_Chromatin',
    'Normal_Nucleoli',
    'Mitoses',
    'Class'
]
```

In [14]:

```
df = pd.read_csv('wisconsin_data.txt', sep=',', names=names, na_values='?')
# we found some ? values, so we replaced it with nan
df
```

Out[14]:

	Sample_code_number	Clump_Thickness	Uniformity_of_Cell_Size	Uniformity_of_Cell_Shape	Marginal_Adhesion	Single_Epithelial_Cell_Size
0	1000025	5	1	1	1	2
1	1002945	5	4	4	5	7
2	1015425	3	1	1	1	2
3	1016277	6	8	8	1	3
4	1017023	4	1	1	3	2
...	...	...	...	...	...	...
694	776715	3	1	1	1	3
695	841769	2	1	1	1	2
696	888820	5	10	10	3	7
697	897471	4	8	6	4	3
698	897471	4	8	8	5	4

699 rows × 11 columns

In [15]:

```
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 699 entries, 0 to 698
Data columns (total 11 columns):
 #   Column                       Non-Null Count  Dtype  
---  ------                       --------------  -----  
 0   Sample_code_number           699 non-null    int64  
 1   Clump_Thickness              699 non-null    int64  
 2   Uniformity_of_Cell_Size      699 non-null    int64  
 3   Uniformity_of_Cell_Shape     699 non-null    int64  
 4   Marginal_Adhesion            699 non-null    int64  
 5   Single_Epithelial_Cell_Size  699 non-null    int64  
 6   Bare_Nuclei                  683 non-null    float64
 7   Bland_Chromatin              699 non-null    int64  
 8   Normal_Nucleoli              699 non-null    int64  
 9   Mitoses                      699 non-null    int64  
 10  Class                        699 non-null    int64  
dtypes: float64(1), int64(10)
memory usage: 60.2 KB
```

In [16]:

```
df.Bare_Nuclei.unique()
```

Out[16]:

```
array([ 1., 10.,  2.,  4.,  3.,  9.,  7., nan,  5.,  8.,  6.])
```

In [17]:

```
# replace the nan with the mean
df['Bare_Nuclei'].fillna(df['Bare_Nuclei'].mean(), inplace=True)
df
```

Out[17]:

	Sample_code_number	Clump_Thickness	Uniformity_of_Cell_Size	Uniformity_of_Cell_Shape	Marginal_Adhesion	Single_Epithelial_Cell_Size
0	1000025	5	1	1	1	2
1	1002945	5	4	4	5	7
2	1015425	3	1	1	1	2
3	1016277	6	8	8	1	3
4	1017023	4	1	1	3	2
...	...	...	...	...	...	...
694	776715	3	1	1	1	3
695	841769	2	1	1	1	2
696	888820	5	10	10	3	7
697	897471	4	8	6	4	3
698	897471	4	8	8	5	4

699 rows × 11 columns

In [18]:

```
df.Bare_Nuclei.unique()
```

Out[18]:

```
array([ 1.        , 10.        ,  2.        ,  4.        ,  3.        ,
        9.        ,  7.        ,  3.54465593,  5.        ,  8.        ,
        6.        ])
```

In [19]:

```
df.describe().T
```

Out[19]:

	count	mean	std	min	25%	50%	75%	max
Sample_code_number	699.0	1.071704e+06	617095.729819	61634.0	870688.5	1171710.0	1238298.0	13454352.0
Clump_Thickness	699.0	4.417740e+00	2.815741	1.0	2.0	4.0	6.0	10.0
Uniformity_of_Cell_Size	699.0	3.134478e+00	3.051459	1.0	1.0	1.0	5.0	10.0
Uniformity_of_Cell_Shape	699.0	3.207439e+00	2.971913	1.0	1.0	1.0	5.0	10.0
Marginal_Adhesion	699.0	2.806867e+00	2.855379	1.0	1.0	1.0	4.0	10.0
Single_Epithelial_Cell_Size	699.0	3.216023e+00	2.214300	1.0	2.0	2.0	4.0	10.0
Bare_Nuclei	699.0	3.544656e+00	3.601852	1.0	1.0	1.0	5.0	10.0
Bland_Chromatin	699.0	3.437768e+00	2.438364	1.0	2.0	3.0	5.0	10.0
Normal_Nucleoli	699.0	2.866953e+00	3.053634	1.0	1.0	1.0	4.0	10.0
Mitoses	699.0	1.589413e+00	1.715078	1.0	1.0	1.0	1.0	10.0
Class	699.0	2.689557e+00	0.951273	2.0	2.0	2.0	4.0	4.0

In [20]:

```
# target vector
y = df['Class'].values//2-1
y
```

Out[20]:

```
array([0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 1, 0, 1, 1, 0, 0, 1, 0, 1, 1,
       0, 1, 0, 1, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 1, 0, 1, 1, 0, 1, 1, 1,
       1, 0, 1, 0, 0, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 0, 1, 1, 0, 1,
       0, 1, 1, 0, 0, 1, 0, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 0, 1, 1, 1, 1, 1, 0, 1,
       0, 1, 1, 1, 0, 0, 0, 1, 0, 0, 0, 0, 1, 1, 1, 0, 1, 0, 1, 0, 0, 0,
       1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 1, 0, 0, 1, 0, 1, 1, 0,
       0, 1, 0, 0, 0, 1, 1, 0, 0, 0, 0, 0, 1, 1, 0, 0, 0, 0, 0, 1, 1, 1,
       0, 1, 0, 1, 0, 0, 0, 1, 1, 0, 1, 1, 1, 0, 1, 1, 0, 0, 0, 0, 0, 0,
       0, 0, 1, 1, 0, 0, 0, 1, 1, 0, 0, 0, 1, 1, 0, 1, 1, 1, 0, 0, 1, 0,
       0, 1, 1, 1, 1, 0, 1, 1, 0, 1, 1, 1, 0, 1, 0, 0, 1, 1, 1, 1, 0, 0,
       0, 0, 0, 0, 1, 1, 0, 0, 0, 1, 0, 1, 1, 1, 0, 0, 0, 0, 1, 1, 1, 1,
       1, 0, 1, 1, 1, 0, 1, 0, 1, 1, 0, 0, 0, 0, 0, 1, 0, 0, 1, 1, 1, 1,
       1, 0, 1, 1, 0, 0, 1, 1, 0, 1, 0, 0, 0, 1, 1, 0, 1, 0, 1, 1, 0, 0,
       1, 0, 0, 0, 1, 0, 0, 0, 1, 1, 0, 0, 1, 0, 0, 1, 0, 0, 1, 0, 1, 1,
       1, 0, 0, 1, 1, 0, 1, 0, 0, 1, 1, 0, 0, 0, 1, 0, 0, 0, 1, 1, 0, 0,
       0, 1, 0, 0, 1, 1, 1, 1, 1, 1, 0, 0, 0, 0, 1, 1, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 1, 0, 0, 0, 0, 1, 0, 0, 0, 0,
       0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 1, 0, 1, 0,
       0, 0, 0, 1, 0, 0, 0, 1, 0, 1, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, 0,
       1, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 1, 0, 1, 1, 1, 0, 0, 0, 0,
       0, 0, 0, 1, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 1, 1,
       0, 0, 0, 1, 1, 1, 0, 1, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       1, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, 0, 1, 0, 0, 1, 1, 0, 0, 0, 0,
       0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 1,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 1, 1, 1, 1,
       0, 0, 1, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, 0, 1, 0, 1, 0, 1, 1, 1, 0,
       1, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 0, 0, 1, 0, 1, 1, 1, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 1, 0, 0, 1, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 1, 1, 1])
```

In [21]:

```
def fit_logreg(x, y, niter=10):
    w = 0 # initial model parameter
    yhat = sigmoid(x*w)
    for it in range(niter):
        ce = -(np.log(yhat)* y + np.log(1-yhat) * (1-y)).sum()
        ce_i = ((yhat - y) * x).sum()
        ce_ii= (yhat * (1-yhat) * x**2).sum()
        w -= ce_i / ce_ii
        yhat = sigmoid(x*w)
        return w, yhat
```

In [22]:

```

def avg_ce(y, yhat):
    ce = -(np.log(yhat)* y + np.log(1-yhat) * (1-y)).sum()
    return ce/len(y)
```

In [23]:

```
for column in names[1:-1]:
    x = df[column]
    w, yhat = fit_logreg(x, y)
    cem = avg_ce(y, yhat)
    print(column)
    print(f'w = {w:.9f} CE(w) = {ce:.9}')
    print(f'CEm(w) = {cem:.9}')
```

```
Clump_Thickness
w = 0.039632874 CE(w) = 3.06038094
CEm(w) = 0.687739208
Uniformity_of_Cell_Size
w = 0.146180893 CE(w) = 3.06038094
CEm(w) = 0.639204697
Uniformity_of_Cell_Shape
w = 0.137765798 CE(w) = 3.06038094
CEm(w) = 0.645652807
Marginal_Adhesion
w = 0.127165565 CE(w) = 3.06038094
CEm(w) = 0.659383857
Single_Epithelial_Cell_Size
w = 0.057453999 CE(w) = 3.06038094
CEm(w) = 0.6868162
Bare_Nuclei
w = 0.132577858 CE(w) = 3.06038094
CEm(w) = 0.633926393
Bland_Chromatin
w = 0.077189590 CE(w) = 3.06038094
CEm(w) = 0.679762996
Normal_Nucleoli
w = 0.134160274 CE(w) = 3.06038094
CEm(w) = 0.651733288
Mitoses
w = 0.071746531 CE(w) = 3.06038094
CEm(w) = 0.689591602
```

In [24]:

```
# 2nd solution Normalized input
def logreg_predict(x, w):
    return sigmoid(x * w)

def logreg_fit(x, y, niter=10):
    w = 0 # initial model parameter
    for it in range(niter):
        yhat = logreg_predict(x, w)
        ce_i = ((yhat - y) * x).sum()
        ce_ii = (yhat * (1 - yhat) * x**2).sum()
        w -= ce_i / ce_ii # Newton step
    return w

def avg_cross_entropy(y, yhat):
    ce = -(np.log(yhat) * y + np.log(1 - yhat) * (1 - y)).sum()
    return ce / len(y)

for column in names[1:-1]:
    se = df[column]
    x = (se - se.mean()).values # input vector
    w = logreg_fit(x, y)
    yhat = logreg_predict(x, w)
    ace = avg_cross_entropy(y, yhat)
    print(f'{column:30} AvgCE={ace:.9f} w={w:.9f}')
```

```
Clump_Thickness                AvgCE=0.390611001 w=0.905912818
Uniformity_of_Cell_Size        AvgCE=0.199170002 w=1.572130112
Uniformity_of_Cell_Shape       AvgCE=0.211668062 w=1.524221657
Marginal_Adhesion              AvgCE=0.359316116 w=1.107418964
Single_Epithelial_Cell_Size    AvgCE=0.351132841 w=1.537879946
Bare_Nuclei                    AvgCE=0.265288430 w=0.979151501
Bland_Chromatin                AvgCE=0.303804235 w=1.542319399
Normal_Nucleoli                AvgCE=0.355869859 w=1.004452002
Mitoses                        AvgCE=0.527654735 w=1.711238337
```

Exercise 4: Repeat the previous experiment using scikit-learn!

In [25]:

```
from sklearn.linear_model import LogisticRegression
from sklearn.metrics import log_loss

for column in names[1:-1]:
    se = df[column]
    x = (se - se.mean()).values # input vector
    cl = LogisticRegression(fit_intercept=False, C=1e12) # define model
    X = x.reshape((-1,1))
    cl.fit(X, y)                                       # train model
    w = cl.coef_[0,0]                                  # extract moddel parameter
    yhat = cl.predict_proba(X)[:,1]                    # make probability prediction
    ace = log_loss(y, yhat)                            # compute average cross entropy

