Berkeley MSSE
MOLECULAR SCIENCE &
SOFTWARE ENGINEERING

Lecture 04:

Linear and Non-Linear Regression

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Machine Learning Algorithms

MSSE 277B, 3 Units

Course Map

Lecture 1: Course Overview and Introduction to Machine Learning

classic ML tools & algorithms

Lecture 2: Bayesian Methods in Machine Learning

Lecture 3: Dimensionality Reduction: Principal Component Analysis

Lecture 4: Linear and Non-linear Regression and Classification

Lecture 5: Unsupervised Learning: Clustering and Gaussian Mixture Models

Lecture 6: Adaptive Learning and Gradient Descent Optimization Algorithms

ANNs/AI/Deep Learning

Lecture 7: Introduction to Artificial Neural Networks - The Perceptron

Lecture 8: Introduction to Artificial Neural Networks - Building Multiple Dense Layers

Lecture 9: Convolutional Neural Networks (CNNs) - Part I

Lecture 10: CNNs - Part II

Lecture 11: Recurrent Neural Networks (RNNs) and Long Short-Term Memory (LSTMs)

Lecture 12: Combining LSTMs and CNNs

Lecture 13: Running Models on GPUs and Parallel Processing

Lecture 14: Project Presentations

Lecture 15: Transformer

Lecture 16: GNN

Outline

Linear Regression

- Mathematical Notation

- What is Linear?

- Some Statistics

- a Python example

Logistic Regression

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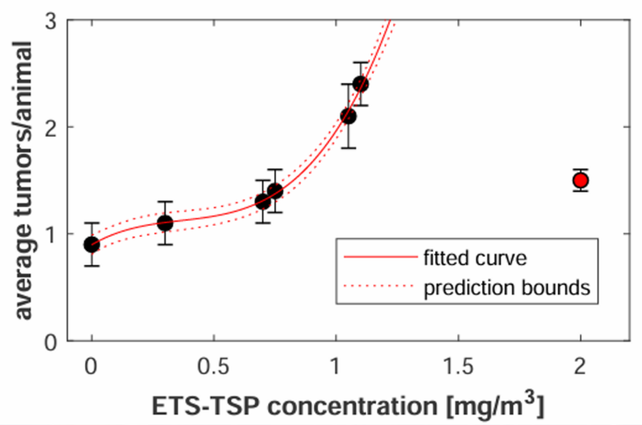
Logistic Regression

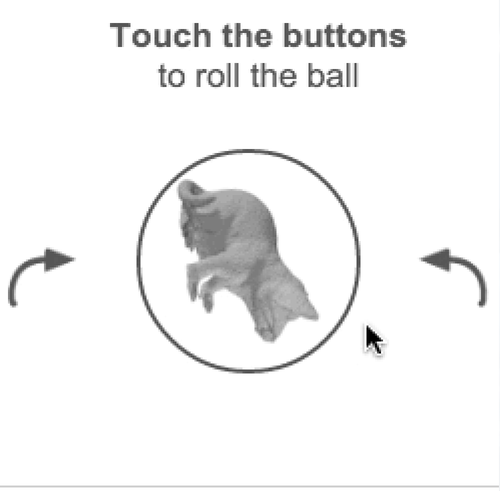
Regression vs Classification

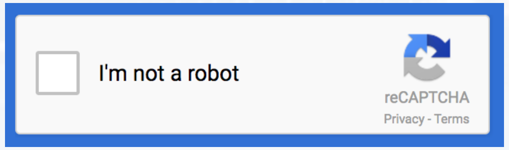
regression



curve fit: finding model parameters by **minimizing** χ^2

$$\chi^2 = \sum_k \frac{(\hat{y}_k - y_k)^2}{\sigma_k^2}$$





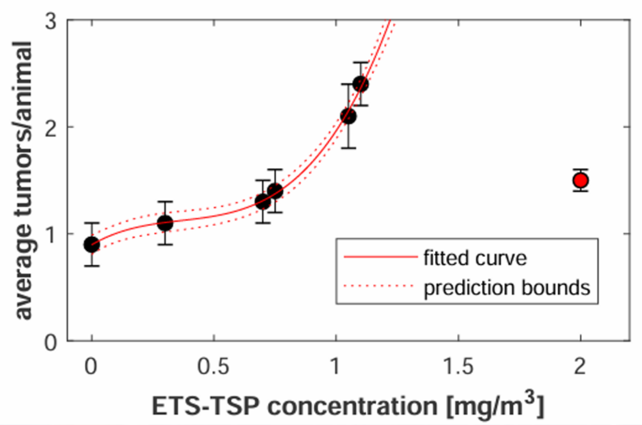
turning an image the right way:

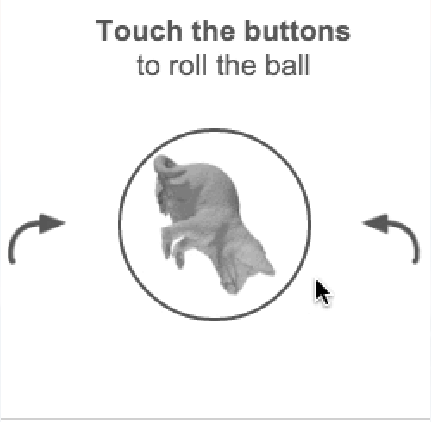
- **maximizing** autocorrelation function
- training an AI

Linear and Non-Linear Regression

Regression vs **Classification**

regression





classification

cat

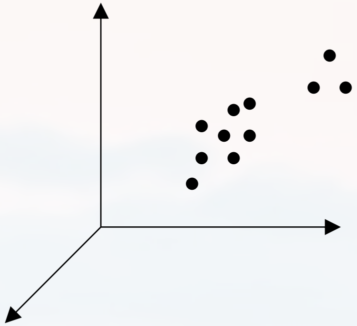
dog

note: we can use (non-linear) regression for classification!

Linear and Non-Linear Regression

idea: data point y_k in *N* dimensional space

→ $y_k = f(x_1, \dots x_n, \dots x_N) + \epsilon$ for each data point *k*



ansatz: $\boxed{y_k = \beta_0 + \sum_{n=1}^{N} \beta_n x_n + \epsilon}$ ***linear*** combination

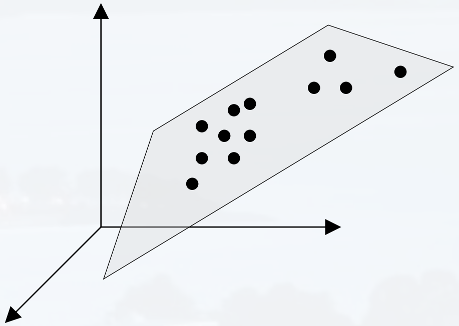
y: response

x: regressors **(assumed to be independent)**

β: factors **(how a regressor contributes to the response)**

β_0: intercept

ε: error **(stochasticity of the data, assumed to be normally dist.)**



Outline

Linear Regression

- Mathematical Notation

- What is Linear?

- Some Statistics

- a Python example

Logistic Regression

Linear and Non-Linear Regression

What is Linear?

y:	**response**
x:	**regressors**
β:	**factors**
$\boldsymbol{\beta_0}$**:**	**intercept**
ε:	**error**

linear ≠ not curved

$$y_k = \beta_0 + \sum_{n=1}^{N} \beta_n \, {x_n}^n \, + \, \epsilon$$

...is still linear

just define: $\bar{x}_n \coloneqq {x_n}^n$

$$y_k = \beta_1 {x_n}^{\beta_2}$$

...is still linear

just use log: $\bar{y}_k = \log(y_k) = \log(\beta_1) + \beta_2 \log(x_n) = \bar{\beta}_1 + \beta_2 \bar{x}_n$

As long as we can recover the linear structure by any transformation → it is linear

in part. log scaling is quite common

examples:

- **log fold change (DESeq/RNASeq)**
- **log odds ratio (comparing models, HMM)**
- **sound → dB is a log unit**
- **log incidence rates (medical studies)**
- **percentiles (medical studies)**
- **.....**

Linear and Non-Linear Regression

y:	**response**
x:	**regressors**
β:	**factors**
$\boldsymbol{\beta_0}$**:**	**intercept**
ε:	**error**

...what is **not** linear?

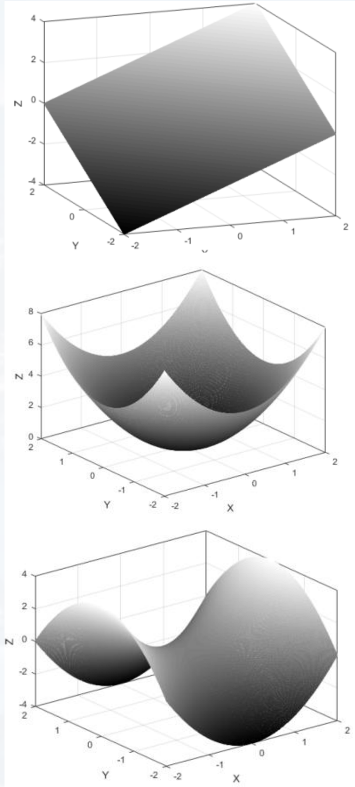
$y_k = \beta_0 + \beta_1 x_n^{\beta_2}$ log trick does not work here

general: linear refers to the **factors**

$y_k = \beta_0 + \beta_1 x_1 + \beta_2 x_2$ 2*D* plane in 3*D* space

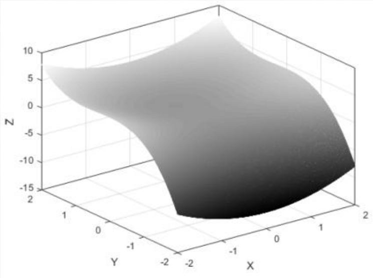
$y_k = \beta_0 + \beta_1 {x_1}^2 + \beta_2 {x_2}^2$ 2*D* parabolic

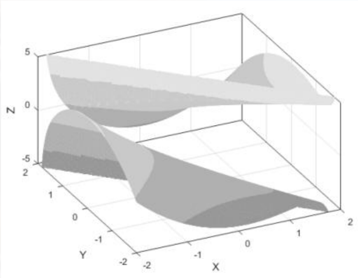
$y_k = \beta_0 + \beta_1 {x_1}^2 - \beta_2 {x_2}^2$ 2*D* hyperbolic



all linear

$$y_k = \beta_0 + \sum_{n=1}^{N} \beta_n x_n + \epsilon$$





...and many more...

Outline

Linear Regression

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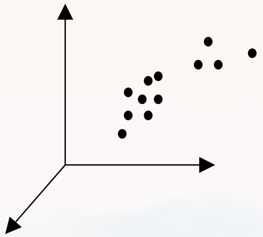
Logistic Regression

Linear and Non-Linear Regression

for *K* data points in *N* dimensional space

$$y_k = \beta_0 + \sum_{n=1}^{N} \beta_n x_n + \epsilon$$



y:	**response**
x:	**regressors**
β:	**factors**
$\boldsymbol{\beta_0}$**:**	**intercept**
ε:	**error**

$$\underbrace{\begin{pmatrix} y_1 \\ \dots \\ y_k \\ \dots \\ \dots \\ y_K \end{pmatrix}}_{Y} = \underbrace{\begin{pmatrix} 1 & x_{11} & x_{12} & \dots & x_{1n} & \dots & x_{1N} \\ \dots & \dots & & & \dots & & \\ 1 & x_{k1} & & & x_{kn} & & \\ 1 & \dots & & & \dots & & \\ 1 & x_{K1} & x_{K2} & \dots & x_{Kn} & \dots & x_{KN} \end{pmatrix}}_{X} \underbrace{\begin{pmatrix} \beta_0 \\ \beta_1 \\ \dots \\ \beta_n \\ \dots \\ \beta_N \end{pmatrix}}_{\beta} + \underbrace{\begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \dots \\ \varepsilon_k \\ \dots \\ \varepsilon_K \end{pmatrix}}_{\varepsilon}$$

$$\boxed{Y = X\beta + \varepsilon}$$

<u>fitting:</u> finding the best β in terms of minimizing the errors

$$\hat{\beta} = \underset{\beta}{argmin} \left\{ \frac{1}{K} \| Y \ - X\beta \|^2 \right\} \qquad (Y - X\beta)^T (Y - X\beta) = \sum_k {\varepsilon_k}^2$$

$$\boxed{Y = X\beta + \varepsilon}$$

y:	**response**
x:	**regressors**
β:	**factors**
$\boldsymbol{\beta_0}$**:**	**intercept**
ε:	**error**

<u>fitting:</u> finding the best β in by minimizing the errors

$$(Y - X\beta)^T(Y - X\beta) = \sum_k {\varepsilon_k}^2$$

$$\frac{\partial}{\partial\beta}\sum_k {\varepsilon_k}^2 = 0 \longrightarrow \beta_{best} = \hat{\beta} = (X^TX)^{-1}X^TY \longrightarrow$$

the model

$$\boldsymbol{\hat{Y}} = \boldsymbol{X\hat{\beta}} = \underbrace{X(X^TX)^{-1}X^T}_{\text{hat matrix } \boldsymbol{H}}Y$$

<u>some properties of the hat matrix:</u>

- $H = H^T$ (symmetry)
- $HH = H \rightarrow H^n = H$ (idempotency)

$$\boldsymbol{\hat{Y}} = \boldsymbol{X\hat{\beta}} = \boldsymbol{X\left(X^TX\right)^{-1}X^TY}$$

all observables!

