Introduction into machine learning and analyzes of Breast Cancer Proteomes

true

September 15th, 2022

Contents

Dataset

About Dataset

information about the data set and the three give files :

Context: This data set contains published iTRAQ proteome profiling of 77 breast cancer samples generated by the Clinical Proteomic Tumor Analysis Consortium (NCI/NIH). It contains expression values for ~12.000 proteins for each sample, with missing values present when a given protein could not be quantified in a given sample.

Content:

- **File:** 77cancerproteomesCPTACitraq.csv
  - **RefSeqaccessionnumber:** RefSeq protein ID (each protein has a unique ID in a RefSeq database)
  - **gene_symbol:** a symbol unique to each gene (every protein is encoded by some gene)
  - **gene_name:** a full name of that gene
  - **Remaining columns:** log2 iTRAQ ratios for each sample (protein expression data, most important), three last columns are from healthy individuals
- **File:** clinicaldatabreast_cancer.csv
  - **First column** "Complete TCGA ID" is used to match the sample IDs in the main cancer proteomes file (see example script).
  - **All other columns** have self-explanatory names, contain data about the cancer classification of a given sample using different methods. 'PAM50 mRNA' classification is being used in the example script.

- **File:** PAM50_proteins.csv
  - **Contains** the list of genes and proteins used by the PAM50 classification system. The column RefSeqProteinID contains the protein IDs that can be matched with the IDs in the main protein expression data set.

Past Research: Original research paper: https://www.researchgate.net/publication/303509927_Proteogenomics_connects_somatic_mutations_to_signaling_in_breast_cancer

Summary: the data were used to assess how the mutations in the DNA are affecting the protein expression landscape in breast cancer. Genes in our DNA are first transcribed into RNA molecules which then are translated into proteins. Changing the information content of DNA has impact on the behavior of the proteome, which is the main functional unit of cells, taking care of cell division, DNA repair, enzymatic reactions and signaling etc. They performed K-means clustering on the protein data to divide the breast cancer patients into sub-types, each having unique protein expression signature. They found that the best clustering was achieved using 3 clusters (original PAM50 gene set yields four different subtypes using RNA data). my question is are there different ways to categorize subtypes of breast cancer other than the PAM50 method, and define them as benign or malignant?

```
# packages
library(pander)
library(tidyr)
library(dplyr)
```

```
##
## Attaching package: 'dplyr'

## The following objects are masked from 'package:stats':
##
##     filter, lag

## The following objects are masked from 'package:base':
##
##     intersect, setdiff, setequal, union
```

```
library(reticulate)
library(here)
```

```
## here() starts at C:/Users/matsp/Documents/Thema-09/Project_thema_09
```

```
library(RcppTOML)
library(ggplot2)
library(gridExtra)
```

```
##
## Attaching package: 'gridExtra'

## The following object is masked from 'package:dplyr':
##
##     combine
```

```
library(stringr)
```

