Introduction into machine learning and analyzes of Breast Cancer Proteomes

true

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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). Are there different ways to categorize breast cancer based on protein expression data, with machine learning being used to classify them as benign or maligned, other than the pam50 proteins?

Exploratory Data Analysis

loading of the data frames 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")

clinical_data <- read.csv(file = "Data/clinical_data_breast_cancer.csv")

pam50_protein_data <- read.csv(file = "Data/PAM50_proteins.csv")

# showing successful loading of data

# only showing first 5 columns of proteomes

pander(head(proteomes_data[1:5], n = 5))</pre>
```

Table 1: Table continues below

$RefSeq_accession_number$	${\rm gene_symbol}$	gene_name	AO.A12D.01TCGA
NP_958782	PLEC	plectin isoform 1	1.096
NP_958785	NA	plectin isoform 1g	1.111
NP_958786	PLEC	plectin isoform 1a	1.111
NP_000436	NA	plectin isoform 1c	1.108
NP_958781	NA	plectin isoform 1e	1.115

C8.A131.01TCGA
2.61
2.65
$2.65 \\ 2.646$
2.646

Table 3: Table continues below

Complete.TCGA.ID	Gender	Age. at. Initial. Pathologic. Diagnosis	ER.Status
TCGA-A2-A0T2	FEMALE	66	Negative
TCGA-A2-A0CM	FEMALE	40	Negative
TCGA-BH-A18V	FEMALE	48	Negative
TCGA-BH-A18Q	FEMALE	56	Negative
TCGA-BH-A0E0	FEMALE	38	Negative

Table 4: Table continues below

PR.Status	HER2.Final.Status	Tumor	${\bf TumorT1.Coded}$	Node	Node.Coded
Negative	Negative	Т3	T_Other	N3	Positive
Negative	Negative	T2	T_Other	N0	Negative
Negative	Negative	T2	T_Other	N1	Positive
Negative	Negative	T2	T_Other	N1	Positive
Negative	Negative	T3	T_Other	N3	Positive

Table 5: Table continues below

Metastasis	Metastasis.Coded	AJCC.Stage	Converted.Stage
M1	Positive	Stage IV	No_Conversion
M0	Negative	Stage IIA	Stage IIA
M0	Negative	Stage IIB	No_Conversion
M0	Negative	Stage IIB	No_Conversion
M0	Negative	Stage IIIC	No_Conversion

Table 6: Table continues below

Survival.Data.Form	Vital.Status	Days. to. Date. of. Last. Contact
followup	DECEASED	240
followup	DECEASED	754
${\rm enrollment}$	DECEASED	1555
${ m enrollment}$	DECEASED	1692
followup	LIVING	133

Table 7: Table continues below

Days.to.date.of.Death	OS.event	OS.Time	PAM50.mRNA
240	1	240	Basal-like
754	1	754	Basal-like
1555	1	1555	Basal-like
1692	1	1692	Basal-like
NA	0	133	Basal-like

Table 8: Table continues below

SigClust.Unsupervised.mRNA	${\bf SigClust. Intrinsic. mRNA}$	miRNA.Clusters
0	-13	3
-12	-13	4
-12	-13	5
-12	-13	5
0	-13	5

Table 9: Table continues below

methylation.Clusters	RPPA.Clusters	CN.Clusters
5	Basal	3
4	Basal	4
5	Basal	1
5	Basal	1
5	Basal	1

Table 10: Table continues below

Integrated.Clusterswith.PAM50.	Integrated.Clustersno.exp.
2	2
2	1
2	2
2	2
2	2

${\bf Integrated. Clusters unsup. exp.}$	
2	
1	
2	
2	
2	

pander(head(pam50_protein_data, n=5))

GeneSymbol	${\bf RefSeqProteinID}$	Species	Gene.Name
MIA	NP_006524	Homo sapiens	melanoma inhibitory activity
FGFR4	NP_002002	Homo sapiens	fibroblast growth factor receptor 4
FGFR4	NP_998812	Homo sapiens	fibroblast growth factor receptor 4
FGFR4	NP_075252	Homo sapiens	fibroblast growth factor receptor 4
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:",nco