<u>evaluating the fit:</u>

$$\hat{\varepsilon} = Y - X\hat{\beta} = Y - \hat{Y} = (I - H)Y$$

$$\hat{\varepsilon}^T\hat{\varepsilon} = [(I - H)Y]^T(I - H)Y = Y^T(I - H)^T(I - H)Y = Y^T(I - H)Y$$

sum of squared errors (SSE)

y:	**response**
x:	**regressors**
β:	**factors**
$\boldsymbol{\beta_0}$**:**	**intercept**
ε:	**error**
***K*:**	**number of data points**
***N*:**	**number of model param**

summary:

the model: $Y = X\beta + \varepsilon$

the fit: $\hat{Y} = X\hat{\beta} = X(X^T X)^{-1} X^T Y$

sum of squared errors (SSE): $\hat{\varepsilon}^T \hat{\varepsilon} = Y^T (I - H) Y$

(after the fit)

mean of squared errors (MSE): $\frac{\hat{\varepsilon}^T \hat{\varepsilon}}{K-N}$

(after the fit)

often fit quality is judged by $R^2 := 1 - \frac{\sum_k (\hat{y}_k - y_k)^2}{\sum_k (y_k - \langle y \rangle)^2}$

or adjusted R^2 $\bar{R}^2 := R^2 - (1 - R^2)\frac{K}{N-K-1}$

and it is said that the fit is good if R^2 is close to one....

...but that is not true...

Linear and Non-Linear Regression

Some Statistics

$\boldsymbol{y_i}$:	**measured value of data point**
$\boldsymbol{\sigma_i}$:	**statistical error of y_i (often aka ey_i)**
$\boldsymbol{\hat{y}_i}$:	**prediction by the model *after the fit***
K :	**number of data points**
N:	**number of fit parameter**

$$\chi^2_{red} = \frac{1}{df}\sum_{i=1}^{K}\left(\frac{y_i - \hat{y}_i}{\sigma_i}\right)^2 \qquad df = K - N - 1$$

def:

$\bar{y}$: mean of the data point values

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

variance data vs model
(aka residual sum of squares)

variance of the data
(aka total sum of squares)

Note: do not confuse R^2 with Pearsons coefficient: $\rho = \frac{cov(x,y)}{\sqrt{var(x)var(y)}}$

Linear and Non-Linear Regression

$$\chi^2_{red} = \frac{1}{df} \sum_{i=1}^{K} \left(\frac{y_i - \hat{y}_i}{\sigma_i} \right)^2$$

$$df = K - N - 1$$

- scales difference between model and data to the error bars
- can be directly translated to a p-value via the Students distribution

H0: the fitted model has in fact generated the data

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

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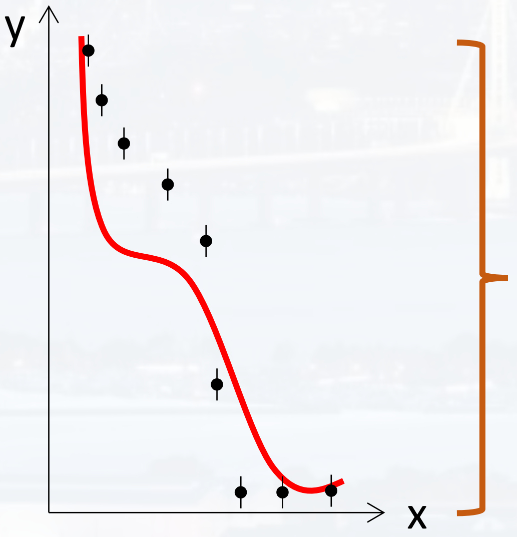

data variance can be huge (i. e. exponential functions)
→ R^2 could be around 1.0 even if fit is completely off!

Linear and Non-Linear Regression

$$\chi^2_{red} = \frac{1}{df} \sum_{i=1}^{K} \left(\frac{y_i - \hat{y}_i}{\sigma_i} \right)^2$$

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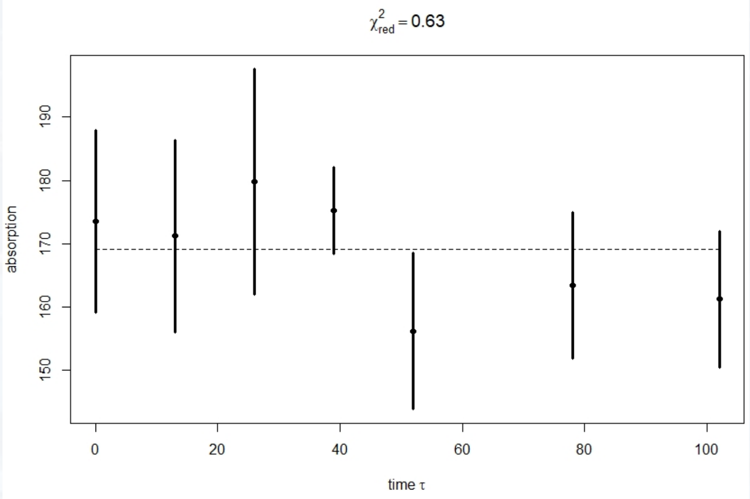
$$R^2 = 1 - \frac{\sum_{i=1}^{K} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{K} (y_i - \bar{y})^2} \qquad \frac{\text{variance data vs model } \textit{(aka residual sum of squares)}}{\text{variance of the data } \textit{(aka total sum of squares)}}$$

$\bar{y}$: mean of the data point values



$$\frac{\text{variance data vs model } \textit{(aka residual sum of squares)}}{\text{variance of the data } \textit{(aka total sum of squares)}} \approx 1 \rightarrow R^2 = 0$$

→ **although the fit is good**

Linear and Non-Linear Regression

$$\chi^2_{red} = \frac{1}{df}\sum_{i=1}^{K}\left(\frac{y_i - \hat{y}_i}{\sigma_i}\right)^2$$

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

variance data vs model
(aka residual sum of squares)

variance of the data
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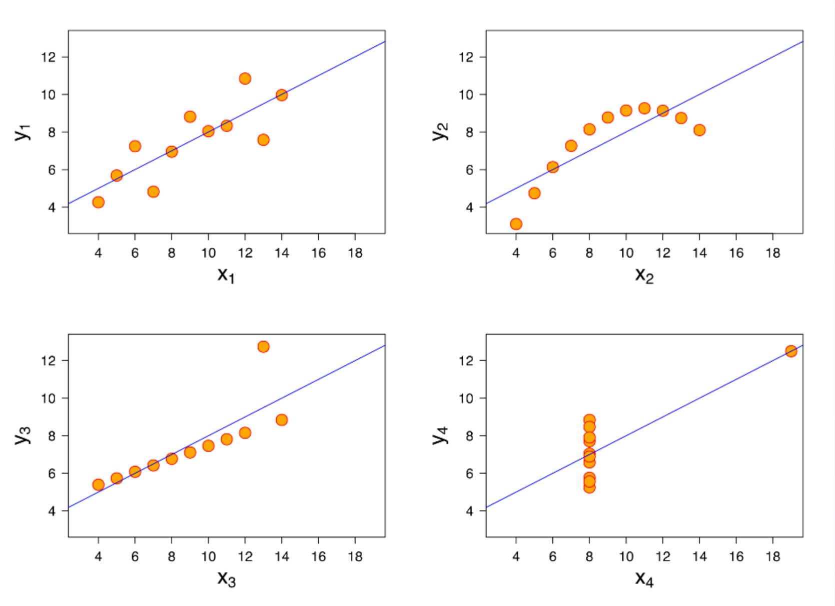
$\bar{y}$: mean of the data point values



all plots: same R^2

Linear and Non-Linear Regression

$$\chi^2_{red} = \frac{1}{df} \sum_{i=1}^{K} \left(\frac{y_i - \hat{y}_i}{\sigma_i} \right)^2$$

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variance data vs model
(aka residual sum of squares)

variance of the data
(aka total sum of squares)

$\bar{y}$: mean of the data point values

conclusion:

- R^2 is not a measure of the fit quality (but χ^2 is)
- error bars are important
- **given a good fit**, R^2 tells how strong the dependent variable responds to the independent variable

Also, Wiki is full of examples…
…and warnings (see “caveats” therein)

regularization:

λ *Lagrangian Multiplier*

$$\hat{\beta} = \underset{\beta}{argmin} \left\{ \frac{1}{K} \|Y - X\beta\|^2 \right\}$$

$$\beta\hat{}= \underset{\beta}{argmin} \left\{ \frac{1}{K} \|Y - X\beta\|^2 + \boldsymbol{\lambda}\|\boldsymbol{\beta}\|^{\mathbf{1}} \right\}$$

the Loss Function
$\boldsymbol{L(X, Y, \lambda)}$

L1 or **L**east **a**bsolute **s**hrinkage and **s**election **o**perator
- encourages **sparsity** of β
- reduces **overfitting**

$$\beta\hat{}= \underset{\beta}{argmin} \left\{ \frac{1}{K} \|Y - X\beta\|^2 + \boldsymbol{\lambda}\|\boldsymbol{\beta}\|^{\mathbf{2}} \right\}$$

L2 or **Ridge**
- **penalizes large $\boldsymbol{\beta}$**

$$\beta\hat{}= \underset{\beta}{argmin} \left\{ \frac{1}{K} \|Y - X\beta\|^2 + \boldsymbol{\lambda\, max(0, -\beta)} \right\}$$