Exploratory Data Analysis

loading of the dataframes and showing the successful loading and its dimensions. note only the first 5 columns of "77_cancer_proteomes_CPTAC_itraq.csv" are shown since after column 4 they are the same type.

```
proteomes_data <- read.csv(file = "Data//77_cancer_proteomes_CPTAC_itraq.csv")
proteomes_data2 <- read.csv(file = "Data//77_cancer_proteomes_CPTAC_itraq_test1.csv")
#py$data <- proteomes_data
clinical_data <- read.csv(file = "Data/clinical_data_breast_cancer.csv")
pam50_protein_data <- read.csv(file = "Data/PAM50_proteins.csv")

# showing succeseful loading of data

# only showing first 5 columns of proteomes
head(proteomes_data[1:5], n = 5)
```

```
##   RefSeq_accession_number gene_symbol          gene_name A0.A12D.01TCGA
## 1               NP_958782        PLEC  plectin isoform 1       1.096131
## 2               NP_958785        <NA> plectin isoform 1g       1.111370
## 3               NP_958786        PLEC plectin isoform 1a       1.111370
## 4               NP_000436        <NA> plectin isoform 1c       1.107561
## 5               NP_958781        <NA> plectin isoform 1e       1.115180
##   C8.A131.01TCGA
## 1       2.609943
## 2       2.650422
## 3       2.650422
## 4       2.646374
## 5       2.646374
```

```
head(clinical_data, n=5)
```

```
##   Complete.TCGA.ID Gender Age.at.Initial.Pathologic.Diagnosis ER.Status
## 1     TCGA-A2-A0T2 FEMALE                                  66  Negative
## 2     TCGA-A2-A0CM FEMALE                                  40  Negative
## 3     TCGA-BH-A18V FEMALE                                  48  Negative
## 4     TCGA-BH-A18Q FEMALE                                  56  Negative
## 5     TCGA-BH-A0E0 FEMALE                                  38  Negative
##   PR.Status HER2.Final.Status Tumor Tumor..T1.Coded Node Node.Coded Metastasis
## 1  Negative          Negative    T3         T_Other   N3   Positive         M1
## 2  Negative          Negative    T2         T_Other   N0   Negative         M0
## 3  Negative          Negative    T2         T_Other   N1   Positive         M0
## 4  Negative          Negative    T2         T_Other   N1   Positive         M0
## 5  Negative          Negative    T3         T_Other   N3   Positive         M0
##   Metastasis.Coded AJCC.Stage Converted.Stage Survival.Data.Form Vital.Status
## 1         Positive   Stage IV   No_Conversion           followup     DECEASED
## 2         Negative  Stage IIA       Stage IIA           followup     DECEASED
## 3         Negative  Stage IIB   No_Conversion         enrollment     DECEASED
## 4         Negative  Stage IIB   No_Conversion         enrollment     DECEASED
```

```
## 5         Negative Stage IIIC   No_Conversion           followup       LIVING
##   Days.to.Date.of.Last.Contact Days.to.date.of.Death OS.event OS.Time
## 1                          240                  240        1     240
## 2                          754                  754        1     754
## 3                         1555                 1555        1    1555
## 4                         1692                 1692        1    1692
## 5                          133                   NA        0     133
##   PAM50.mRNA SigClust.Unsupervised.mRNA SigClust.Intrinsic.mRNA miRNA.Clusters
## 1 Basal-like                         0                     -13              3
## 2 Basal-like                       -12                     -13              4
## 3 Basal-like                       -12                     -13              5
## 4 Basal-like                       -12                     -13              5
## 5 Basal-like                         0                     -13              5
##   methylation.Clusters RPPA.Clusters CN.Clusters
## 1                    5         Basal           3
## 2                    4         Basal           4
## 3                    5         Basal           1
## 4                    5         Basal           1
## 5                    5         Basal           1
##   Integrated.Clusters..with.PAM50. Integrated.Clusters..no.exp.
## 1                                2                           2
## 2                                2                           1
## 3                                2                           2
## 4                                2                           2
## 5                                2                           2
##   Integrated.Clusters..unsup.exp.
## 1                               2
## 2                               1
## 3                               2
## 4                               2
## 5                               2
```

```
head(pam50_protein_data, n=5)
```

```
##   GeneSymbol RefSeqProteinID      Species                          Gene.Name
## 1        MIA       NP_006524 Homo sapiens        melanoma inhibitory activity
## 2      FGFR4       NP_002002 Homo sapiens fibroblast growth factor receptor 4
## 3      FGFR4       NP_998812 Homo sapiens fibroblast growth factor receptor 4
## 4      FGFR4       NP_075252 Homo sapiens fibroblast growth factor receptor 4
## 5     GPR160       NP_055188 Homo sapiens      G protein-coupled receptor 160
```

```
# showing the structure/dimensions of dataframe
cat("77_cancer_proteomes_CPTAC_itraq [ number of rows:", nrow(proteomes_data), "number of columns:",ncol
```

```
## 77_cancer_proteomes_CPTAC_itraq [ number of rows: 12553 number of columns: 86
```

```
cat("clinical_data [ number of rows:", nrow(clinical_data), "number of columns:",ncol(clinical_data),'\n
```

```
## clinical_data [ number of rows: 105 number of columns: 30
```

```
cat("pam50_protein_data [ number of rows:", nrow(pam50_protein_data), "number of columns:",ncol(pam50_p
```

```
## pam50_protein_data [ number of rows: 100 number of columns: 4
```