```
## 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),'\
## 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)
                   12553 obs. of 86 variables:
## 'data.frame':
                                   "NP_958782" "NP_958785" "NP_958786" "NP_000436" ...
## $ RefSeq_accession_number: chr
## $ gene_symbol
                           : chr
                                   "PLEC" NA "PLEC" NA ...
                                   "plectin isoform 1" "plectin isoform 1g" "plectin isoform 1a" "plec
## $ gene_name
                            : chr
## $ AO.A12D.O1TCGA
                           : num
                                   1.1 1.11 1.11 1.11 1.12 ...
## $ C8.A131.O1TCGA
                           : num
                                   2.61 2.65 2.65 2.65 2.65 ...
## $ AO.A12B.O1TCGA
                                   -0.66 -0.649 -0.654 -0.632 -0.64 ...
                            : num
## $ BH.A18Q.02TCGA
                            : num
                                   0.195 0.215 0.215 0.205 0.215 ...
## $ C8.A130.02TCGA
                                   -0.494 -0.504 -0.501 -0.51 -0.504 ...
                            : num
## $ C8.A138.O3TCGA
                                   2.77 2.78 2.78 2.8 2.79 ...
                            : num
## $ E2.A154.O3TCGA
                                   0.863 0.87 0.87 0.866 0.87 ...
                            : num
## $ C8.A12L.O4TCGA
                                   1.41 1.41 1.41 1.41 1.41 ...
                            : num
## $ A2.A0EX.04TCGA
                            : num
                                   1.19 1.19 1.19 1.19 1.2 ...
## $ AO.A12D.O5TCGA
                            : num
                                   1.1 1.1 1.1 1.1 1.09 ...
## $ AN.AO4A.O5TCGA
                                   0.385 0.371 0.371 0.378 0.375 ...
                            : num
                                   0.351 0.367 0.367 0.361 0.371 ...
                            : num
## $ BH.AOAV.O5TCGA
## $ C8.A12T.O6TCGA
                                   -0.205 -0.162 -0.167 -0.184 -0.167 ...
                            : num
## $ A8.A06Z.O7TCGA
                                   -0.496 -0.499 -0.496 -0.492 -0.488 ...
                            : num
## $ A2.AOCM.O7TCGA
                            : 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
                                   -0.913 -0.928 -0.928 -0.932 -0.928 ...
                            : num
## $ AR.AOU4.09TCGA
                            : num
                                   -0.0332 -0.0302 -0.0272 -0.0302 -0.0302 ...
## $ AO.AOJ9.10TCGA
                                   0.02 0.012 0.012 0.0039 0.012 ...
                            : num
## $ AR.A1AP.11TCGA
                                   0.461 0.461 0.461 0.461 0.461 ...
                            : num
## $ AN.AOFK.11TCGA
                                   0.974 0.977 0.977 0.97 0.985 ...
                            : num
## $ AO.AOJ6.11TCGA
                                   0.831 0.857 0.857 0.837 0.865 ...
                            : num
## $ A7.A13F.12TCGA
                                   1.28 1.28 1.28 1.28 1.28 ...
                            : num
## $ BH.AOE1.12TCGA
                                   0.762 0.762 0.766 0.758 0.766 ...
                            : num
## $ A7.AOCE.13TCGA
                                   -1.12 -1.12 -1.13 -1.13 ...
                            : num
## $ A2.A0YC.13TCGA
                                   0.819 0.815 0.815 0.799 0.819 ...
                            : num
## $ AO.AOJC.14TCGA
                                   -0.307 -0.307 -0.307 -0.301 ...
                            : num
## $ A8.A08Z.14TCGA
                                   0.569 0.569 0.569 0.569 ...
                            : num
## $ AR.AOTX.14TCGA
                                   -0.583 -0.573 -0.567 -0.583 -0.573 ...
                            : num
                                   1.87 1.87 1.87 1.86 1.87 ...
## $ A8.A076.15TCGA
                            : num
                                   0.196 0.196 0.196 0.219 0.2 ...
## $ AO.A126.15TCGA
                            : num
## $ BH.AOC1.16TCGA
                                   -0.518 -0.51 -0.507 -0.518 -0.513 ...
                            : num
                            : num 1.17 1.18 1.18 1.17 1.18 ...
## $ A2.A0EY.16TCGA
```

\$ AR.A1AW.17TCGA

: num 0.578 0.582 0.578 0.59 0.586 ...