- **penalizes negative $\boldsymbol{\beta}$**

…and so on

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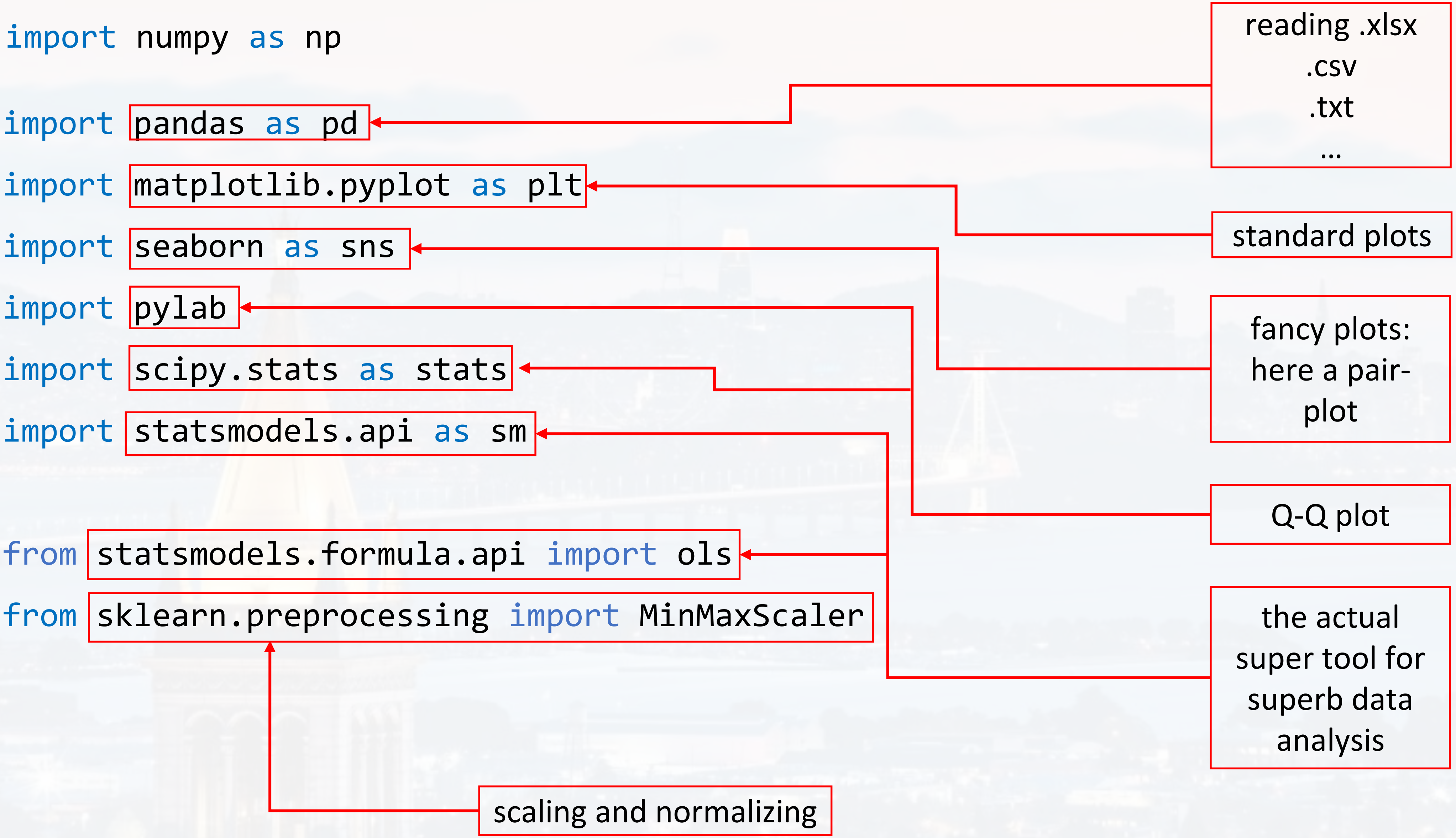
Linear and Non-Linear Regression

a Python Example



```
import numpy as np

import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
import pylab
import scipy.stats as stats
import statsmodels.api as sm

from statsmodels.formula.api import ols
from sklearn.preprocessing import MinMaxScaler
```

reading .xlsx
.csv
.txt
…

standard plots

fancy plots: here a pair-plot

Q-Q plot

the actual super tool for superb data analysis

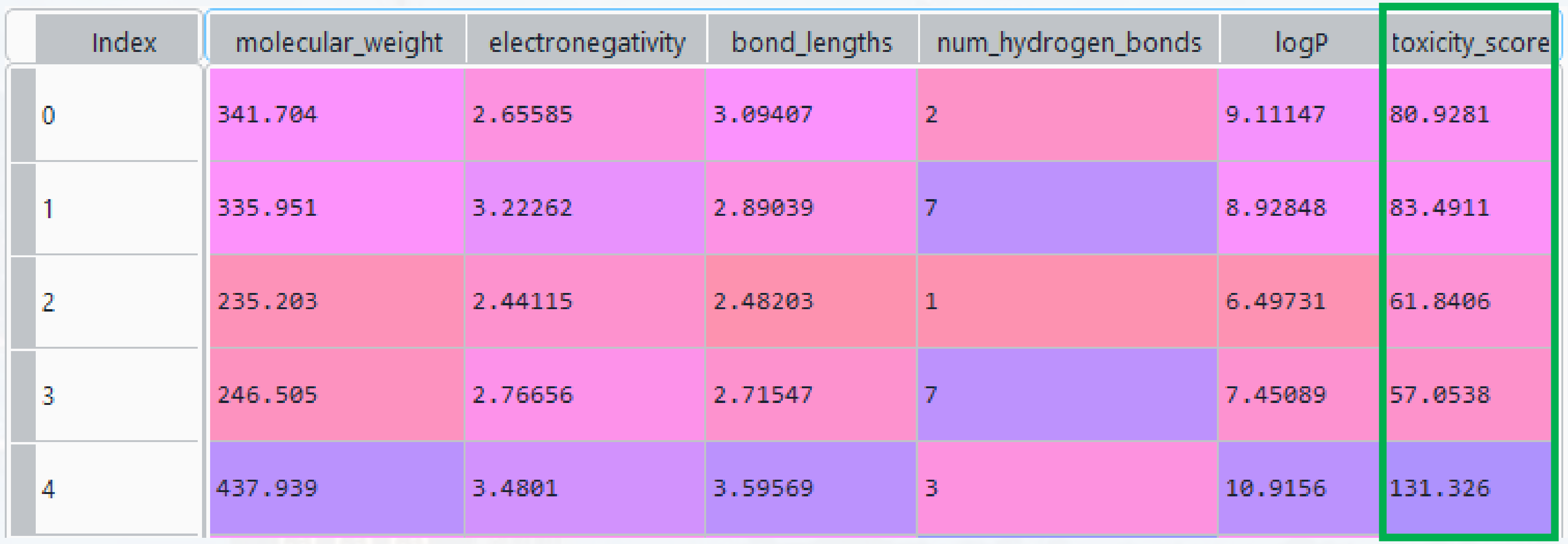
scaling and normalizing

Linear and Non-Linear Regression

a Python Example

1) loading data
2) plotting data
3) scaling data
4) fitting model
5) evaluating model

```
Train   = pd.read_csv("molecular_train_gbc.csv")
Test    = pd.read_csv("molecular_test_gbc.csv")
```



	x_1	x_2	x_3	x_4	x_5	y_k
Index	molecular_weight	electronegativity	bond_lengths	num_hydrogen_bonds	logP	toxicity_score
0	341.704	2.65585	3.09407	2	9.11147	80.9281
1	335.951	3.22262	2.89039	7	8.92848	83.4911
2	235.203	2.44115	2.48203	1	6.49731	61.8406
3	246.505	2.76656	2.71547	7	7.45089	57.0538
4	437.939	3.4801	3.59569	3	10.9156	131.326

$$y_k = \beta_0 + \sum_{n=1}^{N} \beta_n x_n + \epsilon$$

y: toxicity_score

x_n : molecular_weight, electronegativity, bond_lengths, num_hydrogen_bonds, logP

Linear and Non-Linear Regression

a Python Example

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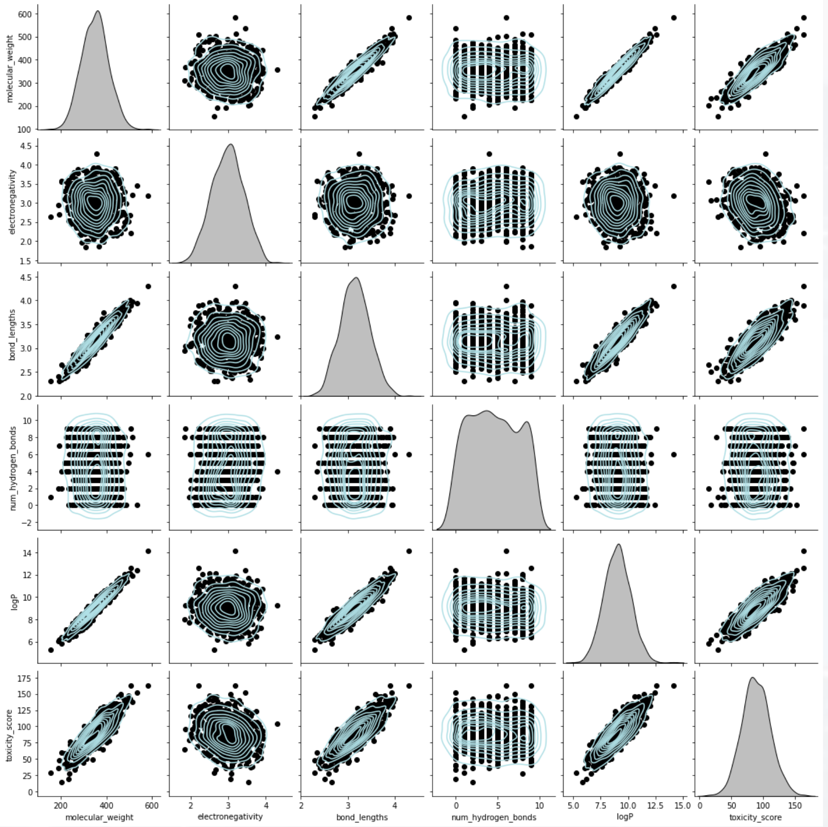
```
Train  = pd.read_csv("molecular_train_gbc.csv")
Test   = pd.read_csv("molecular_test_gbc.csv")


out = sns.pairplot(Train, kind = "kde", \
                   plot_kws = {'color':[176/255, 224/255, 230/255]},\
                   diag_kws = {'color': 'black'})
out.map_offdiag(plt.scatter, color = 'black')
```



Linear and Non-Linear Regression

a Python Example

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```

```
scaler  = MinMaxScaler(feature_range = (0, 1))
TrainS  = scaler.fit_transform(Train)
TestS   = scaler.transform(Test)
```

the scaler returns an np.array
→ convert back to data frame

```
TrainS = pd.DataFrame(TrainS, columns = Train.columns)
TestS  = pd.DataFrame(TestS, columns = Train.columns)
```

Linear and Non-Linear Regression

a Python Example

1) loading data
2) plotting data
3) scaling data
4) fitting model
5) evaluating model

```
TrainS = pd.DataFrame(TrainS, columns = Train.columns)
TestS  = pd.DataFrame(TestS,  columns = Train.columns)
```

```
equation = 'toxicity_score ~ ' + '+'.join(Train.columns[:-1])
print(equation)
```

$$y_k = \beta_0 + \sum_{n=1}^{N} \beta_n x_n + \epsilon$$

```
toxicity_score ~      molecular_weight + electronegativity +
                      bond_lengths + num_hydrogen_bonds + logP
```

```
my_model = ols(equation, data = TrainS).fit()
my_model.summary()
```

OLS (ordinary least squares)

