

# IML Term project paper

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## Introduction

In this project we trained a classifier on a data set of atmospheric measurements. The task is to predict whether new particle formation (NPF) happens or not on a given day based on the atmospheric data. We ran several different kinds of models, assessed through accuracy and perplexity calculations which of these models performed the best, and discuss the results of our analyses.

## Preprocessing of the data

### Initial data analysis

The goal of this assignment is to predict the behavior of a multinomially distributed variable “class4”, which describes new particle formation events on specific observation days. The variable is treated as a multinomial variable divided into four separate groups: no new particle formation (referred to in the dataset as “nonevent”), very clear and strong particle formation events (referred to in the dataset as class “Ia”), other particle formation events where the growth and formation rate could be determined with a sufficiently good confidence level (referred to in the dataset as class “Ib”) and particle formation events where growth and formation rates could either not be defined or there was a possibility that the assessed rates were not sufficiently accurate. For the most part, we are observing a simpler version of this variable instead in the form of a binomial variable, let’s refer to that as “class2”, which is simply divided into no new particle formation events happening and new particle formation events happening.

Our dataset includes 464 observations of this variable as well as corresponding observations to a collection of 103 other variables. These variables include 50 numeric variables which describe the mean measurement related to phenomena such as carbon dioxide concentration, solar radiation and air temperature during a measurement day, 50 numeric variables which describe the corresponding standard deviations to these measurements for those same measurement days, an id listing which runs from 1 to 464, the date of each measurement as well as a logical variable describing whether the other measurements are partly bad. We also notice that some of the 50 types of measurements for which means and standard deviations are calculated are in fact related to the same phenomena but are simply measured at different points. For example, one of the measurements is the amount of carbon dioxide but this is measured at four different heights.

In order to get a preliminary idea of what we are dealing with, let’s visualize some of the variables we’re observing as well as calculate some very simple measurements of these variables. First, let’s download the dataset, define the binomial variable and observe how many of the observation of “class4” fall into specific classes.

```
## [1] "Relative amount of observations in class nonevent: 0.5"
## [1] "Relative amount of observations in class Ia: 0.0732758620689655"
## [1] "Relative amount of observations in class Ib: 0.183189655172414"
## [1] "Relative amount of observations in class II: 0.243534482758621"
```

We observe that half of our observations are days with no new particle formation events, implying that half our observations are days with new particle formation events. Out of the classes related to days with new particle formation events, class I type events are more common than class II type events but class II type events are more common than either class Ia or class Ib type events. And within class type I events, we have more observations of class Ib type events than class Ia type events.

Let's also calculate basic summary statistics for the other measurements

```
##          id          date          class4          partlybad
## Min.    : 1.0    Length:464    Length:464    Mode :logical
## 1st Qu.:116.8    Class :character    Class :character    FALSE:464
## Median :232.5    Mode  :character    Mode  :character
## Mean    :232.5
## 3rd Qu.:348.2
## Max.    :464.0
## C02168.mean    C02168.std    C02336.mean    C02336.std
## Min.    :359.6    Min.    : 0.05397    Min.    :359.1    Min.    : 0.04899
## 1st Qu.:374.4    1st Qu.: 0.84564    1st Qu.:374.4    1st Qu.: 0.78959
## Median :380.8    Median : 1.95273    Median :380.7    Median : 1.89932
## Mean    :382.1    Mean    : 3.12997    Mean    :382.1    Mean    : 2.94065
## 3rd Qu.:389.0    3rd Qu.: 4.42806    3rd Qu.:389.0    3rd Qu.: 4.14100
## Max.    :421.5    Max.    :19.46052    Max.    :421.1    Max.    :17.43986
## C0242.mean    C0242.std    C02504.mean    C02504.std
## Min.    :361.9    Min.    : 0.1115    Min.    :358.8    Min.    : 0.03742
## 1st Qu.:375.4    1st Qu.: 0.9492    1st Qu.:374.3    1st Qu.: 0.78156
## Median :381.6    Median : 2.2723    Median :380.6    Median : 1.75885
## Mean    :383.0    Mean    : 3.9916    Mean    :382.0    Mean    : 2.71896
## 3rd Qu.:389.7    3rd Qu.: 5.9603    3rd Qu.:389.0    3rd Qu.: 3.90350
## Max.    :422.6    Max.    :20.8517    Max.    :419.9    Max.    :16.65607
## Glob.mean    Glob.std    H20168.mean    H20168.std
## Min.    : 3.479    Min.    : 2.166    Min.    : 0.8702    Min.    :0.01335
## 1st Qu.: 61.683    1st Qu.: 41.627    1st Qu.: 3.8563    1st Qu.:0.19028
## Median :194.669    Median :144.928    Median : 5.8639    Median :0.41783
## Mean    :188.905    Mean    :138.933    Mean    : 6.9032    Mean    :0.53393
## 3rd Qu.:303.115    3rd Qu.:222.046    3rd Qu.: 9.4006    3rd Qu.:0.72848
## Max.    :426.457    Max.    :320.099    Max.    :18.7765    Max.    :2.87992
## H20336.mean    H20336.std    H2042.mean    H2042.std
## Min.    : 0.8872    Min.    :0.0110    Min.    : 0.8335    Min.    :0.02013
## 1st Qu.: 3.8345    1st Qu.:0.1846    1st Qu.: 3.8911    1st Qu.:0.18787
## Median : 5.8037    Median :0.4169    Median : 6.0049    Median :0.41841
## Mean    : 6.8349    Mean    :0.5338    Mean    : 7.0239    Mean    :0.54499
## 3rd Qu.: 9.3149    3rd Qu.:0.7380    3rd Qu.: 9.5254    3rd Qu.:0.73381
## Max.    :18.5736    Max.    :2.9379    Max.    :19.2872    Max.    :2.95080
## H20504.mean    H20504.std    H20672.mean    H20672.std
## Min.    : 0.8918    Min.    :0.01125    Min.    : 0.9047    Min.    :0.02052
## 1st Qu.: 3.8171    1st Qu.:0.17681    1st Qu.: 3.7728    1st Qu.:0.17232
## Median : 5.7705    Median :0.41157    Median : 5.7575    Median :0.40763
## Mean    : 6.7958    Mean    :0.53064    Mean    : 6.7678    Mean    :0.53082
## 3rd Qu.: 9.2741    3rd Qu.:0.73216    3rd Qu.: 9.2402    3rd Qu.:0.71825
## Max.    :18.4540    Max.    :2.97439    Max.    :18.4026    Max.    :3.05405
## H2084.mean    H2084.std    NET.mean    NET.std
## Min.    : 0.844    Min.    :0.02052    Min.    : -52.25    Min.    : 1.763
## 1st Qu.: 3.870    1st Qu.:0.18912    1st Qu.: 37.61    1st Qu.: 37.932
## Median : 5.982    Median :0.41437    Median :117.82    Median :127.196
## Mean    : 6.973    Mean    :0.54114    Mean    :117.85    Mean    :121.780
```