```
$ AR.A1AV.17TCGA
                                    -0.76 -0.76 -0.749 -0.736 -0.749 ...
                             : num
##
                                    1.12 1.14 1.14 1.14 1.12 ...
   $ C8.A135.17TCGA
                             : num
   $ A2.A0EV.18TCGA
                                     0.453 0.473 0.473 0.459 0.473 ...
##
                               num
   $ AN.AOAM.18TCGA
                                    1.5 1.51 1.5 1.5 1.5 ...
##
                               num
##
   $ D8.A142.18TCGA
                               num
                                    0.539 0.542 0.542 0.535 0.542 ...
                             :
                                    2.46 2.48 2.48 2.46 2.48 ...
##
   $ AN.AOFL.19TCGA
                             : num
   $ BH.AODG.19TCGA
                                     -0.206 -0.206 -0.206 -0.215 -0.206 ...
                             : num
##
   $ AR.AOTV.2OTCGA
                               num
                                     -1.51 -1.53 -1.53 -1.51 ...
##
   $ C8.A12Z.20TCGA
                                     -0.787 -0.756 -0.756 -0.775 -0.772 ...
                             : num
##
   $ AO.AOJJ.2OTCGA
                               num
                                    0.757 0.781 0.774 0.764 0.771 ...
   $ AO.AOJE.21TCGA
                                    0.56 0.563 0.56 0.542 0.56 ...
                               num
                                     -0.428 -0.406 -0.406 -0.406 -0.406 ...
##
   $ AN.AOAJ.21TCGA
                               num
                             :
##
   $ A7.AOCJ.22TCGA
                                     -1.001 -1.005 -1.005 -0.998 -1.001 ...
                             :
                               num
##
   $ AO.A12F.22TCGA
                               num
                                     -1.95 -1.95 -1.96 -1.95 -1.96 ...
##
   $ A8.A079.23TCGA
                                    1.05 1.05 1.05 1.06 1.05 ...
                               num
##
   $ A2.A0T3.24TCGA
                                     0.584 0.581 0.581 0.587 0.587 ...
                               num
                             :
##
   $ A2.AOYD.24TCGA
                                    0.0638 0.0933 0.0845 0.0667 0.0845 ...
                             :
                               num
##
   $ AR.AOTR.25TCGA
                                     -1.1 -1.11 -1.11 -1.1 -1.11 ...
                             :
                               num
   $ AO.AO3O.25TCGA
##
                                    1.05 1.06 1.06 1.06 1.06 ...
                               num
##
   $ AO.A12E.26TCGA
                             :
                               num
                                    0.265 0.276 0.276 0.278 0.278 ...
##
   $ A8.A06N.26TCGA
                                    0.239 0.25 0.244 0.25 0.25 ...
                               num
   $ A2.AOYG.27TCGA
                                     -0.0782 -0.0681 -0.0714 -0.0579 -0.0647 ...
                               num
   $ BH.A18N.27TCGA
##
                                    1.1 1.1 1.1 1.09 1.11 ...
                               num
                                    0.324 0.327 0.327 0.33 0.327 ...
##
   $ AN.AOAL.28TCGA
                               num
##
   $ A2.A0T6.29TCGA
                               num
                                    0.794 0.818 0.815 0.801 0.818 ...
   $ E2.A158.29TCGA
                               nıım
                                     -1.09 -1.1 -1.1 -1.1 -1.1 ...
##
   $ E2.A15A.29TCGA
                                     2.18 2.18 2.18 2.18 2.18 ...
                               num
##
   $ AO.AOJM.3OTCGA
                                    1.4 1.41 1.41 1.41 1.41 ...
                               num
                             :
##
   $ C8.A12V.30TCGA
                                    0.674 0.689 0.689 0.678 0.689 ...
                               num
##
   $ A2.AOD2.31TCGA
                                    0.1075 0.1042 0.1075 0.0975 0.1042 ...
                             : num
##
   $ C8.A12U.31TCGA
                             :
                               num
                                     -0.482 -0.478 -0.482 -0.471 -0.482 ...
##
   $ AR.A1AS.31TCGA
                                    1.22 1.22 1.22 1.2 1.22 ...
                               num
                             :
##
   $ A8.A09G.32TCGA
                                     -1.52 -1.51 -1.51 -1.52 -1.51 ...
                             :
                               num
##
   $ C8.A131.32TCGA
                                    2.71 2.73 2.74 2.73 2.75 ...
                               num
##
   $ C8.A134.32TCGA
                                     0.14 0.126 0.133 0.112 0.126 ...
                             :
                               num
##
   $ A2.AOYF.33TCGA
                                    0.311 0.296 0.296 0.296 0.296 ...
                             : num
##
   $ BH.AODD.33TCGA
                               num
                                     -0.692 -0.659 -0.664 -0.657 -0.662 ...
##
   $ BH.AOE9.33TCGA
                                    1.47 1.48 1.47 1.46 1.47 ...
                               num
   $ AR.AOTT.34TCGA
                                     -0.511 -0.526 -0.526 -0.533 -0.53 ...
##
                               num
                                     -0.964 -0.938 -0.944 -0.935 -0.935 ...
##
   $ AO.A12B.34TCGA
                               num
                                     -0.488 -0.488 -0.488 -0.504 ...
   $ A2.AOSW.35TCGA
                             : num
   $ AO.AOJL.35TCGA
                                     -0.107 -0.107 -0.107 -0.107 -0.107 ...
##
                               num
                                    -0.0658 -0.0559 -0.0658 -0.0559 -0.0625 ...
##
   $ BH.AOBV.35TCGA
                             : num
##
   $ A2.AOYM.36TCGA
                                    0.656 0.658 0.656 0.656 0.651 ...
                               num
   $ BH.AOC7.36TCGA
                                     -0.552 -0.548 -0.552 -0.552 -0.557 ...
                              : num
##
   $ A2.AOSX.36TCGA
                                     -0.399 -0.393 -0.393 -0.396 ...
                               num
##
   $ 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
                                    0.567 0.579 0.577 0.577 0.577 ...
                               num
```

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:
                                             "TCGA-A2-AOT2" "TCGA-A2-AOCM" "TCGA-BH-A18V" "TCGA-BH-A
   $ Complete.TCGA.ID
                                             "FEMALE" "FEMALE" "FEMALE" ...
## $ Gender
                                      : chr
## $ Age.at.Initial.Pathologic.Diagnosis: int
                                             66 40 48 56 38 57 74 60 61 67 ...
                                             "Negative" "Negative" "Negative" ...
## $ ER.Status
                                      : chr
                                             "Negative" "Negative" "Negative" ...
## $ PR.Status
                                      : chr
## $ HER2.Final.Status
                                             "Negative" "Negative" "Negative" ...
                                      : chr
                                             "T3" "T2" "T2" "T2" ...
## $ Tumor
                                      : chr
                                             "T_0ther" \ "T_0ther" \ "T_0ther" \ "T_0ther" \ \dots
## $ Tumor..T1.Coded
                                      : chr
## $ Node
                                             "N3" "N0" "N1" "N1" ...
                                      : chr
## $ Node.Coded
                                             "Positive" "Negative" "Positive" "Positive" ...
                                      : chr
## $ Metastasis
                                      : chr
                                             "M1" "M0" "M0" "M0" ...
                                             "Positive" "Negative" "Negative" "Negative" ...
##
   $ Metastasis.Coded
                                      : chr
## $ AJCC.Stage
                                             "Stage IV" "Stage IIA" "Stage IIB" "Stage IIB" ...
                                      : chr
                                             "No_Conversion" "Stage IIA" "No_Conversion" "No_Convers
## $ Converted.Stage
                                      : chr
                                             "followup" "followup" "enrollment" "enrollment" ...
## $ Survival.Data.Form
                                      : chr
                                             "DECEASED" "DECEASED" "DECEASED" ...
## $ Vital.Status
                                      : chr
## $ 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
                                             1 1 1 1 0 0 0 0 0 0 ...
                                      : int
## $ OS.Time
                                             240 754 1555 1692 133 309 425 643 775 964 ...
                                             "Basal-like" "Basal-like" "Basal-like" ...
## $ PAM50.mRNA
                                      : chr
## $ SigClust.Unsupervised.mRNA
                                      : int 0 -12 -12 -12 0 0 0 -12 -12 -12 ...
## $ SigClust.Intrinsic.mRNA
                                             -13 -13 -13 -13 -13 -13 -13 -13 -13 ...
                                      : int
## $ 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 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" ...
## $ 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" "fibroblast growth factor fa
```