Linear and Non-Linear Regression

1) loading data
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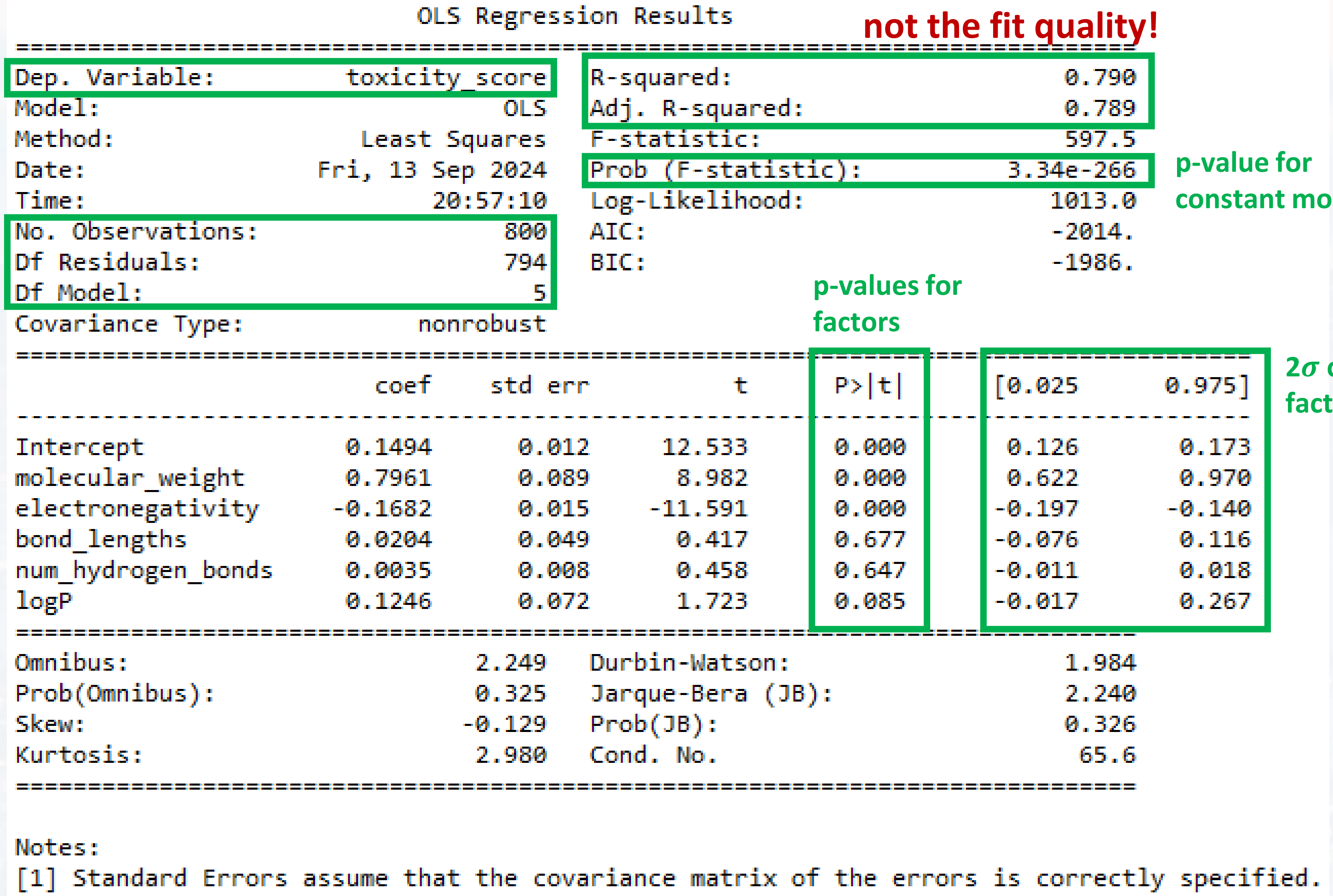
```
my_model.summary()
```



```
                            OLS Regression Results
==============================================================================
Dep. Variable:         toxicity_score   R-squared:                       0.790
Model:                            OLS   Adj. R-squared:                  0.789
Method:                 Least Squares   F-statistic:                     597.5
Date:                Fri, 13 Sep 2024   Prob (F-statistic):          3.34e-266
Time:                        20:57:10   Log-Likelihood:                 1013.0
No. Observations:                 800   AIC:                            -2014.
Df Residuals:                     794   BIC:                            -1986.
Df Model:                           5
Covariance Type:            nonrobust
=========================================================================================
                            coef    std err          t      P>|t|      [0.025      0.975]
-----------------------------------------------------------------------------------------
Intercept                 0.1494      0.012     12.533      0.000       0.126       0.173
molecular_weight          0.7961      0.089      8.982      0.000       0.622       0.970
electronegativity        -0.1682      0.015    -11.591      0.000      -0.197      -0.140
bond_lengths              0.0204      0.049      0.417      0.677      -0.076       0.116
num_hydrogen_bonds        0.0035      0.008      0.458      0.647      -0.011       0.018
logP                      0.1246      0.072      1.723      0.085      -0.017       0.267
==============================================================================
Omnibus:                        2.249   Durbin-Watson:                   1.984
Prob(Omnibus):                  0.325   Jarque-Bera (JB):                2.240
Skew:                          -0.129   Prob(JB):                        0.326
Kurtosis:                       2.980   Cond. No.                         65.6
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
```

not the fit quality!

p-value for constant model

p-values for factors

2σ conf range of factors

number of data points is much larger than the number of regressors

→ degree of freedom approx. no of obs

$$y_k = \beta_0 + \sum_{n=1}^{N} \beta_n x_n + \epsilon$$

Linear and Non-Linear Regression

a Python Example

1) loading data
2) plotting data
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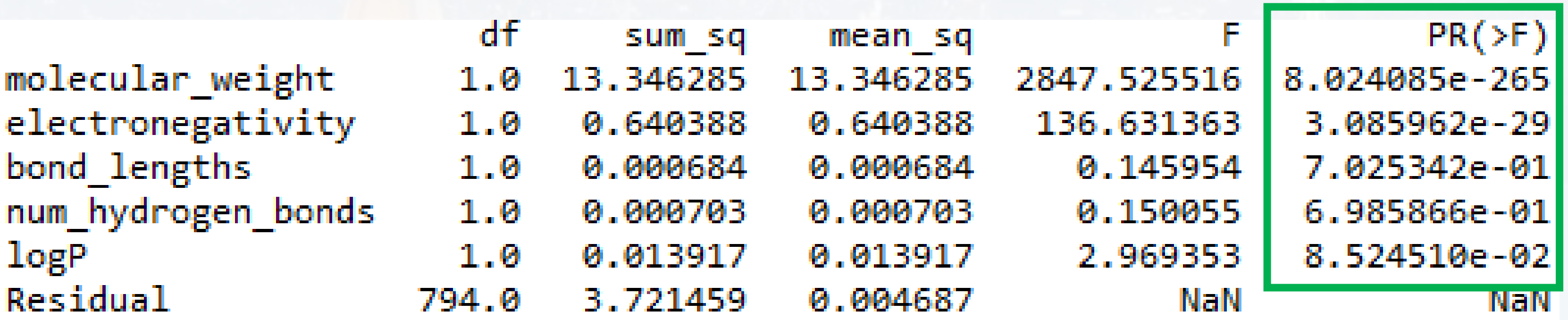
more accurate: determining **the p-values for the factors using ANOVA** for the corresponding residuals

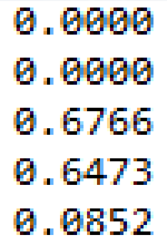
```
table    = sm.stats.anova_lm(my_model, typ = 1)
print(table)
```

$$y_k = \beta_0 + \sum_{n=1}^{N} \beta_n x_n + \epsilon$$



```
                      df     sum_sq    mean_sq            F         PR(>F)
molecular_weight     1.0  13.346285  13.346285  2847.525516  8.024085e-265
electronegativity    1.0   0.640388   0.640388   136.631363   3.085962e-29
bond_lengths         1.0   0.000684   0.000684     0.145954   7.025342e-01
num_hydrogen_bonds   1.0   0.000703   0.000703     0.150055   6.985866e-01
logP                 1.0   0.013917   0.013917     2.969353   8.524510e-02
Residual           794.0   3.721459   0.004687          NaN            NaN
```

vs from t-test



```
0.0000
0.0000
0.6766
0.6473
0.0852
```

Linear and Non-Linear Regression

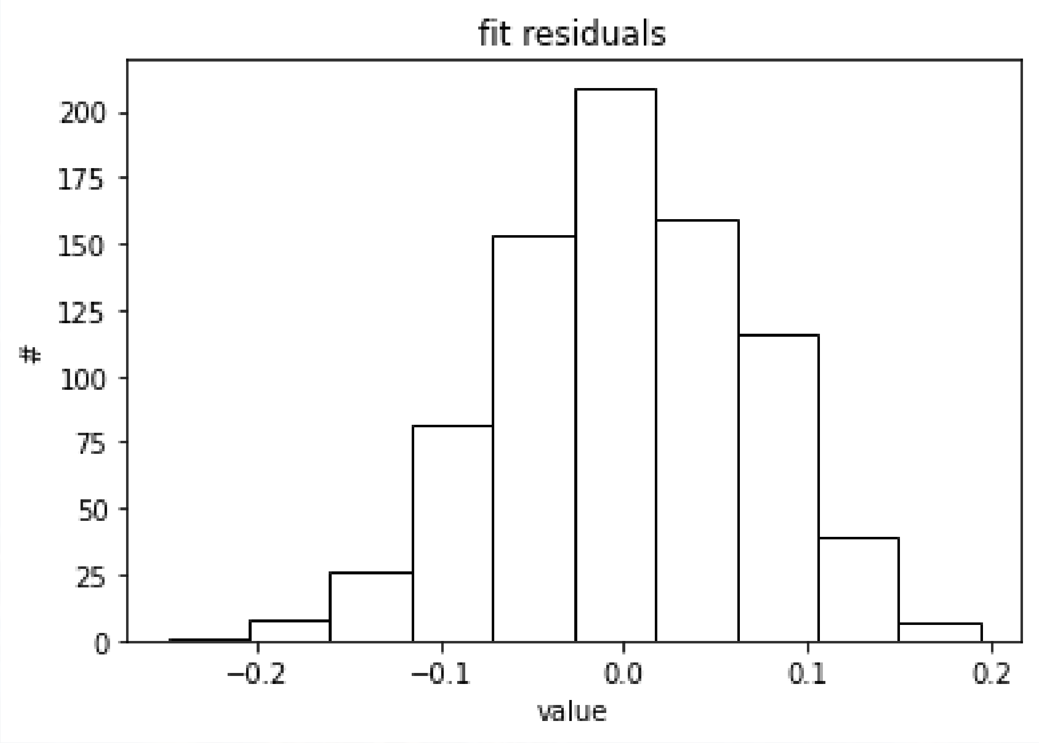
a Python Example

1) loading data
2) plotting data
3) scaling data
4) fitting model
5) evaluating model

$$y_k = \beta_0 + \sum_{n=1}^{N} \beta_n x_n + \epsilon$$

```
residuals = my_model.resid

plt.hist(residuals, color = 'w', edgecolor = 'black')
plt.title('fit residuals')
plt.ylabel('#')
plt.xlabel('value')
plt.show()
```



residuals approx. normally distributed around μ = 0

Linear and Non-Linear Regression

a Python Example

```
residuals = my_model.resid

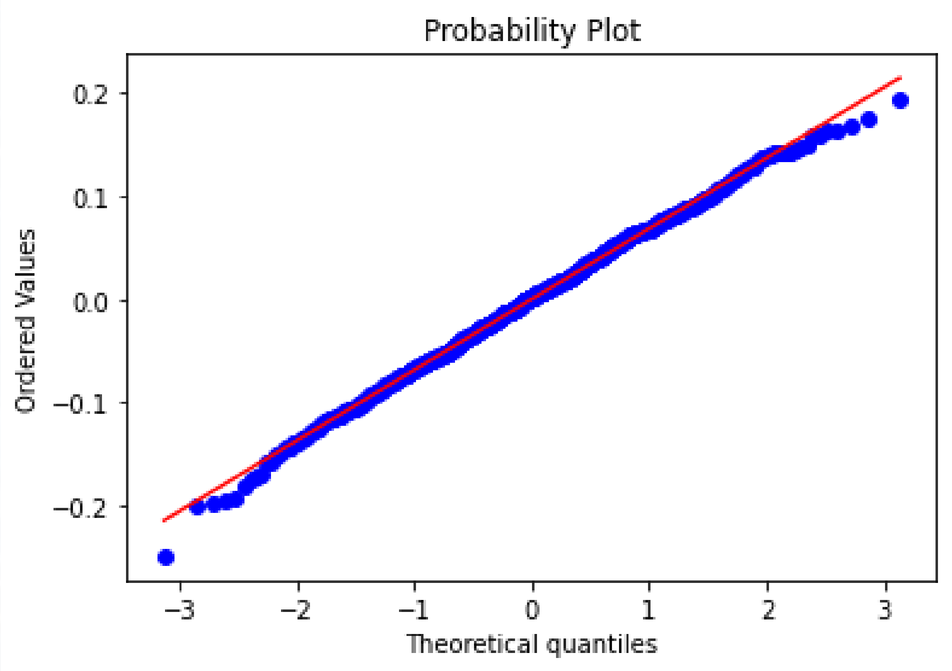
plt.hist(residuals, color = 'w', edgecolor = 'black')
plt.title('fit residuals')
plt.ylabel('#')
plt.xlabel('value')
plt.show()

stats.probplot(residuals, dist = "norm", plot = pylab)
pylab.show()
```