##	3rd Qu.: 9.468	3rd Qu.:0.72392	3rd Qu.:191.00	3rd Qu.:195.107
##	Max. :18.982	Max. :2.87668	Max. :302.83	Max. :262.742
##	N0168.mean	N0168.std	N0336.mean	N0336.std
##	Min. : -0.01438	Min. :0.02096	Min. : -0.01172	Min. :0.02362
##	1st Qu.: 0.02114	1st Qu.:0.05182	1st Qu.: 0.02257	1st Qu.:0.05051
##	Median : 0.04335	Median :0.06355	Median : 0.04455	Median :0.06491
##	Mean : 0.08533	Mean :0.09767	Mean : 0.09048	Mean :0.09471
##	3rd Qu.: 0.08710	3rd Qu.:0.09328	3rd Qu.: 0.09161	3rd Qu.:0.09812
##	Max. : 2.31625	Max. :1.58946	Max. : 2.39429	Max. :0.86861
##	N042.mean	N042.std	N0504.mean	N0504.std
##	Min. : -0.01222	Min. :0.02218	Min. : -0.02333	Min. :0.02535
##	1st Qu.: 0.01890	1st Qu.:0.04952	1st Qu.: 0.02249	1st Qu.:0.05096
##	Median : 0.03717	Median :0.06286	Median : 0.04503	Median :0.06442
##	Mean : 0.06939	Mean :0.09971	Mean : 0.08831	Mean :0.09131
##	3rd Qu.: 0.07428	3rd Qu.:0.09086	3rd Qu.: 0.08847	3rd Qu.:0.09444
##	Max. : 1.90179	Max. :1.01254	Max. : 2.23143	Max. :0.88466
##	N0672.mean	N0672.std	N084.mean	N084.std
##	Min. : -0.01327	Min. :0.02310	Min. : -0.02126	Min. :0.02220
##	1st Qu.: 0.02320	1st Qu.:0.05053	1st Qu.: 0.01726	1st Qu.:0.04941
##	Median : 0.04474	Median :0.06500	Median : 0.03481	Median :0.06098
##	Mean : 0.08599	Mean :0.08921	Mean : 0.07251	Mean :0.09391
##	3rd Qu.: 0.08948	3rd Qu.:0.09387	3rd Qu.: 0.07372	3rd Qu.:0.08700
##	Max. : 1.91714	Max. :0.78343	Max. : 2.06927	Max. :1.37139
##	N0x168.mean	N0x168.std	N0x336.mean	N0x336.std
##	Min. : 0.0949	Min. :0.03606	Min. : 0.0950	Min. :0.0578
##	1st Qu.: 0.5082	1st Qu.:0.21941	1st Qu.: 0.5058	1st Qu.:0.2090
##	Median : 1.0234	Median :0.35092	Median : 1.0187	Median :0.3411
##	Mean : 1.5248	Mean :0.51310	Mean : 1.5156	Mean :0.5137
##	3rd Qu.: 2.0118	3rd Qu.:0.62159	3rd Qu.: 1.9926	3rd Qu.:0.6210
##	Max. :12.6343	Max. :6.26986	Max. :12.5446	Max. :6.0662
##	N0x42.mean	N0x42.std	N0x504.mean	N0x504.std
##	Min. : 0.08883	Min. : 0.06678	Min. : 0.08358	Min. :0.05679
##	1st Qu.: 0.53579	1st Qu.: 0.23237	1st Qu.: 0.49852	1st Qu.:0.20519
##	Median : 1.03089	Median : 0.36963	Median : 1.02123	Median :0.34535
##	Mean : 1.53990	Mean : 0.62994	Mean : 1.50026	Mean :0.52460
##	3rd Qu.: 1.97545	3rd Qu.: 0.70295	3rd Qu.: 1.95752	3rd Qu.:0.62162
##	Max. :12.33232	Max. :12.42314	Max. :12.24750	Max. :5.93928
##	N0x672.mean	N0x672.std	N0x84.mean	N0x84.std
##	Min. : 0.0838	Min. :0.05122	Min. : 0.1005	Min. :0.05788
##	1st Qu.: 0.5002	1st Qu.:0.20901	1st Qu.: 0.5051	1st Qu.:0.22016
##	Median : 1.0066	Median :0.34422	Median : 1.0289	Median :0.35778
##	Mean : 1.4855	Mean :0.50167	Mean : 1.5231	Mean :0.52454
##	3rd Qu.: 1.9644	3rd Qu.:0.59311	3rd Qu.: 2.0045	3rd Qu.:0.65374
##	Max. :12.0379	Max. :5.92112	Max. :12.4547	Max. :6.21296
##	03168.mean	03168.std	0342.mean	0342.std
##	Min. : 3.613	Min. : 0.2163	Min. : 3.465	Min. : 0.2001
##	1st Qu.:26.161	1st Qu.: 1.6010	1st Qu.:25.013	1st Qu.: 1.8771
##	Median :32.507	Median : 3.1526	Median :31.560	Median : 3.5260
##	Mean :32.984	Mean : 3.6238	Mean :31.887	Mean : 4.0472
##	3rd Qu.:39.931	3rd Qu.: 5.1053	3rd Qu.:39.189	3rd Qu.: 5.7574
##	Max. :65.130	Max. :13.5534	Max. :63.968	Max. :13.7123
##	03504.mean	03504.std	03672.mean	03672.std
##	Min. : 3.834	Min. : 0.2116	Min. : 3.848	Min. : 0.2111
##	1st Qu.:27.733	1st Qu.: 1.5723	1st Qu.:28.178	1st Qu.: 1.5831

