Introduction to Machine Learning - Exercise 1

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Problem 1

Task a

Read p1.csv into dataframe and drop columns “id”, “SMILES”, “InChIKey”

```
p1data <- read.csv("data/p1.csv", header=TRUE, sep=",")
p1data <- subset(p1data, select=-c(id, SMILES, InChIKey))
```

Task b

Summary statistics for variables “pSat_PA”, “NumOfConf” and “ChemPot_kJmol”:

	pSat_Pa	NumOfConf	ChemPot_kJmol
	Min. : 0.0000	Min. : 2.00	Min. :-3.160
	1st Qu.: 0.0000	1st Qu.: 73.25	1st Qu.: 9.723
	Median : 0.0001	Median : 172.50	Median :12.781
	Mean : 2.9620	Mean : 223.50	Mean :12.434
	3rd Qu.: 0.0023	3rd Qu.: 324.25	3rd Qu.:15.659
	Max. :562.8970	Max. :1058.00	Max. :28.096

Task c

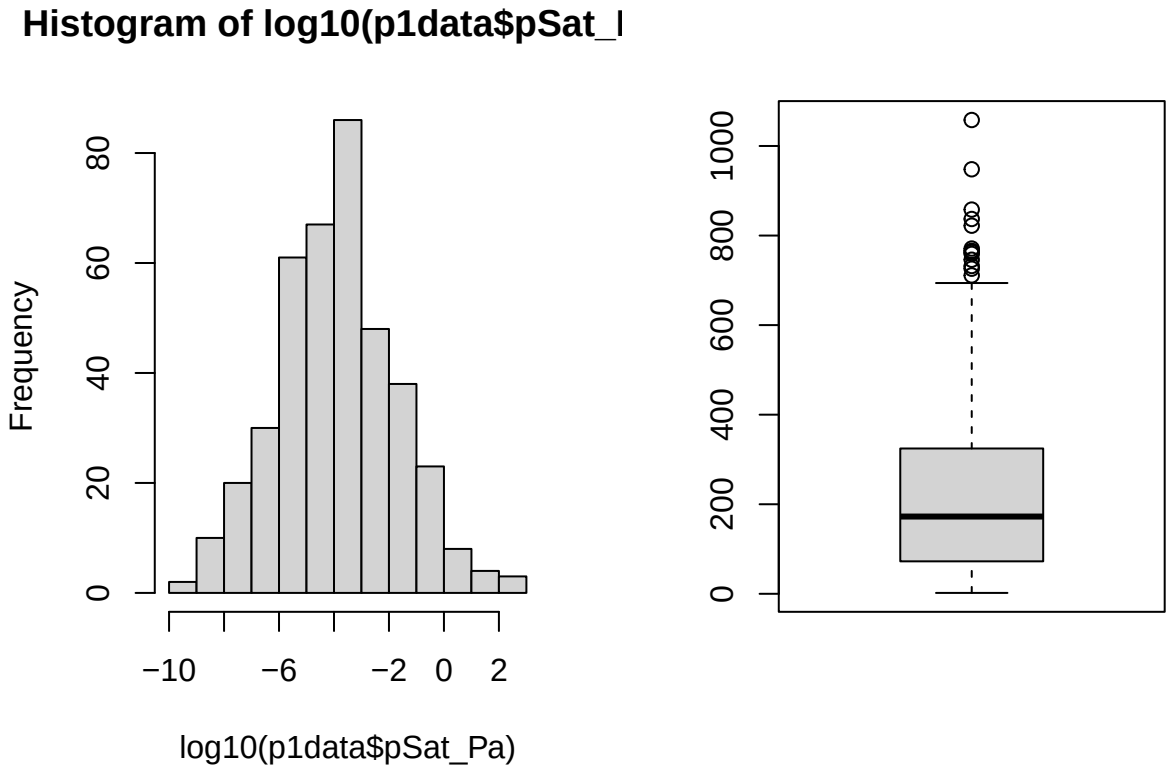
Mean and standard deviation of column ‘ChemPot_kJmol’ are:

[1] “Mean: 12.4344270896”

[1] “Standard deviation: 4.77887217784492”

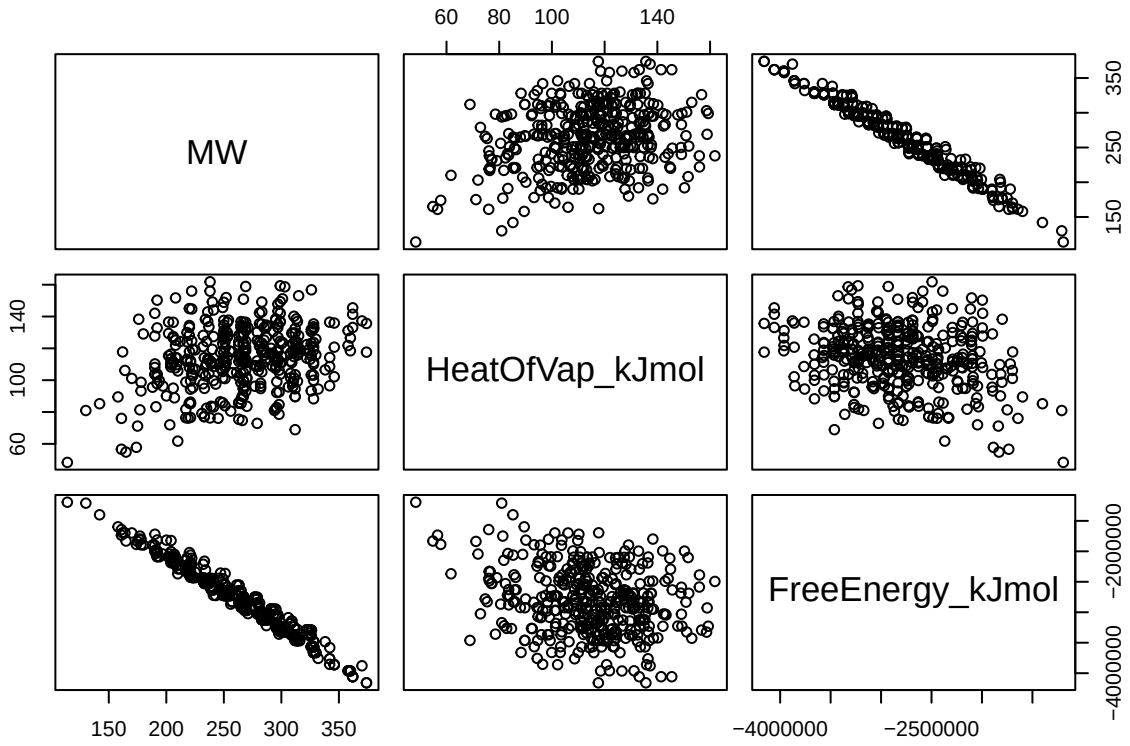
Task d

```
par(mfrow=c(1,2))
hist(log10(p1data$pSat_Pa))
boxplot(p1data$NumOfConf)
```



Task e

```
scatter_subset <- subset(p1data, select=c(MW, HeatOfVap_kJmol, FreeEnergy_kJmol))
pairs(scatter_subset)
```



Problem 2

Task a

Degree	Train	Validation	Test	TestTRVA	CV
0	4.5122613	4.512261	4.512261e+00	4.587239	6.0767506
1	4.0885351	3.494124	5.206372e+00	4.786172	10.5013228
2	0.2185859	7.021118	1.424954e+01	14.791603	0.3622867
3	0.2168190	7.154893	1.383458e+01	14.096042	0.3778728
4	0.1187955	8.776121	1.968113e+01	15.009734	0.4185159
5	0.0965322	7.221166	2.975686e+01	20.134323	0.3094141
6	0.0075741	6.050151	1.564333e+02	12.060633	0.4092672
7	0.0049994	11.394430	1.104038e+03	15.628661	1.2762072
8	0.0020825	407.157118	1.561695e+05	10.979288	17.2093697

Task b

Task c

```
library(rmarkdown)
```