1) loading data
2) plotting data
3) scaling data
4) fitting model
5) evaluating model

residuals approx. normally distributed around μ = 0

$$y_k = \beta_0 + \sum_{n=1}^{N} \beta_n x_n + \epsilon$$



Linear and Non-Linear Regression

a Python Example

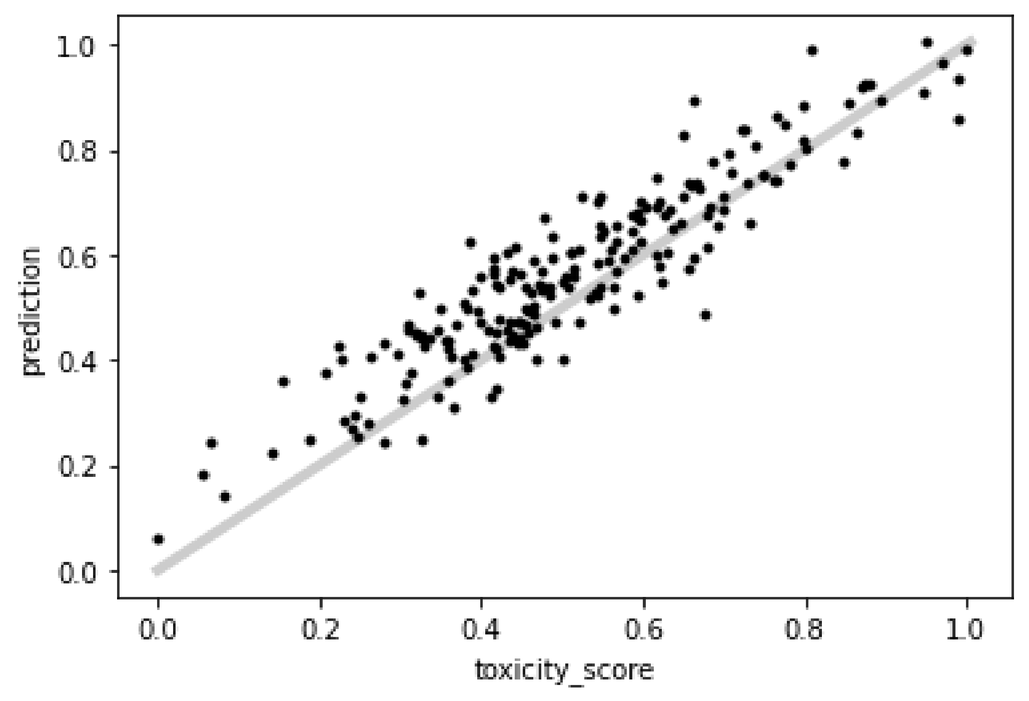
```
Ypred  = my_model.predict(TestS)

higher = np.max([Ypred, TestS.toxicity_score])
lower  = np.min([Ypred, TestS.toxicity_score])

plt.plot([lower, higher], [lower, higher], c = [0, 0, 0, 0.2],\
         linewidth = 4)
plt.scatter(TestS.toxicity_score, Ypred, marker = '.', c = 'k')
plt.ylabel('prediction')
plt.xlabel('toxicity score')
plt.show()
```

1) loading data
2) plotting data
3) scaling data
4) fitting model
5) evaluating model

$$y_k = \beta_0 + \sum_{n=1}^{N} \beta_n x_n + \epsilon$$



Linear and Non-Linear Regression

a Python Example

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plt.xlabel('toxicity score')
plt.show()
```
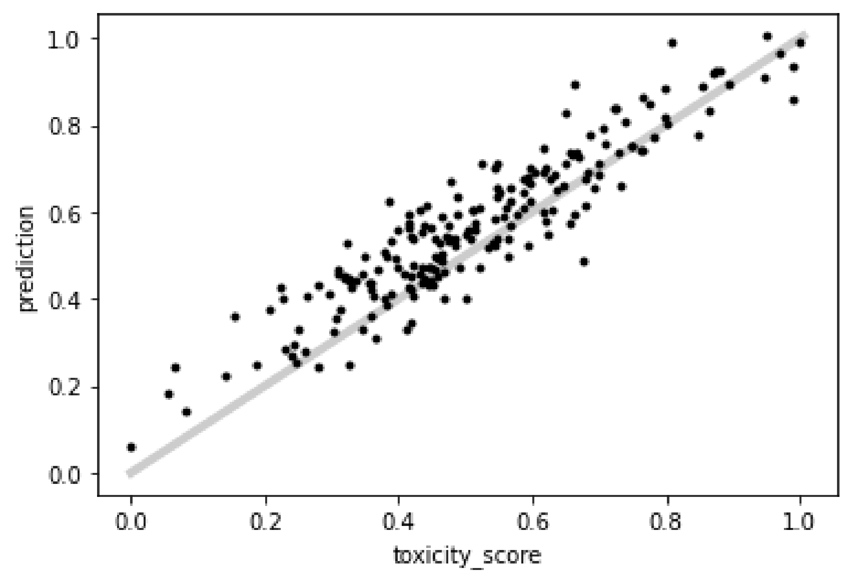

1) loading data
2) plotting data
3) scaling data
4) fitting model
5) evaluating model

$$y_k = \beta_0 + \sum_{n=1}^{N} \beta_n x_n + \epsilon$$