## Median :33.357	Median : 2.9209	Median :33.793	Median : 2.9202
## Mean :33.857	Mean : 3.3877	Mean :34.178	Mean : 3.3024
## 3rd Qu.:40.583	3rd Qu.: 4.7962	3rd Qu.:40.783	3rd Qu.: 4.3776
## Max. :65.777	Max. :12.8208	Max. :65.775	Max. :11.8905
## O384.mean	O384.std	Pamb0.mean	Pamb0.std
## Min. : 3.603	Min. : 0.09849	Min. : 952.8	Min. :0.06661
## 1st Qu.:25.564	1st Qu.: 1.68627	1st Qu.: 983.9	1st Qu.:0.45055
## Median :31.991	Median : 3.27771	Median : 991.6	Median :0.79566
## Mean :32.394	Mean : 3.78074	Mean : 991.2	Mean :1.02577
## 3rd Qu.:39.562	3rd Qu.: 5.42626	3rd Qu.: 997.9	3rd Qu.:1.28511
## Max. :64.505	Max. :13.73501	Max. :1018.8	Max. :5.52491
## PAR.mean	PAR.std	PTG.mean	PTG.std
## Min. : 6.258	Min. : 4.764	Min. : -0.0116443	Min. :0.000000
## 1st Qu.:130.532	1st Qu.: 86.074	1st Qu.: -0.0028799	1st Qu.:0.004029
## Median :387.052	Median :291.060	Median : -0.0002267	Median :0.008191
## Mean :373.349	Mean :275.098	Mean : 0.0001971	Mean :0.009066
## 3rd Qu.:590.161	3rd Qu.:443.805	3rd Qu.: 0.0009356	3rd Qu.:0.013126
## Max. :825.394	Max. :613.025	Max. : 0.0910256	Max. :0.040239
## RGlob.mean	RGlob.std	RHIRGA168.mean	RHIRGA168.std
## Min. : -1.122	Min. : 0.3671	Min. : 27.71	Min. : 0.196
## 1st Qu.:12.910	1st Qu.: 9.3438	1st Qu.: 54.50	1st Qu.: 2.520
## Median :28.933	Median :21.3691	Median : 69.75	Median : 9.022
## Mean :27.834	Mean :18.5654	Mean : 69.49	Mean : 8.480
## 3rd Qu.:42.247	3rd Qu.:27.0129	3rd Qu.: 88.22	3rd Qu.:12.430
## Max. :85.620	Max. :49.7793	Max. :106.02	Max. :23.957
## RHIRGA336.mean	RHIRGA336.std	RHIRGA42.mean	RHIRGA42.std
## Min. : 27.63	Min. : 0.1972	Min. : 29.66	Min. : 0.2724
## 1st Qu.: 53.62	1st Qu.: 2.7418	1st Qu.: 54.98	1st Qu.: 2.1392
## Median : 69.41	Median : 8.7971	Median : 69.73	Median : 9.7053
## Mean : 69.90	Mean : 8.3927	Mean : 70.12	Mean : 8.8841
## 3rd Qu.: 88.82	3rd Qu.:12.3141	3rd Qu.: 87.99	3rd Qu.:13.5341
## Max. :107.44	Max. :24.1008	Max. :103.13	Max. :23.5248
## RHIRGA504.mean	RHIRGA504.std	RHIRGA672.mean	RHIRGA672.std
## Min. : 26.99	Min. : 0.2573	Min. : 26.70	Min. : 0.1943
## 1st Qu.: 53.65	1st Qu.: 2.9149	1st Qu.: 54.56	1st Qu.: 2.9304
## Median : 69.48	Median : 8.5568	Median : 70.02	Median : 8.2752
## Mean : 69.98	Mean : 8.2231	Mean : 70.70	Mean : 8.1227
## 3rd Qu.: 89.07	3rd Qu.:12.1196	3rd Qu.: 90.03	3rd Qu.:12.0411
## Max. :105.74	Max. :23.9752	Max. :104.64	Max. :24.0755
## RHIRGA84.mean	RHIRGA84.std	RPAR.mean	RPAR.std
## Min. : 28.46	Min. : 0.2591	Min. : 0.00	Min. : 0.000
## 1st Qu.: 54.38	1st Qu.: 2.3354	1st Qu.: 9.45	1st Qu.: 7.632
## Median : 69.93	Median : 9.5532	Median : 18.87	Median :14.327
## Mean : 69.65	Mean : 8.7783	Mean : 20.16	Mean :14.093
## 3rd Qu.: 87.93	3rd Qu.:13.1020	3rd Qu.: 26.07	3rd Qu.:17.487
## Max. :103.81	Max. :23.6684	Max. :134.86	Max. :84.203
## S02168.mean	S02168.std	SWS.mean	SWS.std
## Min. : -0.02743	Min. :0.02887	Min. :528.1	Min. : 0.0000
## 1st Qu.: 0.05800	1st Qu.:0.07987	1st Qu.:907.4	1st Qu.: 0.7788
## Median : 0.12286	Median :0.10977	Median :918.5	Median : 1.8926
## Mean : 0.27840	Mean :0.17068	Mean :908.2	Mean : 20.0663
## 3rd Qu.: 0.30154	3rd Qu.:0.18339	3rd Qu.:923.1	3rd Qu.: 16.8917
## Max. : 3.81492	Max. :2.01559	Max. :937.9	Max. :190.6516
## T168.mean	T168.std	T42.mean	T42.std

```
## Min.      :-24.778   Min.      :0.04589   Min.      :-24.883   Min.      :0.05069
## 1st Qu.: -1.530   1st Qu.:0.72766   1st Qu.: -1.510   1st Qu.:0.75975
## Median :  6.402   Median :1.80772   Median :  6.621   Median :1.98491
## Mean    :  5.681   Mean    :1.79699   Mean     :  5.752   Mean     :1.95714
## 3rd Qu.: 13.720   3rd Qu.:2.68334   3rd Qu.: 13.800   3rd Qu.:2.92745
## Max.    : 27.719   Max.    :5.14434   Max.     : 27.889   Max.     :5.09896
##      T504.mean      T504.std      T672.mean      T672.std
## Min.      :-24.017   Min.      :0.05055   Min.      :-23.901   Min.      :0.05258
## 1st Qu.: -1.804   1st Qu.:0.69842   1st Qu.: -1.991   1st Qu.:0.68697
## Median :  6.118   Median :1.71758   Median :  5.959   Median :1.65568
## Mean     :  5.384   Mean     :1.65693   Mean     :  5.189   Mean     :1.59360
## 3rd Qu.: 13.383   3rd Qu.:2.50350   3rd Qu.: 13.040   3rd Qu.:2.35899
## Max.     : 27.276   Max.     :5.06112   Max.     : 27.110   Max.     :4.86725
##      T84.mean      T84.std      UV_A.mean      UV_A.std
## Min.      :-24.875   Min.      :0.0439   Min.      : 0.2959   Min.      : 0.1778
## 1st Qu.: -1.477   1st Qu.:0.7615   1st Qu.:  4.2367   1st Qu.:  2.4317
## Median :  6.577   Median :1.9454   Median :11.3274   Median :  7.5885
## Mean     :  5.767   Mean     :1.9113   Mean     :10.6230   Mean     :  7.4510
## 3rd Qu.: 13.832   3rd Qu.:2.8284   3rd Qu.:16.4605   3rd Qu.:11.8278
## Max.     : 27.939   Max.     :5.1320   Max.     :22.5412   Max.     :16.8305
##      UV_B.mean      UV_B.std      CS.mean      CS.std
## Min.      :0.00514   Min.      :0.003552   Min.      :0.0002433   Min.      :2.727e-05
## 1st Qu.:0.12586   1st Qu.:0.086265   1st Qu.:0.0013907   1st Qu.:2.661e-04
## Median :0.40225   Median :0.334264   Median :0.0023979   Median :4.759e-04
## Mean     :0.42880   Mean     :0.366484   Mean     :0.0029625   Mean     :6.673e-04
## 3rd Qu.:0.66997   3rd Qu.:0.589098   3rd Qu.:0.0039100   3rd Qu.:7.908e-04
## Max.     :1.19727   Max.     :1.055615   Max.     :0.0126701   Max.     :6.277e-03
##      class2
## Mode :logical
## FALSE:232
## TRUE :232
##
##
##
```

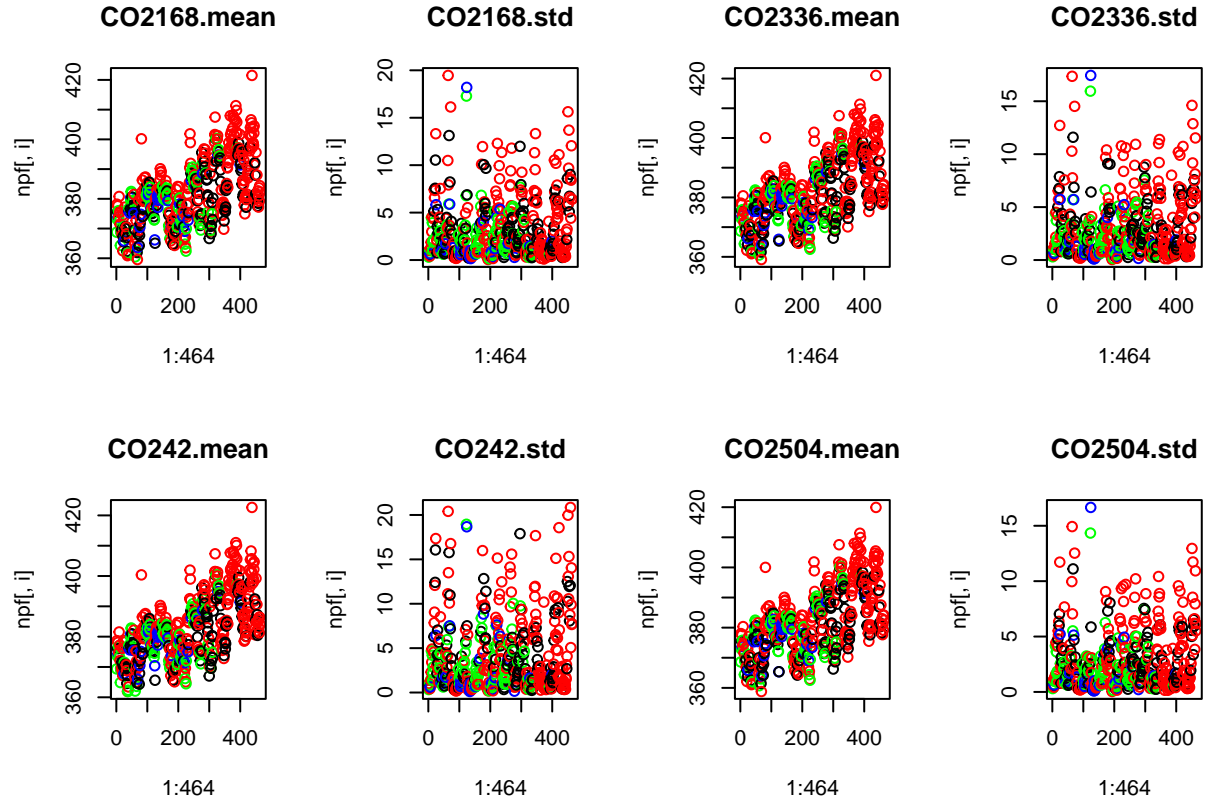
Of particular interest here is that the variable “partlybad” seems to have only observations of type “FALSE”. As a result, we can remove it from the dataset as it gives no extra information. We can also remove the variable id, as the order of the observations is not of interest in our analysis. And on top of this, it is unlikely that we will use the specific dates in relation to the observations either, so we will simply shift that information to be the rownames for the data.