Checking if the Proteomes data has been correctly read.

```
str(proteomes_data)
```

```
## 'data.frame':    12553 obs. of  86 variables:
##  $ RefSeq_accession_number: chr  "NP_958782" "NP_958785" "NP_958786" "NP_000436" ...
##  $ gene_symbol            : chr  "PLEC" NA "PLEC" NA ...
##  $ gene_name              : chr  "plectin isoform 1" "plectin isoform 1g" "plectin isoform 1a" "plec
##  $ A0.A12D.01TCGA         : num  1.1 1.11 1.11 1.11 1.12 ...
##  $ C8.A131.01TCGA         : num  2.61 2.65 2.65 2.65 2.65 ...
##  $ A0.A12B.01TCGA         : num  -0.66 -0.649 -0.654 -0.632 -0.64 ...
##  $ BH.A18Q.02TCGA         : num  0.195 0.215 0.215 0.205 0.215 ...
##  $ C8.A130.02TCGA         : num  -0.494 -0.504 -0.501 -0.51 -0.504 ...
##  $ C8.A138.03TCGA         : num  2.77 2.78 2.78 2.8 2.79 ...
##  $ E2.A154.03TCGA         : num  0.863 0.87 0.87 0.866 0.87 ...
##  $ C8.A12L.04TCGA         : num  1.41 1.41 1.41 1.41 1.41 ...
##  $ A2.A0EX.04TCGA         : num  1.19 1.19 1.19 1.19 1.2 ...
##  $ A0.A12D.05TCGA         : num  1.1 1.1 1.1 1.1 1.09 ...
##  $ AN.A04A.05TCGA         : num  0.385 0.371 0.371 0.378 0.375 ...
##  $ BH.A0AV.05TCGA         : num  0.351 0.367 0.367 0.361 0.371 ...
##  $ C8.A12T.06TCGA         : num  -0.205 -0.162 -0.167 -0.184 -0.167 ...
##  $ A8.A06Z.07TCGA         : num  -0.496 -0.499 -0.496 -0.492 -0.488 ...
##  $ A2.A0CM.07TCGA         : num  0.683 0.694 0.698 0.687 0.687 ...
##  $ BH.A18U.08TCGA         : num  -0.265 -0.252 -0.252 -0.252 -0.252 ...
##  $ A2.A0EQ.08TCGA         : num  -0.913 -0.928 -0.928 -0.932 -0.928 ...
##  $ AR.A0U4.09TCGA         : num  -0.0332 -0.0302 -0.0272 -0.0302 -0.0302 ...
##  $ A0.A0J9.10TCGA         : num  0.02 0.012 0.012 0.0039 0.012 ...
##  $ AR.A1AP.11TCGA         : num  0.461 0.461 0.461 0.461 0.461 ...
##  $ AN.A0FK.11TCGA         : num  0.974 0.977 0.977 0.97 0.985 ...
##  $ A0.A0J6.11TCGA         : num  0.831 0.857 0.857 0.837 0.865 ...
##  $ A7.A13F.12TCGA         : num  1.28 1.28 1.28 1.28 1.28 ...
##  $ BH.A0E1.12TCGA         : num  0.762 0.762 0.766 0.758 0.766 ...
##  $ A7.A0CE.13TCGA         : num  -1.12 -1.12 -1.12 -1.13 -1.13 ...
##  $ A2.A0YC.13TCGA         : num  0.819 0.815 0.815 0.799 0.819 ...
##  $ A0.A0JC.14TCGA         : num  -0.307 -0.307 -0.307 -0.307 -0.301 ...
##  $ A8.A08Z.14TCGA         : num  0.569 0.569 0.569 0.569 0.569 ...
##  $ AR.A0TX.14TCGA         : num  -0.583 -0.573 -0.567 -0.583 -0.573 ...
##  $ A8.A076.15TCGA         : num  1.87 1.87 1.87 1.86 1.87 ...
##  $ A0.A126.15TCGA         : num  0.196 0.196 0.196 0.219 0.2 ...
##  $ BH.A0C1.16TCGA         : num  -0.518 -0.51 -0.507 -0.518 -0.513 ...
##  $ A2.A0EY.16TCGA         : num  1.17 1.18 1.18 1.17 1.18 ...
##  $ AR.A1AW.17TCGA         : num  0.578 0.582 0.578 0.59 0.586 ...
##  $ AR.A1AV.17TCGA         : num  -0.76 -0.76 -0.749 -0.736 -0.749 ...
##  $ C8.A135.17TCGA         : num  1.12 1.14 1.14 1.14 1.12 ...
##  $ A2.A0EV.18TCGA         : num  0.453 0.473 0.473 0.459 0.473 ...
##  $ AN.A0AM.18TCGA         : num  1.5 1.51 1.5 1.5 1.5 ...
##  $ D8.A142.18TCGA         : num  0.539 0.542 0.542 0.535 0.542 ...
##  $ AN.A0FL.19TCGA         : num  2.46 2.48 2.48 2.46 2.48 ...
```