```
mean_dev = np.sum( abs(TestS.toxicity_score - Ypred) )/len(Ypred)
print(mean_dev)
```

5%

Outline

Linear Regression

- Mathematical Notation

- What is Linear?

- Some Statistics

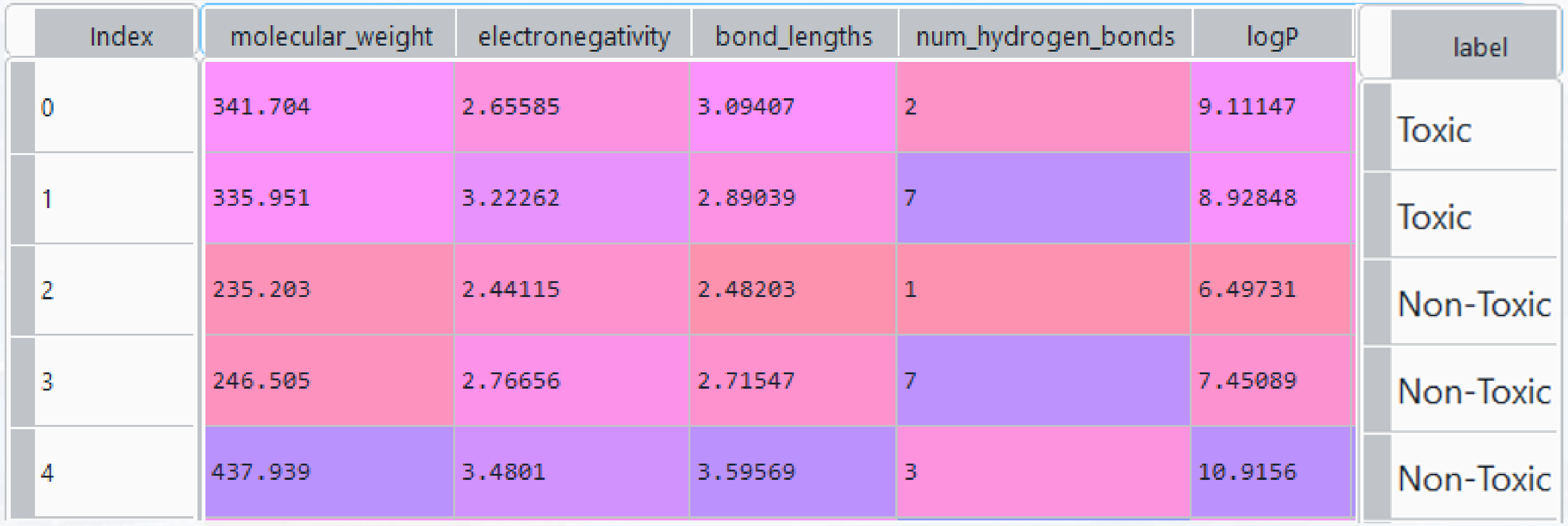
- a Python example

Logistic Regression

<u>linear model:</u> regressors are continuous or categorical, response is continuous

<u>logistic model:</u> response is **categorical**

y: response
x: regressors **(assumed to be independent)**
β: factors
β_0: intercept
ε: error **(stochasticity of the data, assumed to be normally dist.)**



Index	molecular_weight	electronegativity	bond_lengths	num_hydrogen_bonds	logP	label
0	341.704	2.65585	3.09407	2	9.11147	Toxic
1	335.951	3.22262	2.89039	7	8.92848	Toxic
2	235.203	2.44115	2.48203	1	6.49731	Non-Toxic
3	246.505	2.76656	2.71547	7	7.45089	Non-Toxic
4	437.939	3.4801	3.59569	3	10.9156	Non-Toxic

Linear and Non-Linear Regression

y:	response
x:	regressors **(assumed to be independent)**
β:	factors
β_0:	intercept
ε:	error **(stochasticity of the data, assumed to be normally dist.)**

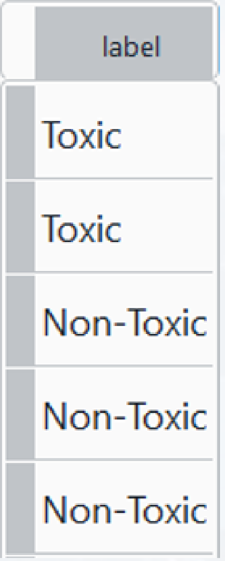
<u>linear model:</u> regressors are continuous or categorical, response is continuous

<u>logistic model:</u> response is **categorical**

dichotomic model:

probability to be in state A) → ***p***

probability to be in state B) → ***1 - p***



label
Toxic
Toxic
Non-Toxic
Non-Toxic
Non-Toxic

<u>ansatz:</u>

$$\boxed{log\left(\frac{p}{1-p}\right) = \beta_0 + \sum_{n=1}^{N} \beta_n x_n + \epsilon}$$

log odds ratio: linear model

Linear and Non-Linear Regression

Logistic Regression

y:	response
x:	regressors **(assumed to be independent)**
β:	factors
β_0:	intercept
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dichotomic model:

probability to be in state A) → ***p***

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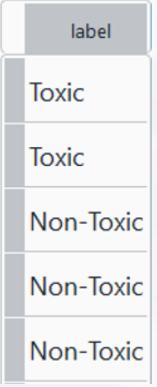

label
Toxic
Toxic
Non-Toxic
Non-Toxic
Non-Toxic

ansatz:

$$\boxed{log\left(\frac{p}{1-p}\right) = \beta_0 + \sum_{n=1}^{N} \beta_n x_n + \epsilon}$$

log odds ratio: linear model

→ probability for being in a certain state

$$\boxed{p = \frac{e^{\beta_0+\beta_1 x_1+\cdots}}{1+e^{\beta_0+\beta_1 x_1+\cdots}}}$$

often:

$$\boxed{logit(p) = log\left(\frac{p}{1-p}\right)}$$

examples:

- probability that a gene has been mutated
- probability of being diseased (cancer, alzheimer etc) as function of age, environmental influence etc ...
- Verhulst equation: $N(t) = N_0 \frac{e^{rt}}{C+e^{rt}}$
- activation functions in ANNs

Logistic Regression

$$log\left(\frac{p}{1-p}\right) = \beta_0 + \sum_{n=1}^{N} \beta_n x_n + \epsilon$$

y:	response
x:	regressors **(assumed to be independent)**
β:	factors
β_0:	intercept
ε:	error **(stochasticity of the data, assumed to be normally dist.)**

Note: one can derive the logit function from max. entropy too!

$$\boxed{p = \frac{e^{\beta_0+\beta_1 x_1+\cdots}}{1+e^{\beta_0+\beta_1 x_1+\cdots}} = \frac{1}{1+e^{-\beta_0-\beta_1 x_1-\cdots}}}$$

onset of Alzheimer’s disease (AD) is a function of ***age*** and years spent in ***education***
(and other risk factors we ignore here for the sake of simplicity)

education: $\mathrm{d} = x_1$ [yrs]
age: $a = x_2$ [yrs]

model: $p_{AD} = \frac{1}{1+e^{-\beta_0-\beta_1 d-\beta_2 a}}$

+ data set + fit → $\beta_0 = +0.1$
$\beta_1 = -1.5$
$\beta_2 = +0.12$

- *positive* value → *increasing p*
- *negative* value → *decreasing p*
- intercept: “background” prevalence, not related to environmental/internal conditions

Logistic Regression

y:	response
x:	regressors **(assumed to be independent)**
β:	factors
β_0:	intercept
ε:	error **(stochasticity of the data, assumed to be normally dist.)**

model: $p_{AD} = \frac{1}{1+e^{-\beta_0-\beta_1 d-\beta_2 a}}$

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age: $a = x_2$ [yrs]

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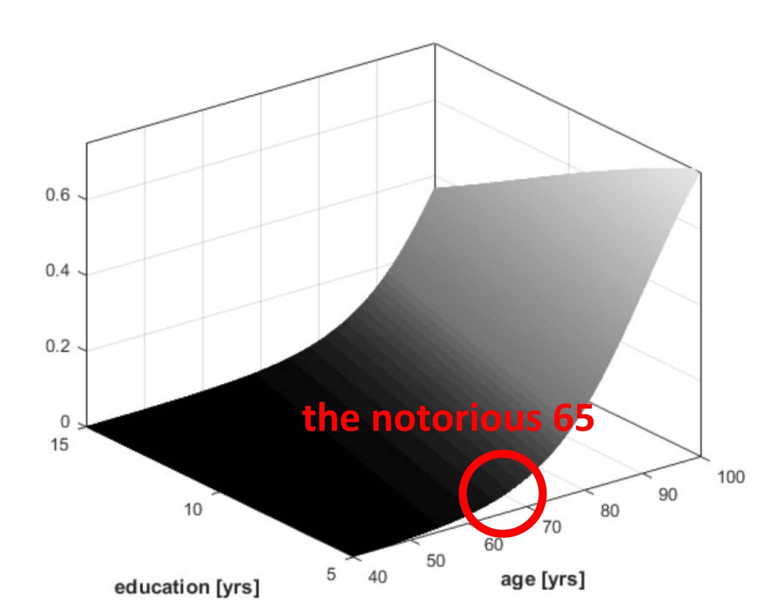


the notorious 65

example: ***65yrs*** old person, ***8yrs*** spent in education

→ $p_{AD} = 1.6\%$

65yrs old person, ***13yrs*** spent in education

→ $p_{AD} = 0.001\%$

<u>How does education compensate aging?</u>

$$p_{AD}(d+\bar{d}, a+\bar{a}) = p_{AD}(d,a)$$

→ $\bar{a} = 12.5\,\bar{d}$

hence, one more year prolonged education compensates 12.5 years of aging

(warning: don't confuse correlation with causation here!)

Linear and Non-Linear Regression

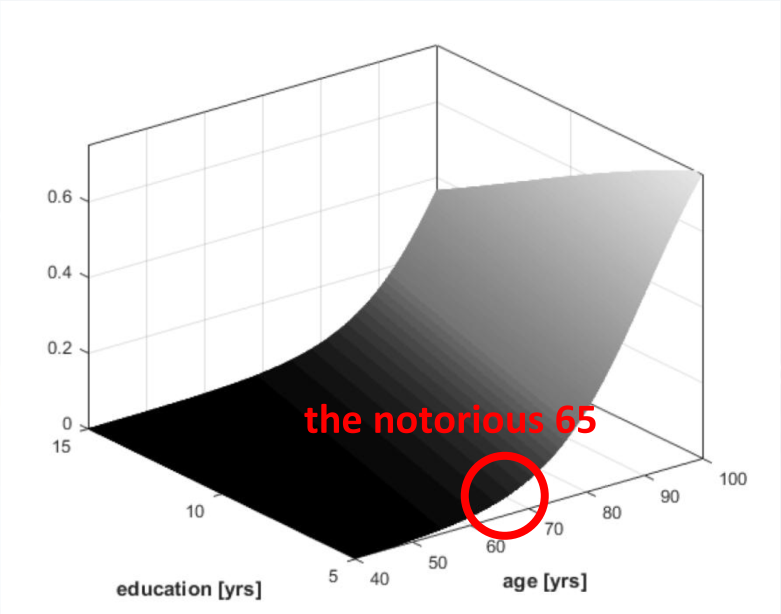
y:	response
x:	regressors **(assumed to be independent)**
β:	factors
β_0:	intercept
ε:	error **(stochasticity of the data, assumed to be normally dist.)**

model: $$p_{AD} = \frac{1}{1+e^{-\beta_0-\beta_1 d-\beta_2 a}}$$

education: $\mathrm{d} = x_1$ [yrs]

age: $a = x_2$ [yrs]

$$\beta_0 = +0.1$$
$$\beta_1 = -1.5$$
$$\beta_2 = +0.12$$



the notorious 65

How does the risk of onset changes *per year*?

relative change:

$$\frac{p_{AD}(a+1)-p_{AD}(a)}{p_{AD}(a)} \approx e^{\beta_2}-1 \approx 12.7\%$$

$p_{AD} \ll 1$ (hence, for small Δa and "young" ages, i. e. below ≈ 80yrs)

the risk of getting AD increases by 12.7% every year

(warning: does not mean that it increases by 127% in ten yrs – we made an approximation!)

y:	response
x:	regressors **(assumed to be independent)**
β:	factors
β_0:	intercept
ε:	error **(stochasticity of the data, assumed to be normally dist.)**

model: $$p_{AD} = \frac{1}{1+e^{-\beta_0-\beta_1 d-\beta_2 a}}$$

education: $\mathrm{d} = x_1$ [yrs]

age: $a = x_2$ [yrs]

$$\beta_0 = +0.1$$
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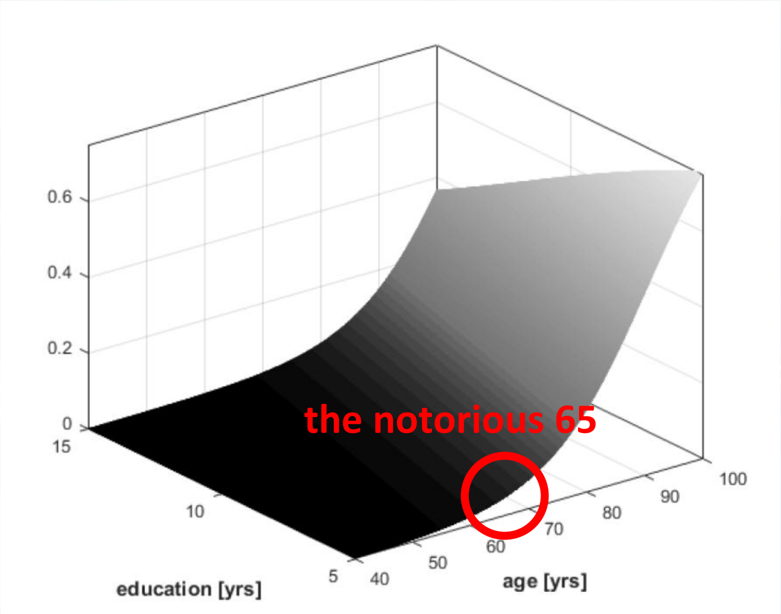


the notorious 65

How does the risk of onset changes *per year*?

more precise: relative change of the odds ratio

$$\frac{\frac{\partial}{\partial x_i}\left(\frac{p_{AD}}{1-p_{AD}}\right)}{\frac{p_{AD}}{1-p_{AD}}} = \beta_i$$

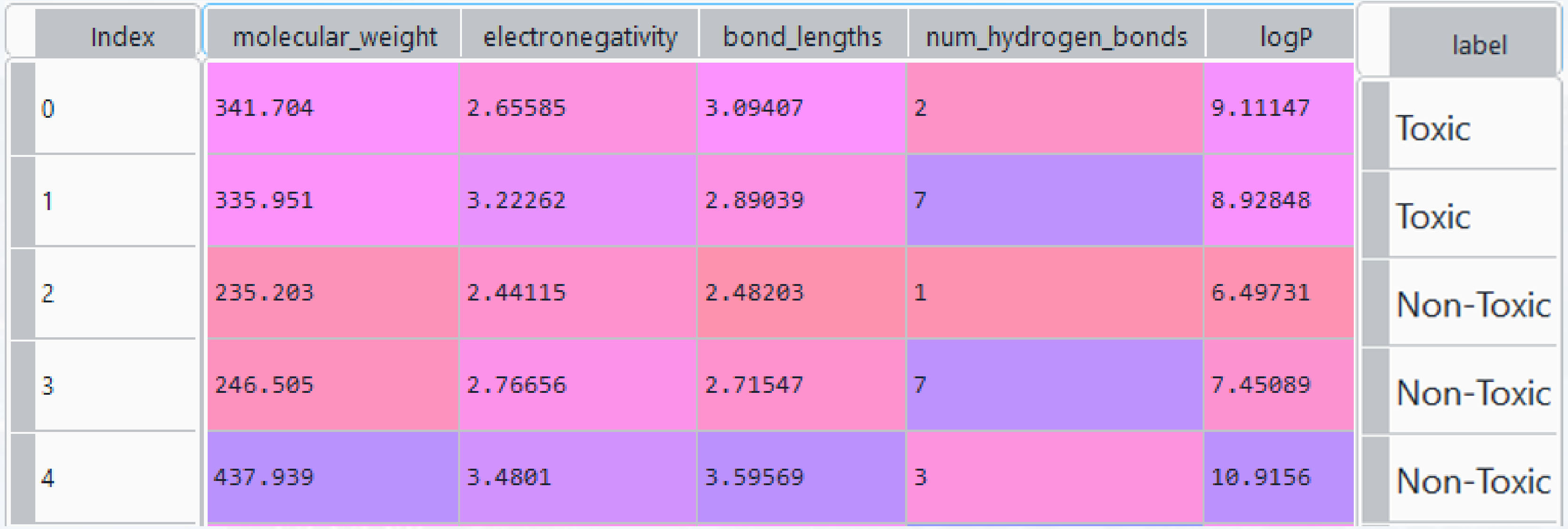
x_i is the desired regressor, for example, age again (x_2)

the factors $\boldsymbol{\beta_i}$ indicate how strong (and in which direction) *p* changes wrt a regressor $\boldsymbol{x_i}$

1) loading data
2) plotting data
3) scaling data
4) fitting model
5) evaluating model

let us return to the molecule data set:

```
Train   = pd.read_csv("molecular_train_gbc_cat.csv")
Test    = pd.read_csv("molecular_test_gbc_cat.csv")
```



Index	molecular_weight	electronegativity	bond_lengths	num_hydrogen_bonds	logP	label
0	341.704	2.65585	3.09407	2	9.11147	Toxic
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4	437.939	3.4801	3.59569	3	10.9156	Non-Toxic

```
import statsmodels.api as sm
```

1) loading data
2) plotting data
3) scaling data
4) fitting model
5) evaluating model

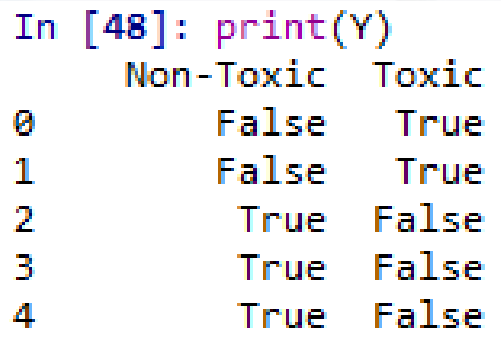
it is the same data set → plotting and scaling is as before