    print(f'{column:30} AvgCE={ace:.9f} w={w:.9f}')
```

```
Clump_Thickness                AvgCE=0.390611001 w=0.905912814
Uniformity_of_Cell_Size        AvgCE=0.199170002 w=1.572130109
Uniformity_of_Cell_Shape       AvgCE=0.211668062 w=1.524221656
Marginal_Adhesion              AvgCE=0.359316116 w=1.107418964
Single_Epithelial_Cell_Size    AvgCE=0.351132841 w=1.537879938
Bare_Nuclei                    AvgCE=0.265288430 w=0.979151504
Bland_Chromatin                AvgCE=0.303804235 w=1.542318627
Normal_Nucleoli                AvgCE=0.355869859 w=1.004451975
Mitoses                        AvgCE=0.527654735 w=1.711237945
```

Exercise 5: Introduce a 70-30% train-test split and re-run the experiment!

In [26]:

```python
from sklearn.model_selection import ShuffleSplit
# another way of set test size is: train_test_split
tr, te = next(ShuffleSplit(test_size=0.3, random_state=42).split(df))
tr, te
```

Out[26]:

```
(array([357, 648, 291, 420, 177, 456, 444,  83, 453, 354, 495, 575,  79,
         23,  15, 381, 292, 275, 653, 314, 519, 137, 485, 483,  33, 662,
        257,   9,  22, 543, 221, 404, 684, 334,  84, 335, 247, 582, 620,
        203, 196, 660, 327, 399,  93, 587, 294, 265, 375, 184, 636, 512,
        153,  75, 332,  68, 615, 188, 236,  88, 590, 117, 125, 571, 238,
          0, 691, 530, 630, 608, 278, 116, 228, 697, 319, 274, 692, 144,
        382, 426, 631, 500, 268, 465,  46, 261, 195, 698, 583, 107, 462,
        609, 531, 100, 350, 624, 333, 179, 304, 349, 149, 124, 551, 605,
        185, 428, 558, 689, 344, 644, 142, 141, 393, 320,  19, 172, 632,
        312, 650,  12, 305,  25, 518, 169, 479, 411, 245, 298, 434, 272,
        154, 126, 538, 341, 287, 113, 367, 173, 355,  57, 443, 222, 280,
         17, 405, 322, 255, 417, 669, 190, 439, 616, 490,  94, 180, 301,
        641, 511, 642, 451, 429,   5, 685,  45, 398, 525, 171,  16,  48,
        675, 639,   3, 449, 412, 316, 643, 283, 581, 285, 677, 225,  26,
        547, 263,  50, 364, 229,  37, 157, 237, 670, 374, 370, 175, 591,
        480, 513, 194, 593, 601, 425, 445, 448, 674, 580, 599,  67, 534,
        168, 447, 162, 309, 193, 478, 365, 383, 629, 535, 152, 488, 497,
        226, 457, 557, 103, 421, 678, 527,  74, 115, 407, 673, 119,  53,
        151, 403, 658, 207, 687, 487, 468, 537,   8, 572,  36, 452, 139,
        253, 303, 523, 526, 368,  59, 111, 597, 503, 493, 262, 586, 297,
        414, 150, 433, 576, 440, 266, 607, 359, 619,  38, 127, 423, 416,
        307, 198, 351, 494, 146, 450, 647, 522, 419, 442, 621, 147, 585,
        348, 463, 325, 186, 123, 602,  96, 143, 239, 394, 469, 197,  97,
        371, 324, 279, 293, 400, 122, 183, 202, 438, 246, 415, 618, 129,
        402, 549, 541, 219, 634, 529, 637, 536, 386, 676, 509, 267, 441,
        496, 112, 232, 606, 373, 233, 550, 317, 410, 623, 358, 258, 282,
        376, 384, 224, 683, 568, 472, 347, 505, 688, 645, 628, 594, 556,
         85, 242, 159, 524,  35, 540, 170, 596, 588, 657,  95, 563, 240,
        574, 460, 553, 611, 206, 392, 397, 589, 217,   4, 622, 546,  98,
        573, 406, 502,  47,  32, 200, 134,  27, 613, 230, 489, 378, 288,
        418, 391, 592, 498, 138,  62, 471, 128, 679, 520,  64,  14, 156,
         40, 492, 379, 187, 216,  52, 337, 295, 251, 461, 455, 696, 269,
        201, 161, 555, 401, 476, 105, 565, 389,   1, 652, 561,  80, 205,
         34, 508, 427, 454, 366,  91, 339, 564, 345, 241,  13, 315, 600,
        387, 273, 166, 693, 646, 484, 682, 504, 243, 566, 562, 189, 475,
        510,  58, 474, 560, 252,  21, 313, 459, 160, 276, 191, 385, 413,
        491, 343, 308, 661, 130, 663,  99, 372,  87, 458, 330, 214, 466,
        121, 614,  20,  71, 106, 270, 435, 102]),
 array([158, 499, 396, 155, 321, 212, 234, 289, 300, 356, 672, 328, 199,
         78, 598, 569, 446, 506, 626, 603, 360, 338, 668, 290, 284, 331,
        477,  54, 248, 223, 133, 640, 136, 109, 181, 432, 554, 482, 516,
        132, 176,  72, 254, 577, 649, 595, 666, 352,  76, 148, 346,  90,
        681,  10,  63, 635, 656, 174, 256, 667,  31, 369, 570,  77, 532,
        548, 211,  55, 135, 671, 340,   2, 227,  81, 473, 694, 665, 604,
        120, 311, 204, 244, 686, 271, 131, 680,  60, 310,  30,  69, 651,
        390,  44, 625,  70, 515, 654, 249, 209, 165, 470, 164, 507, 323,
         65, 409,  49, 118, 192,  39, 259, 422,   6, 101, 542, 299, 395,
        501, 318, 145, 486, 353, 208, 695, 361,  86, 664, 481, 633,  41,
        108, 690,  56, 424, 514,  24, 218, 431, 281, 110,  82,  51, 220,
        559, 544, 302, 552, 215, 235,  18, 250, 260, 430, 264,  61, 213,
        377,  29, 182, 306, 388, 329, 437, 296, 584, 342, 436, 579, 326,
        362, 617, 578, 231, 336, 655, 163, 286, 612, 517, 464, 277, 408,
        104, 114, 627, 545, 467,  92,   7,  89, 528, 380, 521, 539, 363,
        638, 140,  28,  43,  42,  73, 167, 210, 610,  66,  11, 659, 567,
        178, 533]))
```

In [27]:

```python
for column in names[1:-1]:
    se = df[column]
    x = (se - se.mean()).values # input vector
    cl = LogisticRegression(fit_intercept=False, C=1e12) # define model
    X = x.reshape((-1,1))
    cl.fit(X[tr], y[tr])                              # train model (on training set)
    w = cl.coef_[0,0]                                 # extract moddel parameter
    yhat = cl.predict_proba(X)[:,1]                   # make probability prediction
    ace = log_loss(y[te], yhat[te])                   # compute average cross entropy (on test set)

    print(f'{column:30} AvgCE={ace:.9f} w={w:.9f}')
```

```
Clump_Thickness                AvgCE=0.335747286 w=0.826808279
Uniformity_of_Cell_Size        AvgCE=0.176748276 w=1.515755629
Uniformity_of_Cell_Shape       AvgCE=0.217456999 w=1.535220556
Marginal_Adhesion              AvgCE=0.300066855 w=1.024555296
Single_Epithelial_Cell_Size    AvgCE=0.350178198 w=1.527215223
Bare_Nuclei                    AvgCE=0.311173420 w=1.008497031
Bland_Chromatin                AvgCE=0.306641746 w=1.453926694
Normal_Nucleoli                AvgCE=0.362623274 w=1.024082073
Mitoses                        AvgCE=0.491826787 w=1.562289264
```

Multivariate Logistic Regression

The previous approach can be generalized to allows multiple input features.

- model's prediction: $\hat{y} = \sigma(Xw)$
- objective function: $CE(w) = -\log(\hat{y})^T y - \log(1-\hat{y})^T(1-y)$
- gradient vector: $\frac{d}{dw}CE(w) = X^T(\hat{y} - y)$
- Hessian matrix: $\left(\frac{d}{dw}\right)^2 CE(w) = X^T \mathrm{diag}\left(\hat{y}(1-\hat{y})\right) X$
- Newton-step: $w_{\mathrm{new}} = w - \left[\left(\frac{d}{dw}\right)^2 CE(w)\right]^{-1} \left[\frac{d}{dw}CE(w)\right]$

Similarly to linear regression, the bias term can be handled by introducing a constant 1 feature.

Exercise 6: Train a multivariate logistic regression model on the training set and measure its cross-entropy on the test set! Implement the training algorithm without using scikit-learn!

In [28]:

```python
# input matrix
X = df[names[1:-1]].values
# target vector
y = df['Class'].values//2-1
print(X.shape)

# initial model
w = np.zeros(X.shape[1])

# prediction
yhat = sigmoid(X @ w)

# gradient of cross-entropy
g = X.T @ (yhat - y)
g
```

```
(699, 9)
```

Out[28]:

```
array([-190.        , -488.5       , -460.        , -356.        ,
       -153.        , -591.23206442, -239.5       , -411.        ,
        -68.5       ])
```

In [30]:

```
# Hessian matrix of cross-entropy
H = X.T * (yhat * (1 - yhat)) @ X
H
```

Out[30]:

```
array([[4794.        , 3386.75      , 3432.        , 2849.25      ,
        3050.5       , 3775.85285505, 3323.        , 3017.25      ,
        1522.        ],
       [3386.75      , 3341.75      , 3192.        , 2610.25      ,
        2648.       , 3258.81039531, 2864.25      , 2745.75      ,
        1289.5       ],
       [3432.        , 3192.        , 3339.        , 2584.75      ,
        2629.        , 3312.26354319, 2857.5       , 2746.25      ,
        1281.25       ],
       [2849.25      , 2610.25      , 2584.75      , 2799.5       ,
        2239.        , 2932.19875549, 2496.25      , 2324.25      ,
        1136.5       ],
       [3050.5       , 2648.        , 2629.        , 2239.        ,
        2663.        , 2801.06039531, 2512.5       , 2353.25      ,
        1210.75       ],
       [3775.85285505, 3258.81039531, 3312.26354319, 2932.19875549,
        2801.06039531, 4459.50834264, 3165.30819912, 2883.99121523,
        1349.67862372],
       [3323.        , 2864.25      , 2857.5       , 2496.25      ,
        2512.5       , 3165.30819912, 3102.75      , 2587.5       ,
        1206.        ],
       [3017.25      , 2745.75      , 2746.25      , 2324.25      ,
        2353.25      , 2883.99121523, 2587.5       , 3063.5       ,
        1187.75       ],
       [1522.        , 1289.5       , 1281.25      , 1136.5       ,
        1210.75      , 1349.67862372, 1206.        , 1187.75      ,
         954.75       ]])
```

In [33]:

```
# Newton-step
w -= np.linalg.solve(H, g)
w
```

Out[33]:

```
array([-0.5109304 ,  1.11234173,  0.27328331,  0.04948115, -0.97918294,
        0.73256627, -0.72881045,  0.41669609, -0.28989454])
```

In [34]:

```
# Newton Loop
w = np.zeros(X.shape[1])
niter = 10
for it in range(niter):
    # prediction
    yhat = sigmoid(X @ w)
    # cross-entropy
    ce = -np.log(yhat) @ y - np.log(1 - yhat) @ (1 - y)
    # gradient of cross-entropy
    g = X.T @ (yhat - y)
    # Hessian matrix of cross-entropy
    H = X.T * (yhat * (1 - yhat)) @ X
    print(it, ce)
    # Newton-step
    w -= np.linalg.solve(H, g)
```

```
0 484.50987921140165
1 320.0112328042882
2 285.73437841351625
3 277.70418009292183
4 277.0625947428168
5 277.05704693001366
6 277.0570464294203
7 277.0570464294203
8 277.0570464294204
9 277.0570464294203
```

In [38]:

```
def cross_entropy(y, yhat):
    return -np.log(yhat) @ y - np.log(1 - yhat) @ (1 - y)

def logreg_m_fit(X, y, niter=10):
    w = np.zeros(X.shape[1])
    for it in range(niter):
        # prediction
        yhat = sigmoid(X @ w)
        # cross-entropy
        ce = cross_entropy(y, yhat)
        # gradient of cross-entropy
        g = X.T @ (yhat - y)
        # Hessian matrix of cross-entropy
        H = X.T * (yhat * (1 - yhat)) @ X
        print(it, ce)
        # Newton-step
        w -= np.linalg.solve(H, g)
    return w
```

In [39]:

```
w = logreg_m_fit(X[tr], y[tr])
w
```

```
0 338.9489712938133
1 219.31492649580565
2 194.84385525659366
3 189.2334455179607
4 188.79436565306744
5 188.79058752143467
6 188.7905871820355
7 188.79058718203555
8 188.79058718203555
9 188.79058718203552
```

Out[39]:

```
array([-0.37775352,  0.81513883,  0.24794682, -0.00703306, -0.7267206 ,
        0.585522  , -0.43993472,  0.32078896, -0.23507939])
```

In [41]:

```
# testing
yhat = sigmoid(X @ w)
cross_entropy(y[te], yhat[te])
```

Out[41]:

```
92.3437344981877
```

In [45]:

```
w
```

Out[45]:

```
array([-0.37775352,  0.81513883,  0.24794682, -0.00703306, -0.7267206 ,
        0.585522  , -0.43993472,  0.32078896, -0.23507939])
```

Exercise 7: Use scikit-learn for training the model and compare the results against the previous experiment's results!

In [54]:

```
from sklearn.linear_model import LogisticRegression

cl = LogisticRegression(fit_intercept=False, C=1e12) # no bies, no regularization
cl.fit(X[tr], y[tr])
yhat = cl.predict_proba(X)[:,1]
ce = cross_entropy(y[te], yhat[te])
print (ce, ce / len(te))
```

```
28.330792605335226 0.4105911971787714
```

In [44]:

```
cl.coef_[0]
```

Out[44]:

```
array([-0.37775325,  0.81513397,  0.24796104, -0.00703901, -0.72671579,
        0.58551021, -0.43993414,  0.32079127, -0.23508148])
```

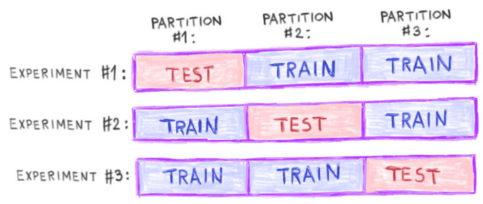
In [ ]:

```

```

K-Fold Cross-Validation

- Idea: Randomly split the data to K roughly equal partitions and run K experiments!
- In the i-th experiment, partition i is used as the test set and all other partitions as the training set.
- In the end, the scores obtained from the K experiments are averaged.
- K-fold cross-validation is slower but more reliable than the simple train-test split.
- In the *stratified* variant of the method, the same distribution of labels is enforced in every partition.



Exercise 8: Replace the train-test split to 10-fold cross valiadtion and re-run the last experiment!

In [50]:

```
from sklearn.model_selection import KFold
from sklearn.metrics import log_loss

cv = KFold(10, shuffle=True, random_state=42)
```

In [51]:

```
scores = []
for tr, te in cv.split(X):
    cl = LogisticRegression(fit_intercept=False, C=1e12) # no bies, no regularization
    cl.fit(X[tr], y[tr])
    yhat = cl.predict_proba(X)[:,1]
    score = log_loss(y[te], yhat[te])
    scores.append(score)
```

In [52]:

```
scores
```

Out[52]:

```
[0.3103854498633047,
 0.5013502260500776,
 0.492728969735146,
 0.34584544309166304,
 0.5820155518006203,
 0.3244320020003381,
 0.4848963100207666,
 0.3690964445150554,
 0.38712987311278146,
 0.41059119717877135]
```

In [53]:

```
np.mean(scores)
```

Out[53]:

```
0.4208471467368525
```