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 = ";")
pander(cancer_proteomes_CPTAC_codebook)</pre>
```

Column	Description	data.type	unit
RefSeq_accession_number	RefSeq protein ID	string	NA
$gene_symbol$	Gene abbreviation code	string	NA
$gene_name$	Name of the gene	string	NA
Remaining columns	$\log 2 iTRAQ ratios$	float	NA

pander(clinical_data_codebook)

Table 14: Table continues below

Column	Description
Complete_TCGA_ID	TCGA ID
Gender	Gender
Age_at_Initial_Pathologic_Diagnosis	Age at Initial Pathologic Diagnosis
ER Status	Estrogen receptor Status
PR Status	Progesterone receptor Status
HER2 Final Status	Human Epidermal growth factor Receptor 2
Tumor	Tumor
Tumor-T1 Coded	Tumor-T1 Coded
Node	Node
Node-Coded	Node-Coded
Metastasis	Metastasis
Metastasis-Coded	Metastasis-Coded
AJCC Stage	American Joint Committee on Cancer Stage
Converted Stage	Converted Stage
Survival Data Form	Survival Data Form
Vital Status	Vital Status
Days to Date of Last Contact	Days to Date of Last Contact
Days to date of Death	Days to date of Death
OS event	OS event $0 = NO$, $1 = YES$
OS Time	OS Time
PAM50 mRNA	PAM50 mRNA
SigClust Unsupervised mRNA	SigClust Unsupervised mRNA
SigClust Intrinsic mRNA	SigClust Intrinsic mRNA
miRNA Clusters	miRNA Clusters
methylation Clusters	methylation Clusters
RPPA Clusters	RPPA Clusters
CN Clusters	CN Clusters
Integrated Clusters (with PAM50)	Integrated Clusters (with PAM50)
Integrated Clusters (no exp)	Integrated Clusters (no exp)
Integrated Clusters (unsup exp)	Integrated Clusters (unsup exp)

type	data.type	unit
name	chr	NA
name	chr	NA
Descriptive	int	Years
Descriptive	chr	NA
Time	int	Days
Time	int	Days
Descriptive	int	NA
Time	int	Hours
Descriptive	chr	NA
Count	int	NA
Descriptive	chr	NA
Count	int	NA

pander(PAM50_protein_codebook)

Column	Description	type	unit
GeneSymbol	Gene abbreviation	chr	NA
RefSeqProteinID	Unique reference identifier	chr	NA
Species	Species	chr	latin name
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
change_sample_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, change_sample_name)
cat("Old name:",column_names[[4]],",New name:",names(proteomes_data)[[4]])</pre>
```