```
X = sm.add_constant(TrainS)
```

adding the intercept

```
Y = pd.get_dummies(Train['label'])
```

Python needs True/False as categorical



```
In [48]: print(Y)
     Non-Toxic  Toxic
0        False   True
1        False   True
2         True  False
3         True  False
4         True  False
```

$$p = \frac{e^{\beta_0+\beta_1 x_1+\cdots}}{1+e^{\beta_0+\beta_1 x_1+\cdots}}$$

```
my_model = sm.GLM(Y, X, family = sm.families.Binomial()).fit()

my_model.summary()
```

we have two states: toxic / non-toxic

GLM: general linear model

Linear and Non-Linear Regression

Logistic Regression

1) loading data
2) plotting data
3) scaling data
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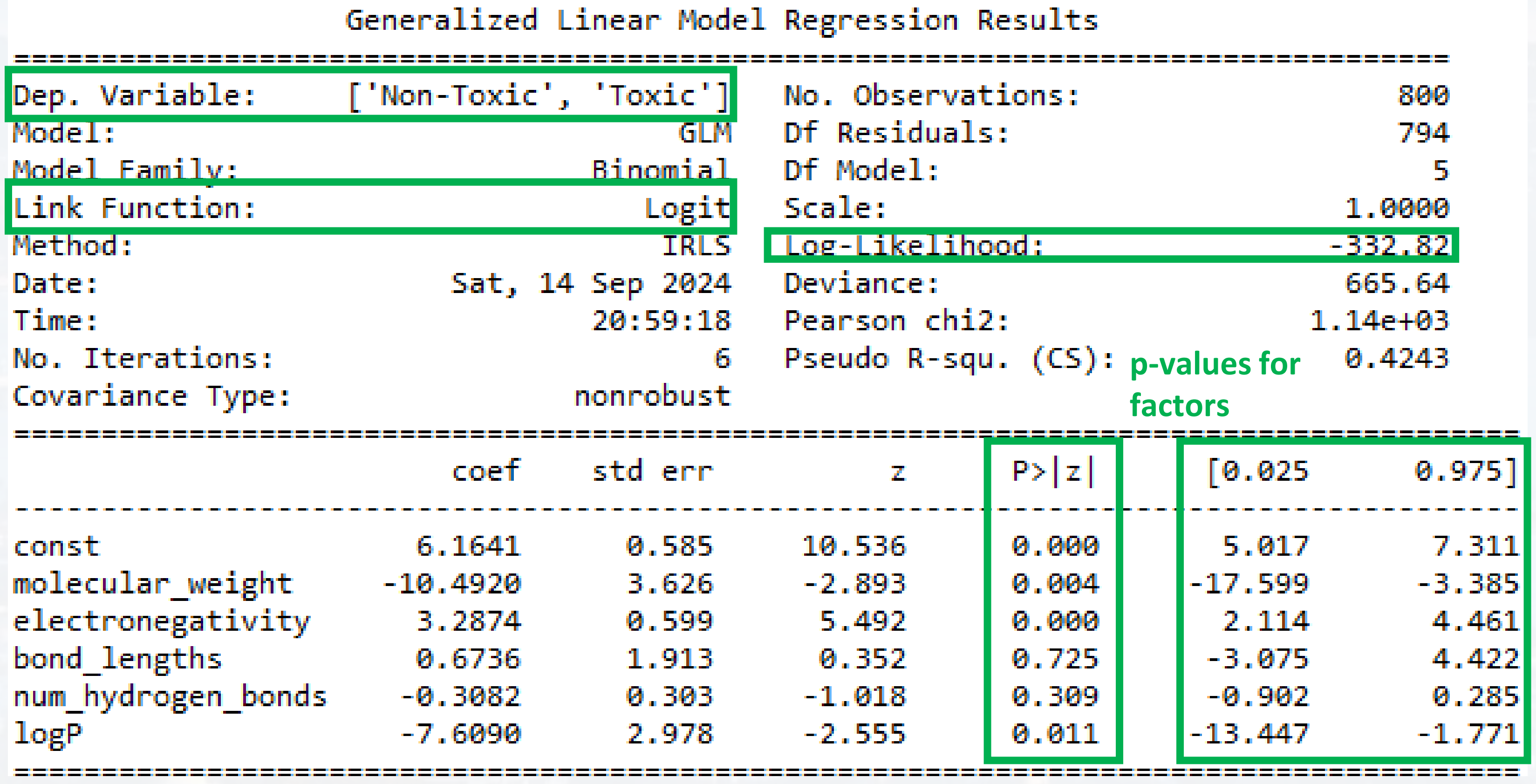
it is the same data set → plotting and scaling is as before

```
X = sm.add_constant(TrainS)
Y = pd.get_dummies(Train['label'])

my_model = sm.GLM(Y, X, family = sm.families.Binomial()).fit()
my_model.summary()
```

$$p = \frac{e^{\beta_0+\beta_1 x_1+\cdots}}{1+e^{\beta_0+\beta_1 x_1+\cdots}}$$



```
                 Generalized Linear Model Regression Results
==============================================================================
Dep. Variable:      ['Non-Toxic', 'Toxic']   No. Observations:             800
Model:                                 GLM   Df Residuals:                 794
Model Family:                     Binomial   Df Model:                       5
Link Function:                       Logit   Scale:                     1.0000
Method:                               IRLS   Log-Likelihood:           -332.82
Date:                     Sat, 14 Sep 2024   Deviance:                  665.64
Time:                             20:59:18   Pearson chi2:             1.14e+03
No. Iterations:                          6   Pseudo R-squ. (CS):        0.4243
Covariance Type:                 nonrobust
=======================================================================================
                          coef    std err          z      P>|z|      [0.025      0.975]
---------------------------------------------------------------------------------------
const                   6.1641      0.585     10.536      0.000       5.017       7.311
molecular_weight      -10.4920      3.626     -2.893      0.004     -17.599      -3.385
electronegativity       3.2874      0.599      5.492      0.000       2.114       4.461
bond_lengths            0.6736      1.913      0.352      0.725      -3.075       4.422
num_hydrogen_bonds     -0.3082      0.303     -1.018      0.309      -0.902       0.285
logP                   -7.6090      2.978     -2.555      0.011     -13.447      -1.771
=======================================================================================
```

p-value for constant model

p-values for factors

2σ conf range of factors

accuracy: How ***often*** did the model make the correct prediction.

cross-entropy: How ***certain*** was the model when making the prediction.

1) loading data
2) plotting data
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1) loading data
2) plotting data
3) scaling data
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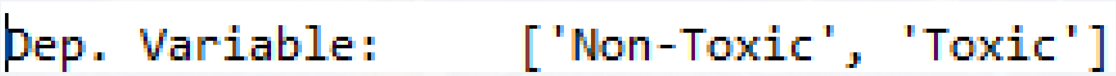
accuracy: How ***often*** did the model make the correct prediction.

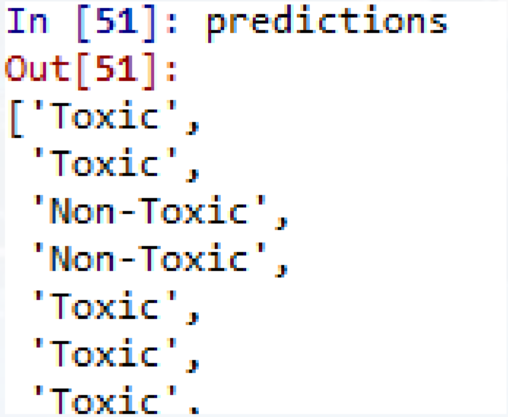
cross-entropy: How ***certain*** was the model when making the prediction.

```
predProbs   = my_model.predict(sm.add_constant(TestS))

Pred        = np.round(predProbs).astype(int)
predictions = ['Non-Toxic' if i==1 else 'Toxic' for i in Pred]
```

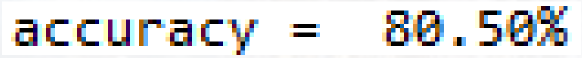


```
Dep. Variable:      ['Non-Toxic', 'Toxic']
```



```
In [51]: predictions
Out[51]:
['Toxic',
 'Toxic',
 'Non-Toxic',
 'Non-Toxic',
 'Toxic',
 'Toxic',
 'Toxic',
```

```
TestY       = Test['label']
accuracy    = 100*(TestY == predictions).sum()/len(predictions)
print(f'accuracy = {accuracy: .2f}%')
```



```
accuracy =  80.50%
```

Linear and Non-Linear Regression

Logistic Regression

1) loading data
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accuracy: How ***often*** did the model make the correct prediction.

cross-entropy: How ***certain*** was the model when making the prediction.

accuracy is ≈ 80% But does it depend on the class? → **confusion matrix**

<u>ideal world:</u>

true label	**non-toxic**	**toxic**
non-toxic	**100%**	**0%**
toxic	**0%**	**100%**

predicted label

```
from sklearn.metrics import confusion_matrix, ConfusionMatrixDisplay
```

1) loading data
2) plotting data
3) scaling data
4) fitting model
5) evaluating model

accuracy: How ***often*** did the model make the correct prediction.

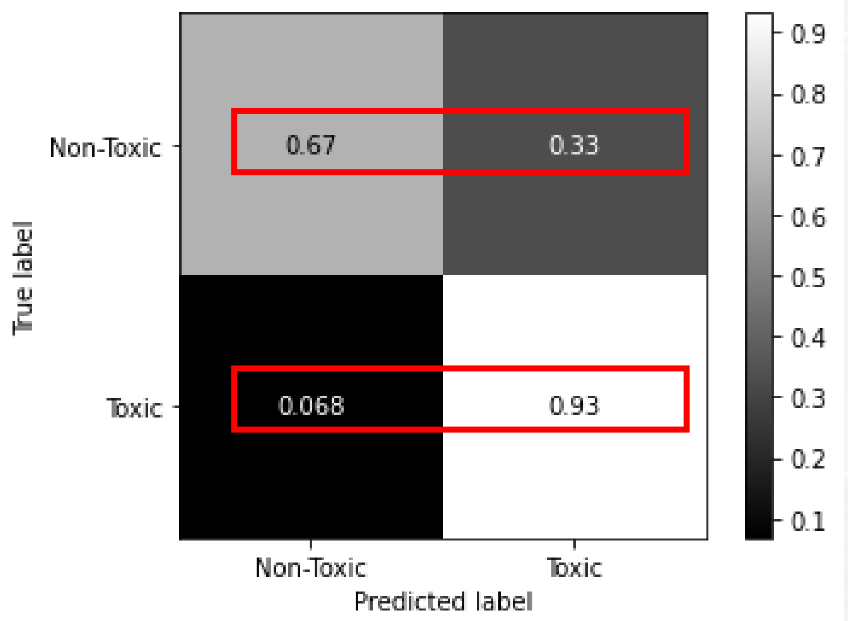
cross-entropy: How ***certain*** was the model when making the prediction.

accuracy is ≈ 80% But does it depend on the class? → **confusion matrix**

two labels