```
##  $ BH.A0DG.19TCGA         : num  -0.206 -0.206 -0.206 -0.215 -0.206 ...
##  $ AR.A0TV.20TCGA         : num  -1.51 -1.53 -1.53 -1.53 -1.51 ...
##  $ C8.A12Z.20TCGA         : num  -0.787 -0.756 -0.756 -0.775 -0.772 ...
##  $ A0.A0JJ.20TCGA         : num  0.757 0.781 0.774 0.764 0.771 ...
##  $ A0.A0JE.21TCGA         : num  0.56 0.563 0.56 0.542 0.56 ...
##  $ AN.A0AJ.21TCGA         : num  -0.428 -0.406 -0.406 -0.406 -0.406 ...
##  $ A7.A0CJ.22TCGA         : num  -1.001 -1.005 -1.005 -0.998 -1.001 ...
##  $ A0.A12F.22TCGA         : num  -1.95 -1.95 -1.96 -1.95 -1.96 ...
##  $ A8.A079.23TCGA         : num  1.05 1.05 1.05 1.06 1.05 ...
##  $ A2.A0T3.24TCGA         : num  0.584 0.581 0.581 0.587 0.587 ...
##  $ A2.A0YD.24TCGA         : num  0.0638 0.0933 0.0845 0.0667 0.0845 ...
##  $ AR.A0TR.25TCGA         : num  -1.1 -1.11 -1.11 -1.1 -1.11 ...
##  $ A0.A03O.25TCGA         : num  1.05 1.06 1.06 1.06 1.06 ...
##  $ A0.A12E.26TCGA         : num  0.265 0.276 0.276 0.278 0.278 ...
##  $ A8.A06N.26TCGA         : num  0.239 0.25 0.244 0.25 0.25 ...
##  $ A2.A0YG.27TCGA         : num  -0.0782 -0.0681 -0.0714 -0.0579 -0.0647 ...
##  $ BH.A18N.27TCGA         : num  1.1 1.1 1.1 1.09 1.11 ...
##  $ AN.A0AL.28TCGA         : num  0.324 0.327 0.327 0.33 0.327 ...
##  $ A2.A0T6.29TCGA         : num  0.794 0.818 0.815 0.801 0.818 ...
##  $ E2.A158.29TCGA         : num  -1.09 -1.1 -1.1 -1.1 -1.1 ...
##  $ E2.A15A.29TCGA         : num  2.18 2.18 2.18 2.18 2.18 ...
##  $ A0.A0JM.30TCGA         : num  1.4 1.41 1.41 1.41 1.41 ...
##  $ C8.A12V.30TCGA         : num  0.674 0.689 0.689 0.678 0.689 ...
##  $ A2.A0D2.31TCGA         : num  0.1075 0.1042 0.1075 0.0975 0.1042 ...
##  $ C8.A12U.31TCGA         : num  -0.482 -0.478 -0.482 -0.471 -0.482 ...
##  $ AR.A1AS.31TCGA         : num  1.22 1.22 1.22 1.2 1.22 ...
##  $ A8.A09G.32TCGA         : num  -1.52 -1.51 -1.51 -1.52 -1.51 ...
##  $ C8.A131.32TCGA         : num  2.71 2.73 2.74 2.73 2.75 ...
##  $ C8.A134.32TCGA         : num  0.14 0.126 0.133 0.112 0.126 ...
##  $ A2.A0YF.33TCGA         : num  0.311 0.296 0.296 0.296 0.296 ...
##  $ BH.A0DD.33TCGA         : num  -0.692 -0.659 -0.664 -0.657 -0.662 ...
##  $ BH.A0E9.33TCGA         : num  1.47 1.48 1.47 1.46 1.47 ...
##  $ AR.A0TT.34TCGA         : num  -0.511 -0.526 -0.526 -0.533 -0.53 ...
##  $ A0.A12B.34TCGA         : num  -0.964 -0.938 -0.944 -0.935 -0.935 ...
##  $ A2.A0SW.35TCGA         : num  -0.488 -0.488 -0.488 -0.488 -0.504 ...
##  $ A0.A0JL.35TCGA         : num  -0.107 -0.107 -0.107 -0.107 -0.107 ...
##  $ BH.A0BV.35TCGA         : num  -0.0658 -0.0559 -0.0658 -0.0559 -0.0625 ...
##  $ A2.A0YM.36TCGA         : num  0.656 0.658 0.656 0.656 0.651 ...
##  $ BH.A0C7.36TCGA         : num  -0.552 -0.548 -0.552 -0.552 -0.557 ...
##  $ A2.A0SX.36TCGA         : num  -0.399 -0.393 -0.393 -0.393 -0.396 ...
##  $ X263d3f.I.CPTAC        : num  0.599 0.607 0.604 0.604 0.604 ...
##  $ blcdb9.I.CPTAC         : num  -0.191 -0.184 -0.186 -0.186 -0.167 ...
##  $ c4155b.C.CPTAC         : num  0.567 0.579 0.577 0.577 0.577 ...
```