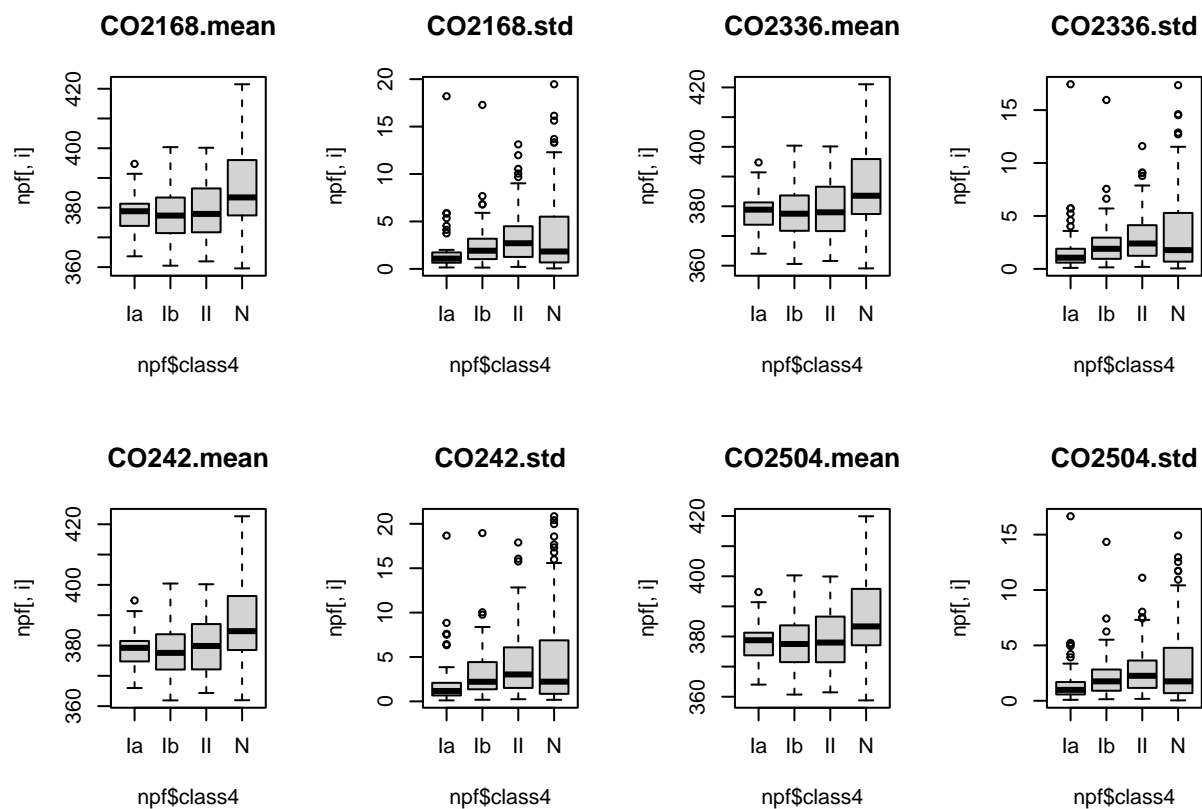
Now we are left with our variable of interest, as well as 100 explanatory variables.

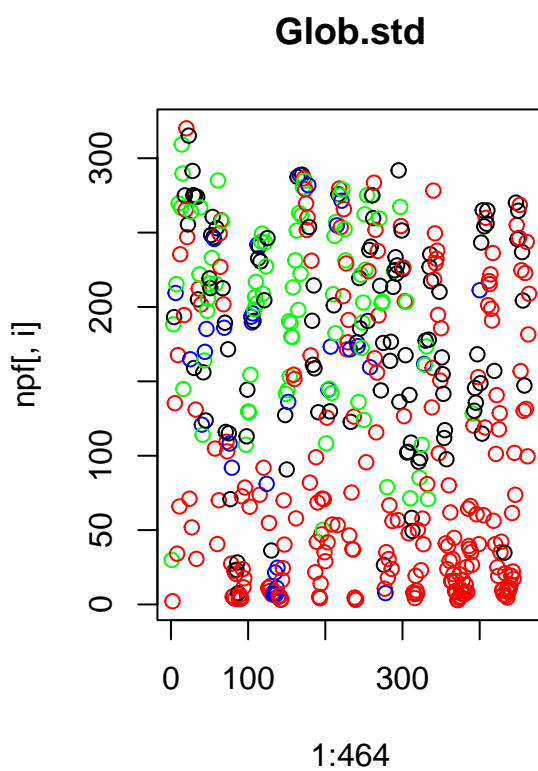
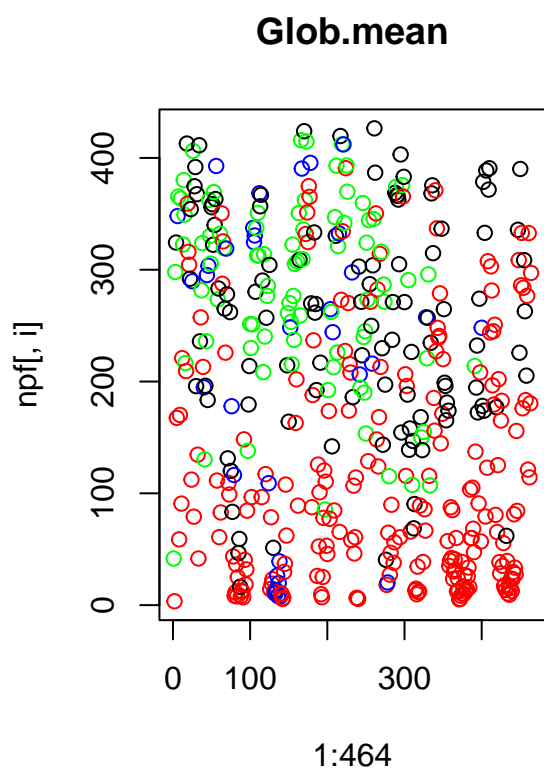
%Mitä teemme tälle, haluammeko viitata tähän visualisointien ja nimien suhteen vai onko ideaalia, että teemme omat visualisointimme, jotka esittelemme tekstissä? % (Sara) Ainakin jos tehdään omat visualisoinnit, mielestäni tämän voi poistaa. Visualisointien kanssa kuitenkin miettisin, että mitä todella halutaan näyttää/kertoa, ja tukeeko kyseinen tai kyseiset visualisoinnit tätä. Eli jos visualisointeja halutaan, niin mitä ja miksi, ja miten ne liittyvät luokitteluun ja partikkeleiden muodostumiseen tai muuten tukevat projektityön päämääriä. We also familiarized ourselves with the data through the [smear.avaa.scs.fi](http://smear.avaa.scs.fi) webpage that offers further visualizations details about the data and the measurement site, and with the variable names and details available at [wiki.helsinki.fi](http://wiki.helsinki.fi).

Let’s next visualize some our explanatory variables via boxplots and scatterplots to get a deeper understanding of them. For the sake of simplicity, these visualizations grouped by the phenomena being measured. In order to also preliminarily look at how these variables behave in relation to new particle formation events, we’ll also look at said measurements behave in relation to variable “class4”. In terms of the boxplots,