Old name: AO.A12D.O1TCGA , 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

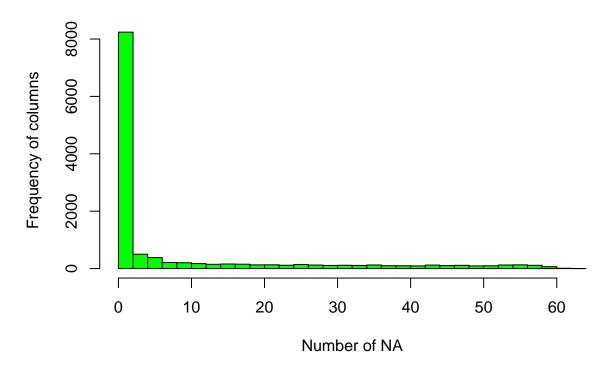
proteomes_data_numerical_transposed[number of rows: 83 number of columns: 12553

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

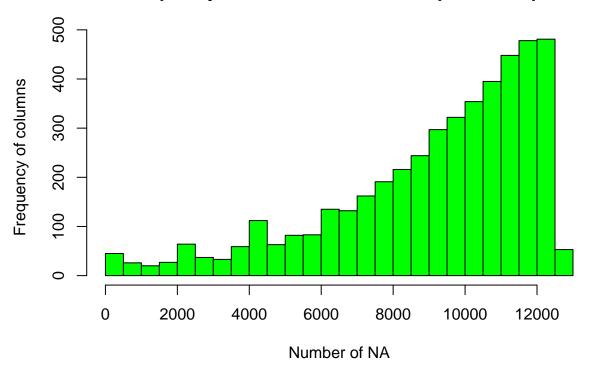
cleaning

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

Frequency of number of NA values per RefSeqID



Frequency of number of NA values per RefSeqID



```
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

as we can see from te reports generated by the code we can see that the filtereing of NA was succesfull.

```
rownames(clinical_data) <- clinical_data$Complete.TCGA.ID

clinical_data <- clinical_data[,-1]

data <- merge(clinical_data, proteomes_data_numerical_transposed, by = 0)

#data <- clinical_data %>% inner_join(proteomes_data,by="Complete.TCGA.ID")

#ggplot(pam50_protein_data, aes(PAM50.mRNA, col = PAM50.mRNA, fill = PAM50.mRNA, alpha=0.7)) + geom_bar
```

clinical_data\$Vital.Status <- factor(clinical_data\$Vital.Status)
summary(clinical_data\$Vital.Status)</pre>

DECEASED LIVING ## 11 94