Nothing strange about the Proteomes dat everything seems to be read correct.

Checking if the clinical data has been correctly read.

```
str(clinical_data)
```

```
## 'data.frame':    105 obs. of  30 variables:
##  $ Complete.TCGA.ID                  : chr  "TCGA-A2-A0T2" "TCGA-A2-A0CM" "TCGA-BH-A18V" "TCGA-BH-A
##  $ Gender                            : chr  "FEMALE" "FEMALE" "FEMALE" "FEMALE" ...
##  $ Age.at.Initial.Pathologic.Diagnosis: int  66 40 48 56 38 57 74 60 61 67 ...
```

```
##  $ ER.Status                          : chr  "Negative" "Negative" "Negative" "Negative" ...
##  $ PR.Status                          : chr  "Negative" "Negative" "Negative" "Negative" ...
##  $ HER2.Final.Status                  : chr  "Negative" "Negative" "Negative" "Negative" ...
##  $ Tumor                              : chr  "T3" "T2" "T2" "T2" ...
##  $ Tumor..T1.Coded                    : chr  "T_Other" "T_Other" "T_Other" "T_Other" ...
##  $ Node                               : chr  "N3" "N0" "N1" "N1" ...
##  $ Node.Coded                         : chr  "Positive" "Negative" "Positive" "Positive" ...
##  $ Metastasis                         : chr  "M1" "M0" "M0" "M0" ...
##  $ Metastasis.Coded                   : chr  "Positive" "Negative" "Negative" "Negative" ...
##  $ AJCC.Stage                         : chr  "Stage IV" "Stage IIA" "Stage IIB" "Stage IIB" ...
##  $ Converted.Stage                    : chr  "No_Conversion" "Stage IIA" "No_Conversion" "No_Conversi
##  $ Survival.Data.Form                 : chr  "followup" "followup" "enrollment" "enrollment" ...
##  $ Vital.Status                       : chr  "DECEASED" "DECEASED" "DECEASED" "DECEASED" ...
##  $ Days.to.Date.of.Last.Contact       : int  240 754 1555 1692 133 309 425 643 775 964 ...
##  $ Days.to.date.of.Death              : int  240 754 1555 1692 NA NA NA NA NA NA ...
##  $ OS.event                           : int  1 1 1 1 0 0 0 0 0 0 ...
##  $ OS.Time                            : int  240 754 1555 1692 133 309 425 643 775 964 ...
##  $ PAM50.mRNA                         : chr  "Basal-like" "Basal-like" "Basal-like" "Basal-like" ...
##  $ SigClust.Unsupervised.mRNA         : int  0 -12 -12 -12 0 0 0 -12 -12 -12 ...
##  $ SigClust.Intrinsic.mRNA            : int  -13 -13 -13 -13 -13 -13 -13 -13 -13 -13 ...
##  $ miRNA.Clusters                     : int  3 4 5 5 5 5 3 5 2 5 ...
##  $ methylation.Clusters               : int  5 4 5 5 5 5 5 5 5 5 ...
##  $ RPPA.Clusters                      : chr  "Basal" "Basal" "Basal" "Basal" ...
##  $ CN.Clusters                        : int  3 4 1 1 1 1 1 1 1 3 ...
##  $ Integrated.Clusters..with.PAM50.   : int  2 2 2 2 2 2 2 2 2 2 ...
##  $ Integrated.Clusters..no.exp.       : int  2 1 2 2 2 2 2 2 2 2 ...
##  $ Integrated.Clusters..unsup.exp.    : int  2 1 2 2 2 2 2 2 2 2 ...
```