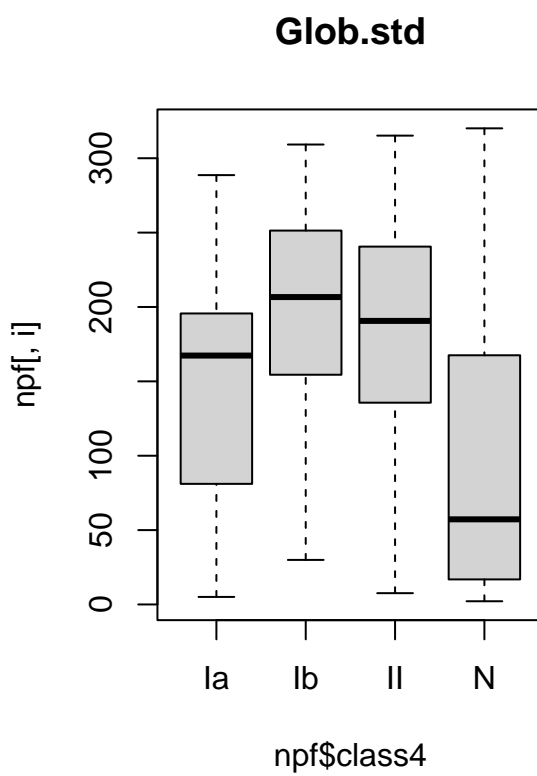
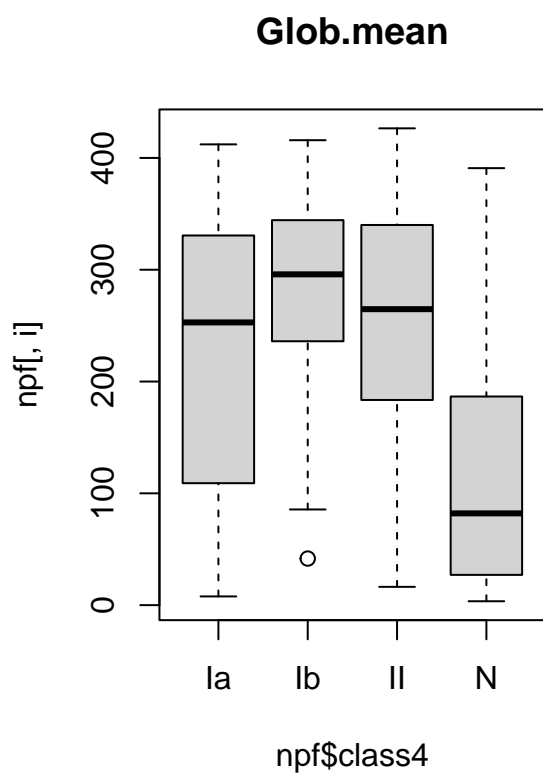
the boxplots are divided into groups by variable class4, and in terms of the scatterplots, the following colors represent different classes: red represents nonevent days, blue represents days with type Ia NPF events, green represents days with type Ib NPF events and black represents days with type II NPF events:

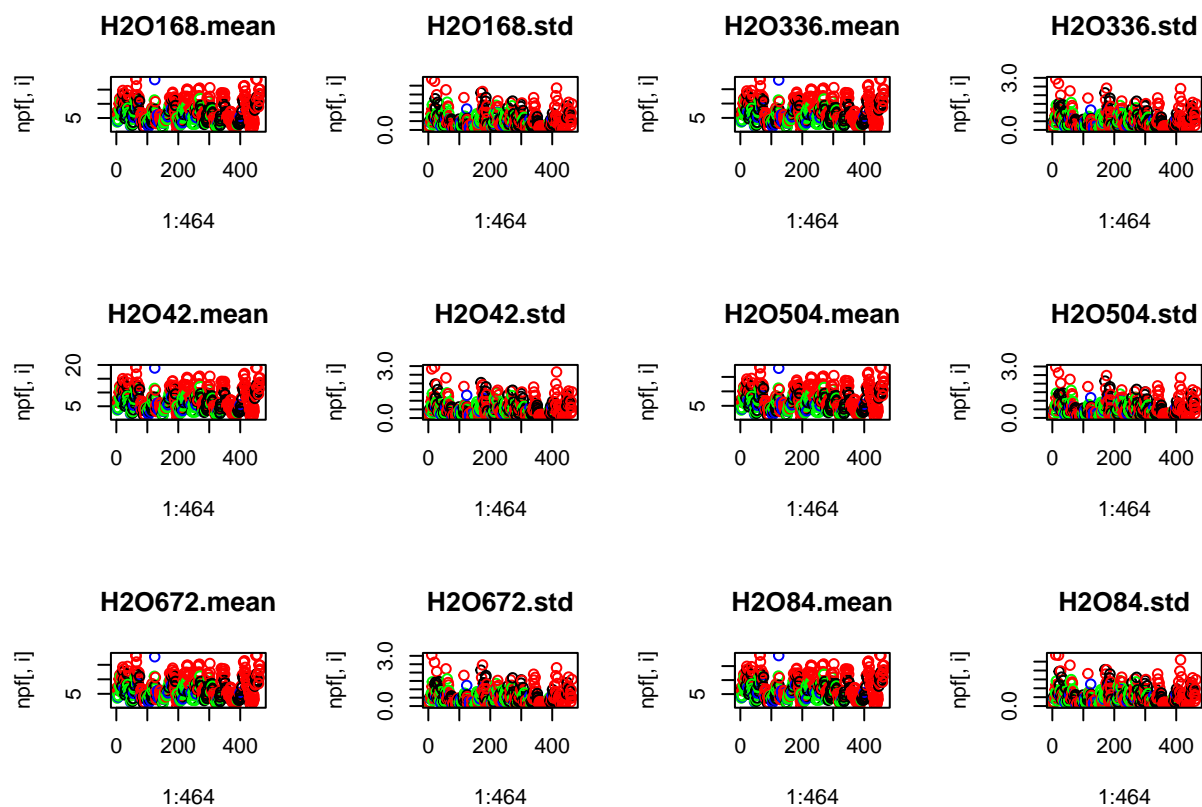


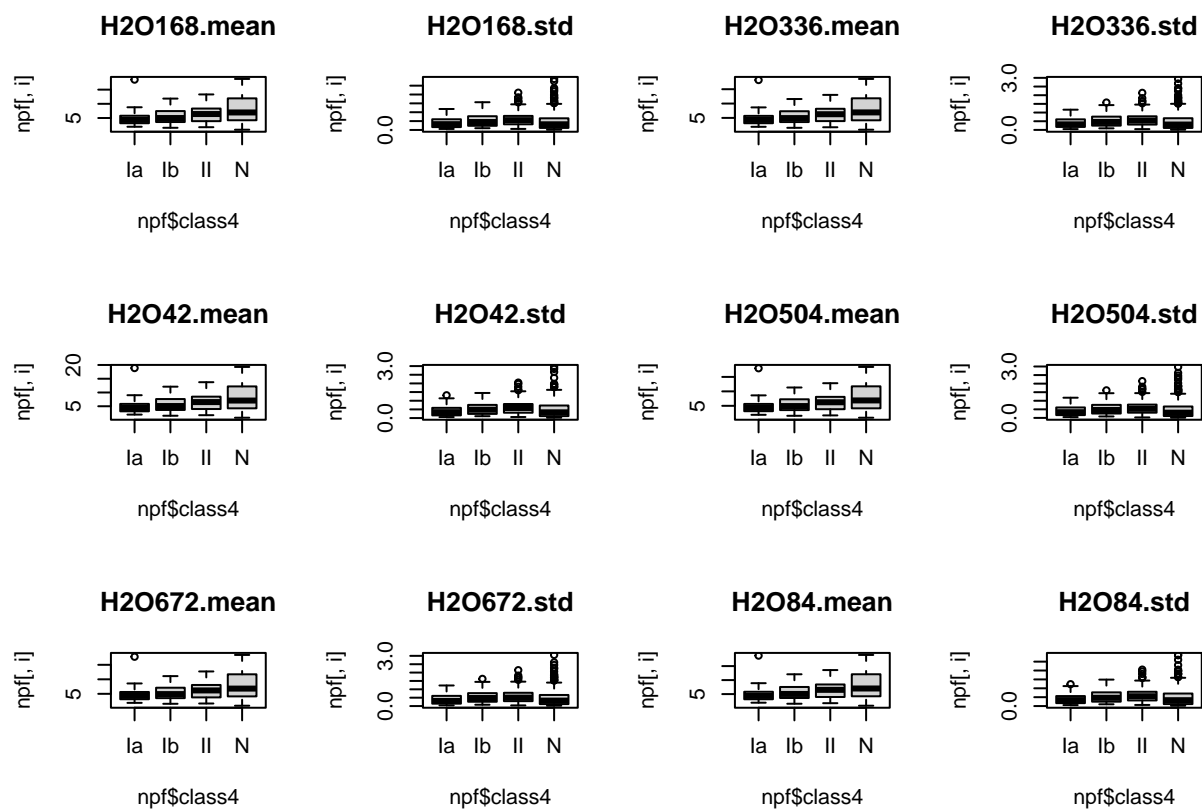


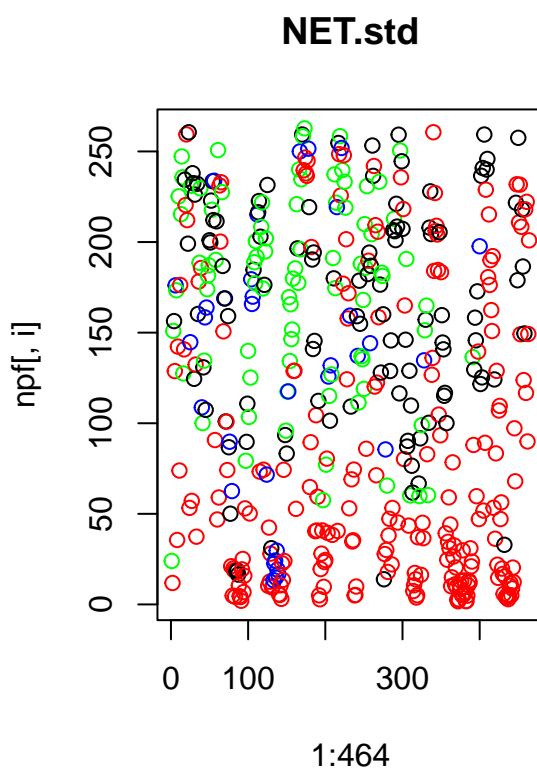
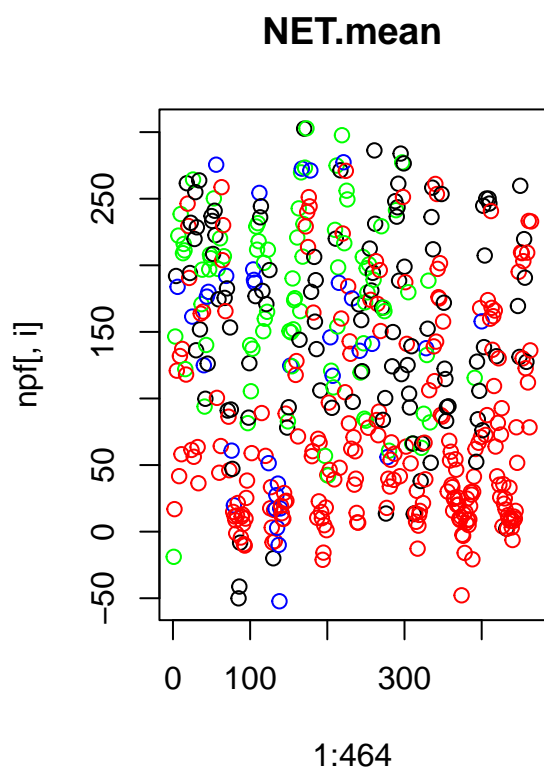


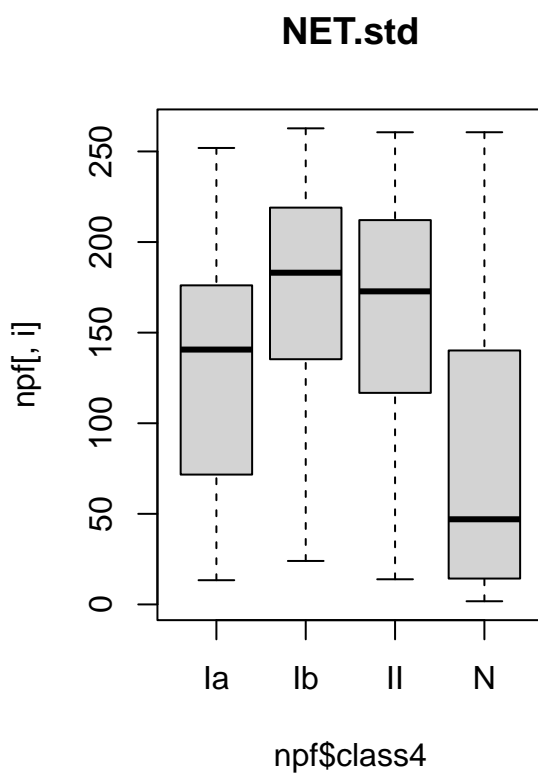
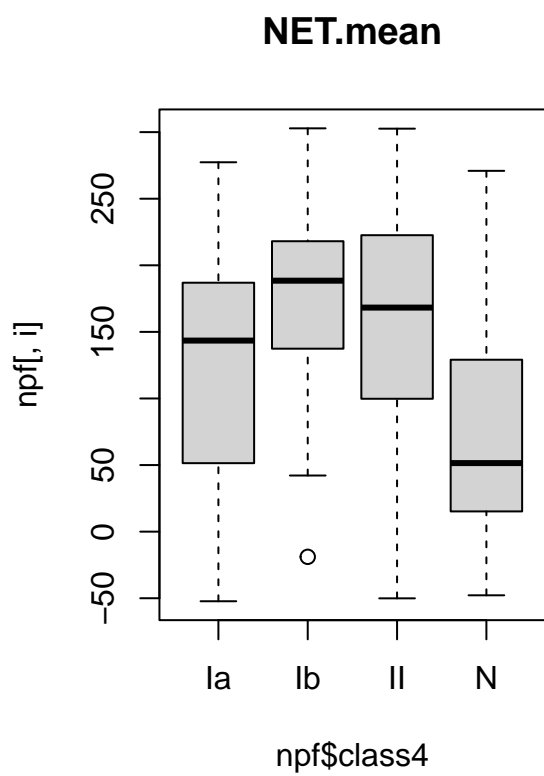