```
L = ['Non-Toxic', 'Toxic']

cm   = confusion_matrix(TestY, predictions, labels = L, normalize = 'true')
disp = ConfusionMatrixDisplay(confusion_matrix = cm, display_labels = L)
disp.plot(cmap = 'gray')
plt.show()
```



Linear and Non-Linear Regression

accuracy: How ***often*** did the model make the correct prediction.

cross-entropy: How ***certain*** was the model when making the prediction.

1) loading data
2) plotting data
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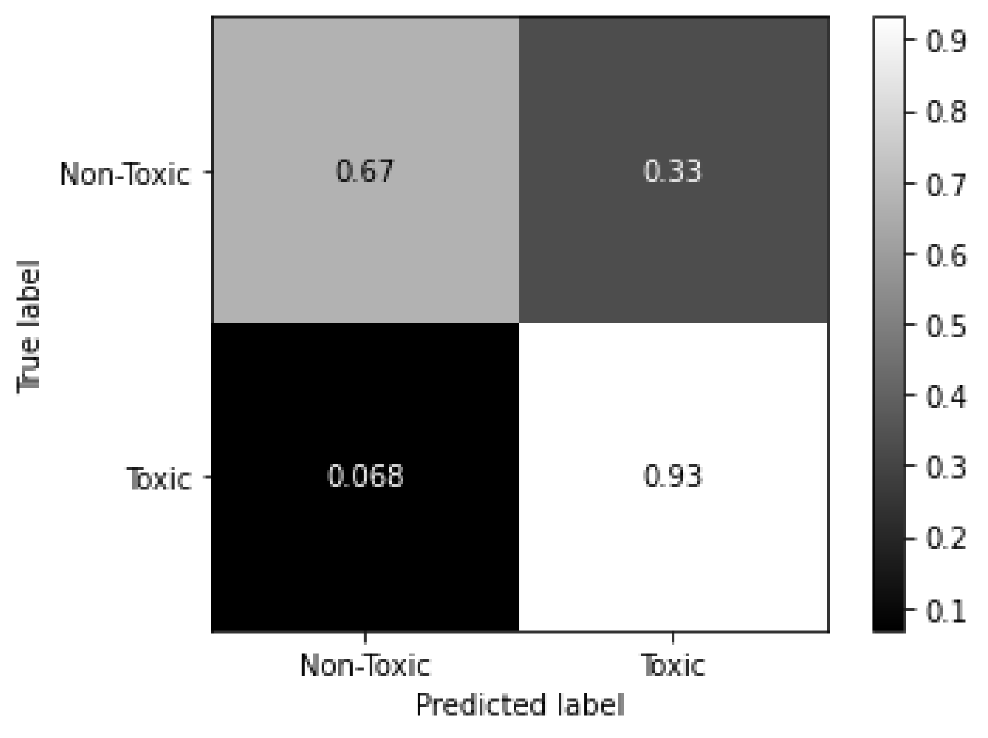
4) fitting model
5) evaluating model

accuracy is ≈ 80% But does it depend on the class? → **confusion matrix**



		predicted label	
		non-toxic	**toxic**
true label	**non-toxic**	**100%**	**0%**
	toxic	**0%**	**100%**

Linear and Non-Linear Regression

Logistic Regression

accuracy: How *often* did the model make the correct prediction.

cross-entropy: How ***certain*** was the model when making the prediction.

1) loading data
2) plotting data
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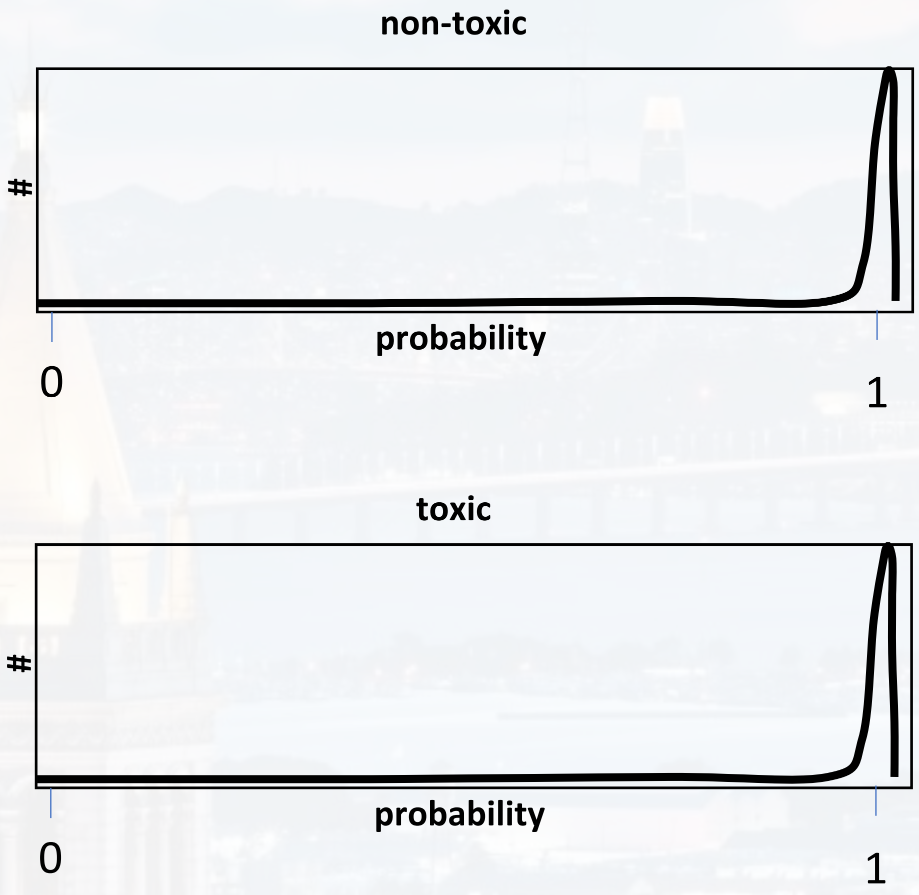
5) evaluating model

ideal world:



1) loading data
2) plotting data
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accuracy: How *often* did the model make the correct prediction.

cross-entropy: How ***certain*** was the model when making the prediction.

```
PredProbs = np.vstack((predProbs, 1 - predProbs))

fig, ax = plt.subplots(len(L), 1, sharex = True)
fig.set_figheight(6)
fig.subplots_adjust(hspace = 0.5)
fig.suptitle('entropy')
for i, l in enumerate(L):
    idx = [k for k, y in enumerate(TestY) if y == l]
    idx = np.array(idx)
    (value, where) = np.histogram(PredProbs[i,idx],\
                                  bins = np.arange(0, 1, 0.01),\
                                  density = True)
    w = 0.5*(where[1:] + where[:-1])
    ax[i].plot(w, value, 'k-')
    ax[i].set_ylabel('frequency')
    ax[i].set_title(l)
ax[len(L)-1].set_xlabel('probability')
plt.show()
```

Linear and Non-Linear Regression

accuracy: How ***often*** did the model make the correct prediction.

cross-entropy: How ***certain*** was the model when making the prediction.

1) loading data
2) plotting data
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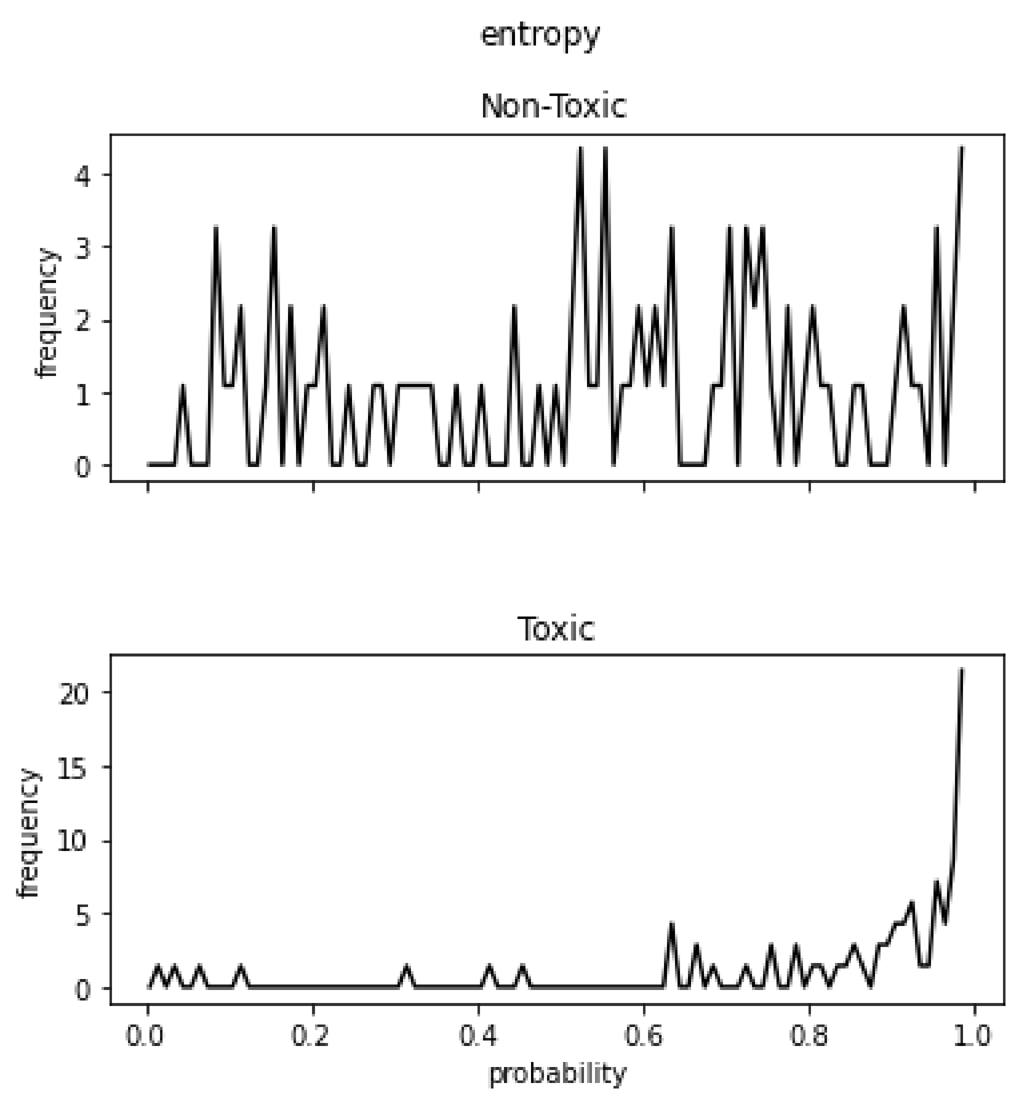
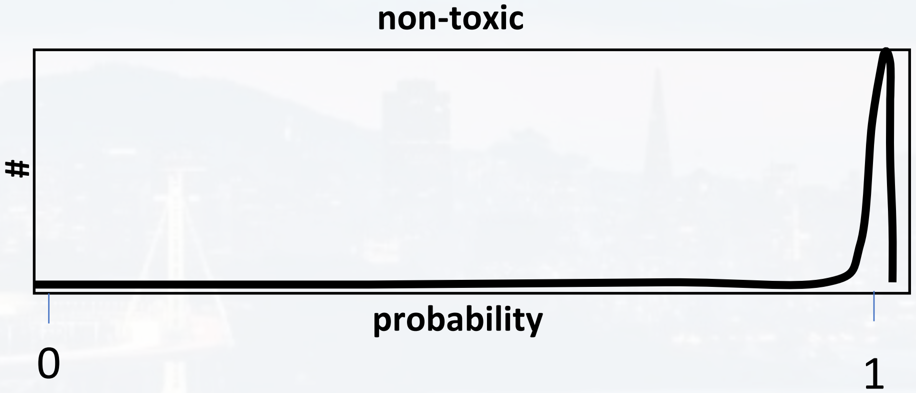
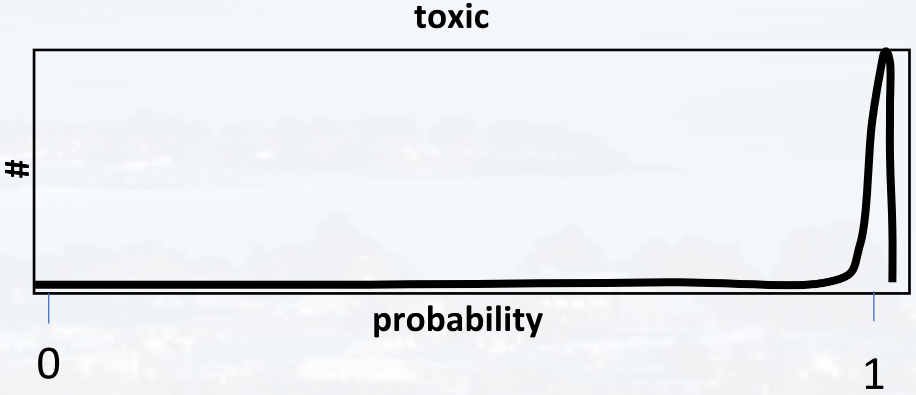
5) evaluating model







Thank you very much for your attention!