Nothing strange about the clinical data everything seems to be read correct.

Checking if the pam50 protein data has been correctly read.

```
str(pam50_protein_data)
```

```
## 'data.frame':    100 obs. of  4 variables:
##  $ GeneSymbol     : chr  "MIA" "FGFR4" "FGFR4" "FGFR4" ...
##  $ RefSeqProteinID: chr  "NP_006524" "NP_002002" "NP_998812" "NP_075252" ...
##  $ Species        : chr  "Homo sapiens" "Homo sapiens" "Homo sapiens" "Homo sapiens" ...
##  $ Gene.Name      : chr  "melanoma inhibitory activity" "fibroblast growth factor receptor 4" "fibrol
```

Nothing strange about the pam50 protein data everything seems to be read correct.

codebook

loading of the created codebooks for the three dataframes. showing also its contents and successful loading

```
cancer_proteomes_CPTAC_codebook <- read.csv2("Data/77_cancer_proteomes_CPTAC_codebook.txt")
clinical_data_codebook <- read.csv2("Data/clinical_data_breast_cancer_codebook.txt")
PAM50_protein_codebook <- read.csv2("Data/PAM50_protein_codebook.txt", sep = ";")


cancer_proteomes_CPTAC_codebook
```

```
##                    Column            Description data.type unit
## 1 RefSeq_accession_number      RefSeq protein ID    string   NA
## 2             gene_symbol Gene abbreviation code    string   NA
## 3                gene_name       Name of the gene    string   NA
## 4       Remaining columns      log2 iTRAQ ratios     float   NA
```

```
clinical_data_codebook
```

```
##                                Column                                Description
## 1                     Complete_TCGA_ID                                   TCGA ID
## 2                               Gender                                     Gender
## 3  Age_at_Initial_Pathologic_Diagnosis      Age at Initial Pathologic Diagnosis
## 4                            ER Status                 Estrogen receptor Status
## 5                            PR Status             Progesterone receptor Status
## 6                    HER2 Final Status Human Epidermal growth factor Receptor 2
## 7                                Tumor                                    Tumor
## 8                     Tumor--T1 Coded                           Tumor--T1 Coded
## 9                                Node                                     Node
## 10                         Node-Coded                                Node-Coded
## 11                         Metastasis                                Metastasis
## 12                   Metastasis-Coded                          Metastasis-Coded
## 13                         AJCC Stage American Joint Committee on Cancer Stage
## 14                   Converted Stage                           Converted Stage
## 15                  Survival Data Form                        Survival Data Form
## 16                        Vital Status                              Vital Status
## 17       Days to Date of Last Contact            Days to Date of Last Contact
## 18              Days to date of Death                   Days to date of Death
## 19                           OS event                  OS event 0= NO, 1= YES
## 20                            OS Time                                 OS Time
## 21                         PAM50 mRNA                              PAM50 mRNA
## 22          SigClust Unsupervised mRNA              SigClust Unsupervised mRNA
## 23             SigClust Intrinsic mRNA                 SigClust Intrinsic mRNA
## 24                      miRNA Clusters                           miRNA Clusters
## 25               methylation Clusters                    methylation Clusters
## 26                       RPPA Clusters                            RPPA Clusters
## 27                         CN Clusters                              CN Clusters
## 28    Integrated Clusters (with PAM50)        Integrated Clusters (with PAM50)
## 29        Integrated Clusters (no exp)            Integrated Clusters (no exp)
## 30     Integrated Clusters (unsup exp)         Integrated Clusters (unsup exp)
##           type data.type  unit
## 1         name       chr  <NA>
## 2         name       chr  <NA>
## 3  Descriptive       chr  <NA>
## 4  Descriptive       chr  <NA>
## 5  Descriptive       chr  <NA>
## 6  Descriptive       chr  <NA>
## 7  Descriptive       chr  <NA>
## 8  Descriptive       chr  <NA>
## 9  Descriptive       chr  <NA>
## 10 Descriptive       chr  <NA>
## 11 Descriptive       chr  <NA>
## 12 Descriptive       chr  <NA>
## 13 Descriptive       chr  <NA>
## 14 Descriptive       chr  <NA>
```

```
## 15 Descriptive       chr  <NA>
## 16 Descriptive       chr  <NA>
## 17        Time       int  Days
## 18        Time       int  Days
## 19 Descriptive       int  <NA>
## 20        Time       int Hours
## 21 Descriptive       chr  <NA>
## 22       Count       int  <NA>
## 23       Count       int  <NA>
## 24       Count       int  <NA>
## 25       Count       int  <NA>
## 26 Descriptive       chr  <NA>
## 27       Count       int  <NA>
## 28       count       int  <NA>
## 29       count       int  <NA>
## 30       count       int  <NA>
```

```
PAM50_protein_codebook
```

```
##            Column                  Description type       unit
## 1      GeneSymbol            Gene abbreviation  chr       <NA>
## 2 RefSeqProteinID Unique reference identifier   chr       <NA>
## 3         Species                       Species  chr latin name
## 4       Gene.Name             Name of the gene  chr       <NA>
```