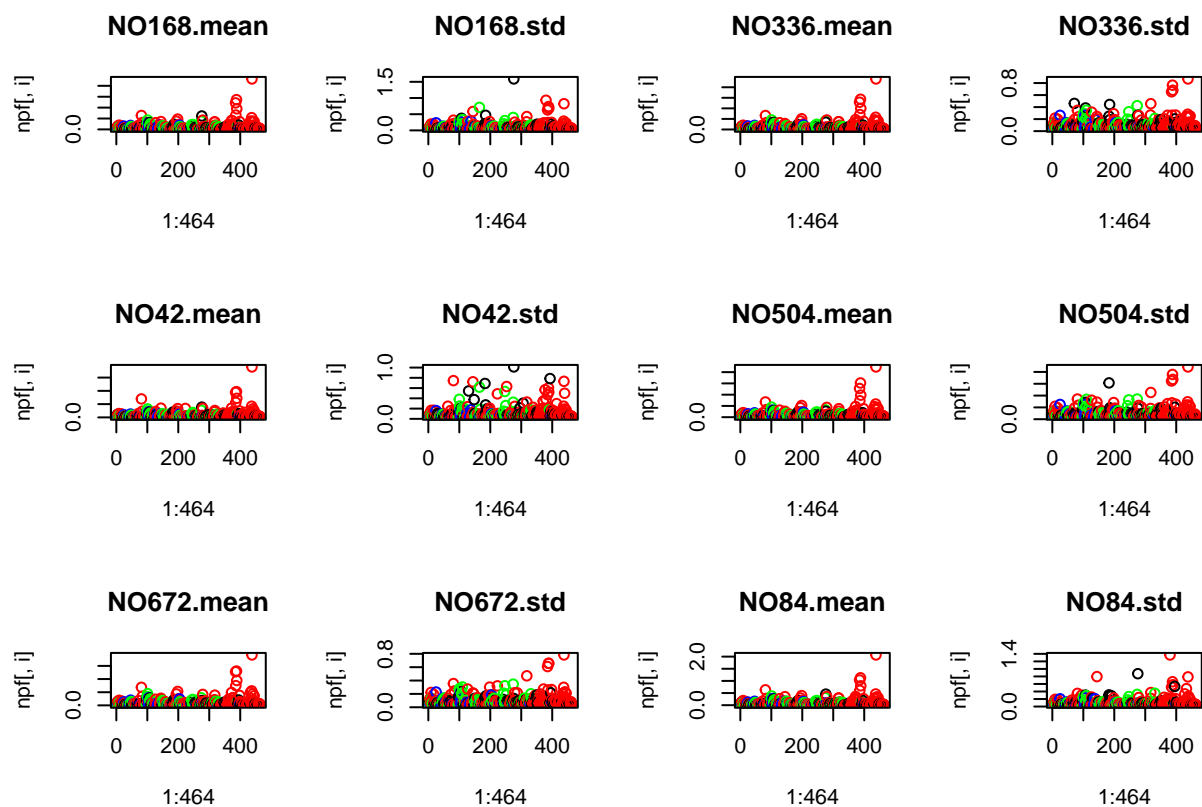


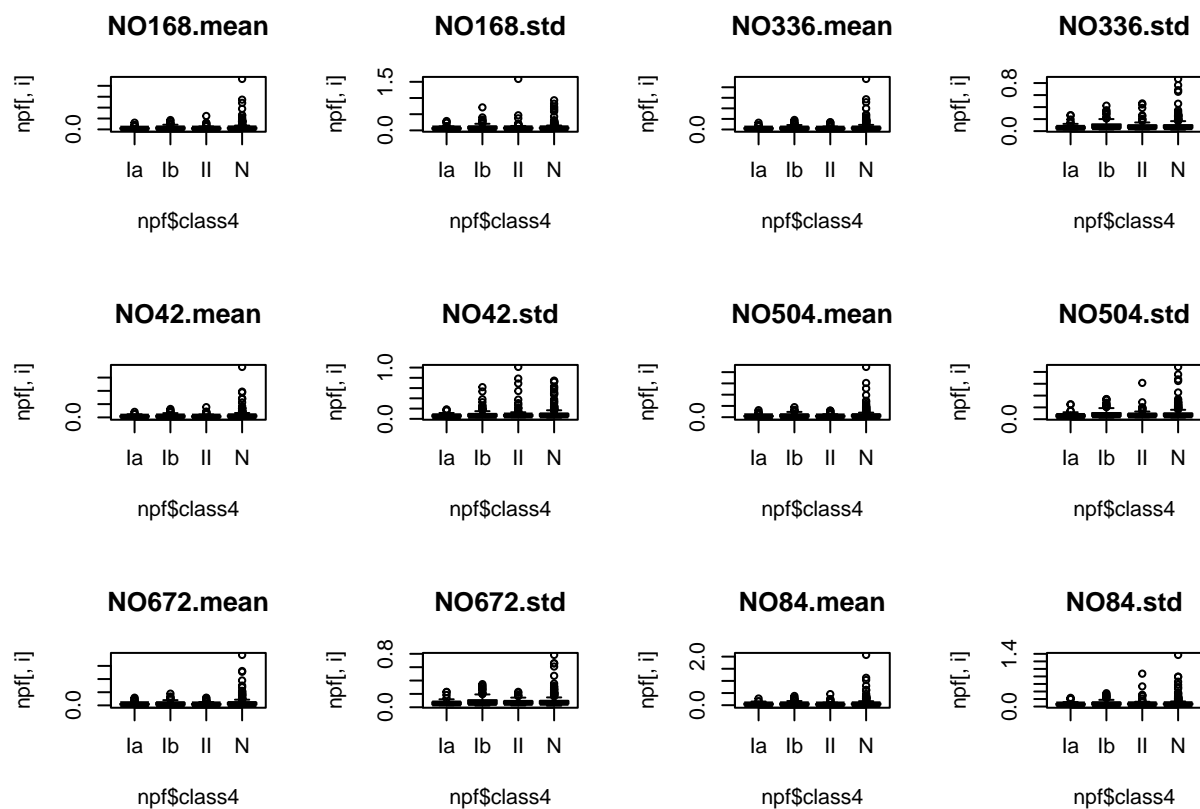


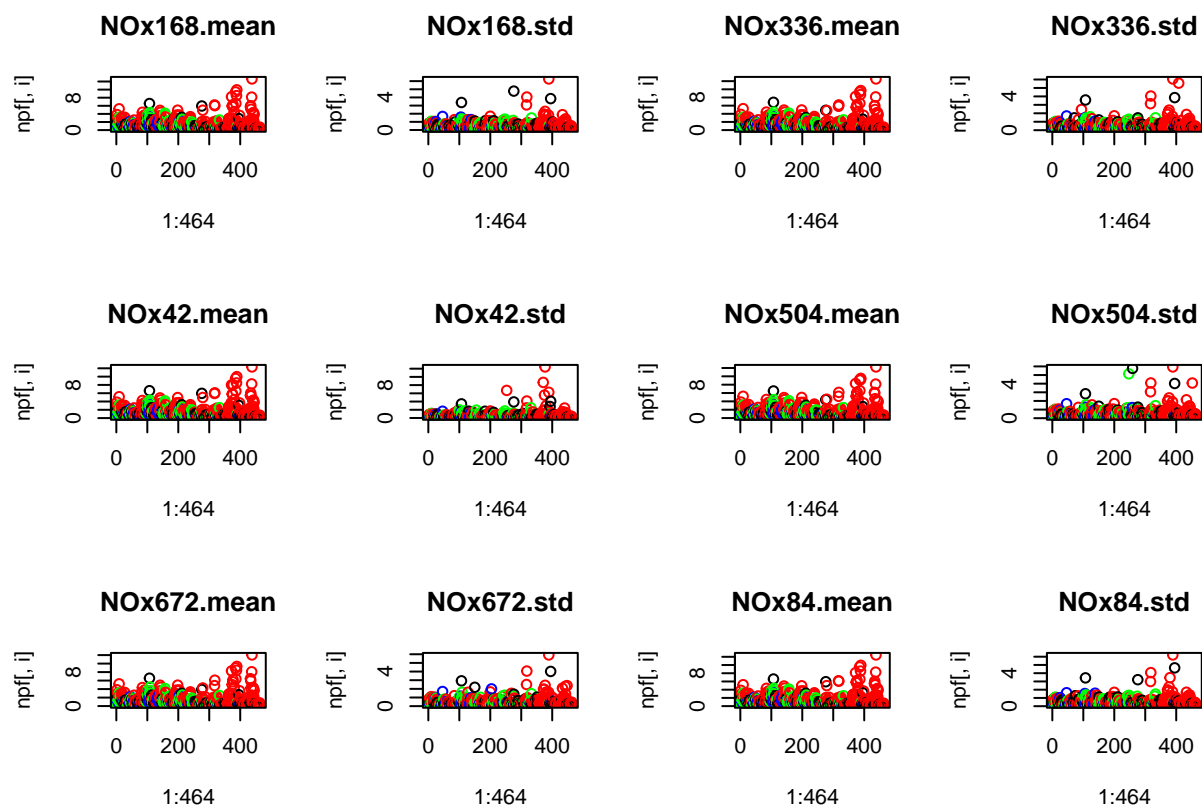