Data observation

there are 12553 rows in the data, these are proteins identifiable with a RefSeq ID number and have 86 columns of witch the last 83 are samples(with named with their identifiers and the last three from healthy individuals. to further use the data i shall reshape it to make the rows samples and each column a protein

Data cleaning and altering

altering sample names

the alteration of sample names to corespondent to the clinical data names is needed for further comparison and analyses. this is done by changing the column names to that of the same format of the clinical data. this is done with some regex magic

```
# storing a list of the column names
column_names <- names(proteomes_data)

# function
ch_sp_name <- function (x){
  #search for TCGA name,if found split and make new name
    if(grepl("TCGA",x) == TRUE){
      temp_list <- as.list(strsplit(x, '[_|-|.]')[[1]])
      x <- str_c(c('TCGA',temp_list[[1]],temp_list[[2]]),collapse = '-')
    }
return (x)
}
```

```
# changing of the colnames
colnames(proteomes_data) <- lapply(column_names, ch_sp_name)
cat("Old name:",column_names[[4]],",New name:",names(proteomes_data)[[4]])
```

```
## Old name: AO.A12D.01TCGA ,New name: TCGA-AO-A12D
```

this output show to conversion has been succesfull

numerical data frame

now we need to make a data frame with only the numerical data for the ease of analyzes

```
# first making a data frame with only the numerical data, samples start at column number 4 til the end
proteomes_data_numerical <- proteomes_data[4:86]
```

Transposing

transposing the created data frame "proteomes_data_numerical", and adding the refseq ID as column name

```
proteomes_data_numerical_transposed <- as.data.frame(t(proteomes_data_numerical))
colnames(proteomes_data_numerical_transposed) <- proteomes_data$RefSeq_accession_number

# checking is succesfull
cat("proteomes_data_numerical_transposed[ number of rows:", nrow(proteomes_data_numerical_transposed),
    "number of columns:",ncol(proteomes_data_numerical_transposed),'\n')
```

```
## proteomes_data_numerical_transposed[ number of rows: 83 number of columns: 12553
```

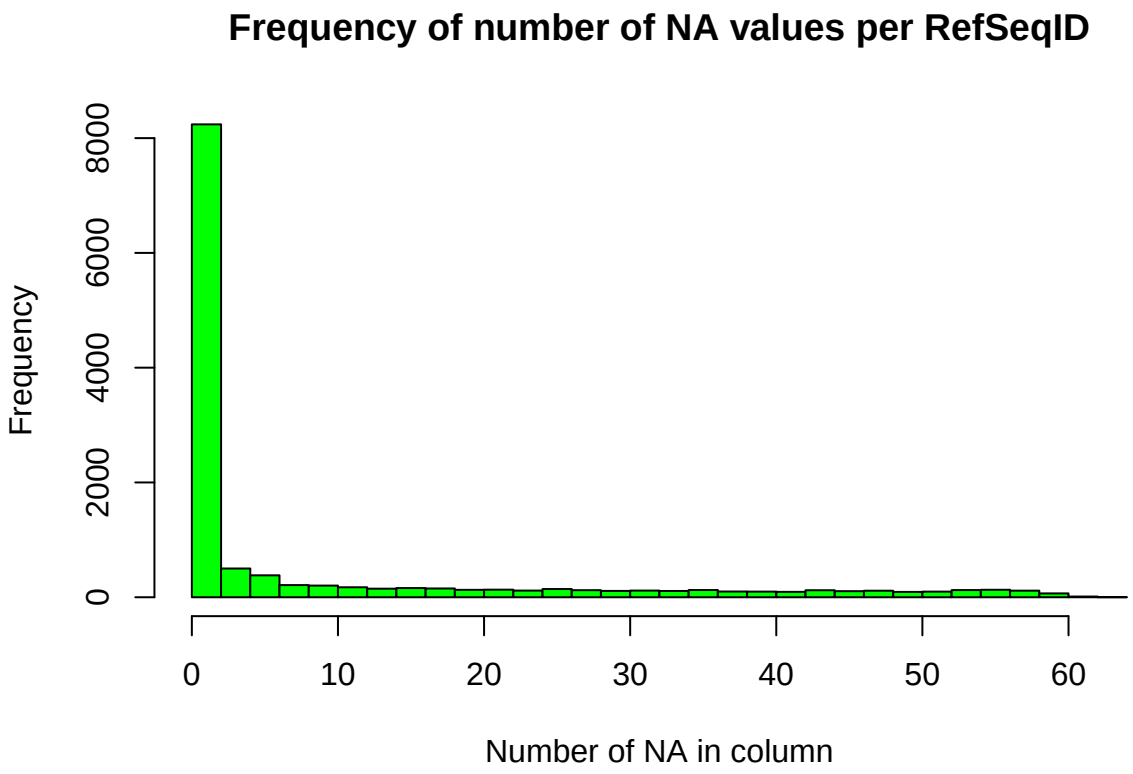
```
# lets add a healthy group and cancer, the last 3 columns where from healtyh poeple
# *see content section for the reference
proteomes_data_numerical_transposed$sample_type <- "Cancer"
proteomes_data_numerical_transposed$sample_type[81:83] <- "Healthy"
```

cleaning

since there are NA values in the data lets see how much

```
count_na_func <- function(x) sum(is.na(x))
# getting NA values per RefSeqID(column)
Na_per_col <- sapply(proteomes_data_numerical_transposed,count_na_func)

hist(Na_per_col, breaks = 40,
     xlab = "Number of NA in column",
     ylab = "Frequency",
     main = "Frequency of number of NA values per RefSeqID",
     col = "green")
```




```
cat("number of proteins with NA values in them:", sum(Na_per_col > 0), '\n' )
```

```
## number of proteins with NA values in them: 4559
```

```
# TODO  decide how many NA values are permitted per protein
proteomes_filtered_data <- proteomes_data_numerical_transposed[Na_per_col < 8]
cat("number of proteins with 8 or more NA values in them and deleted from data:",
    sum(Na_per_col > 8), '\n')
```

```
## number of proteins with 8 or more NA values in them and deleted from data: 3219
```

```
cat("proteomes_filtered_data[number of rows:",
    nrow(proteomes_filtered_data),
    "number of columns:",
    ncol(proteomes_filtered_data),'\n')
```

```
## proteomes_filtered_data[number of rows: 83 number of columns: 9200
```