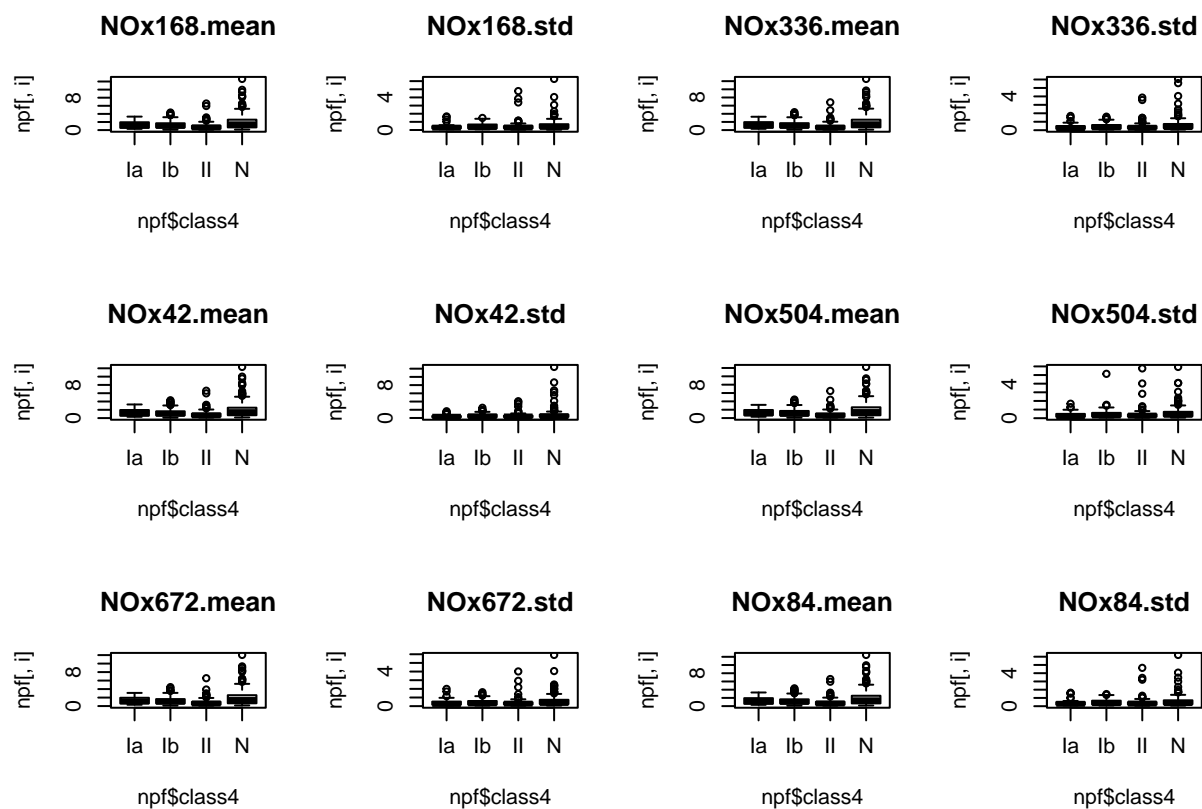


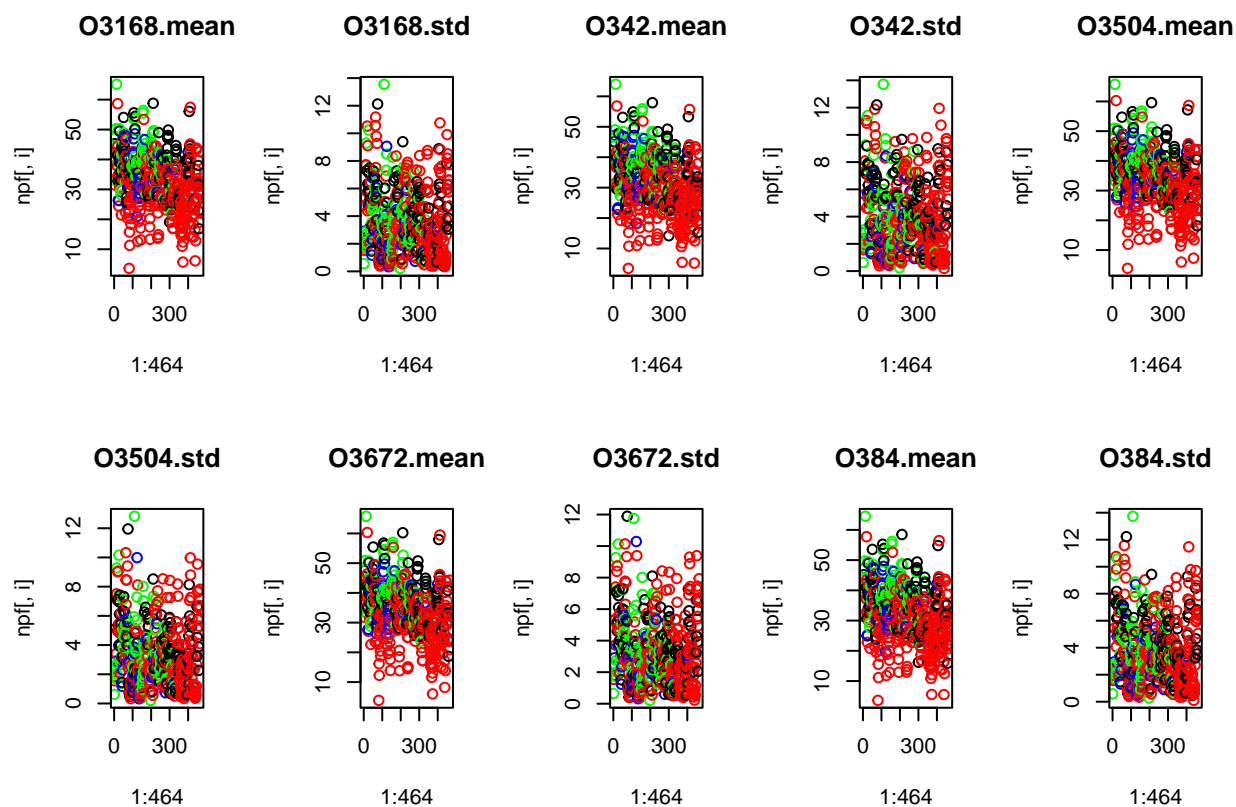


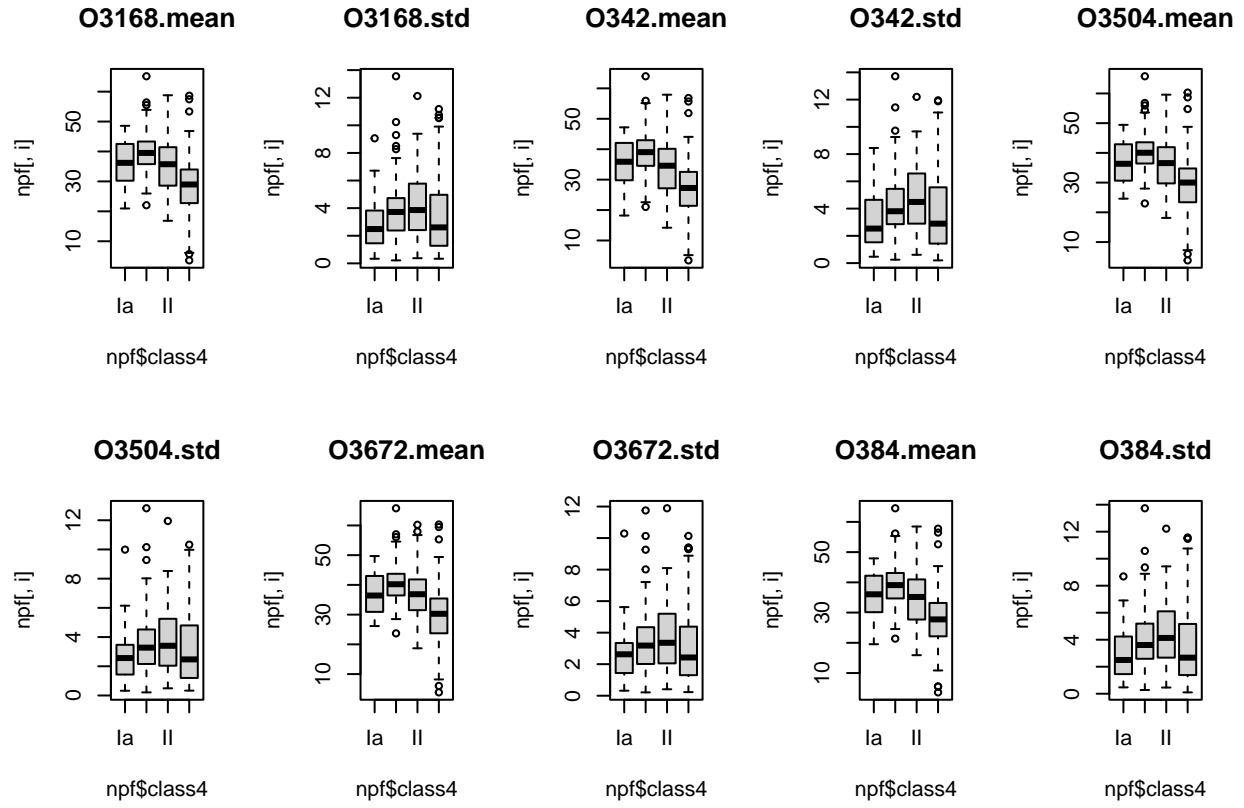


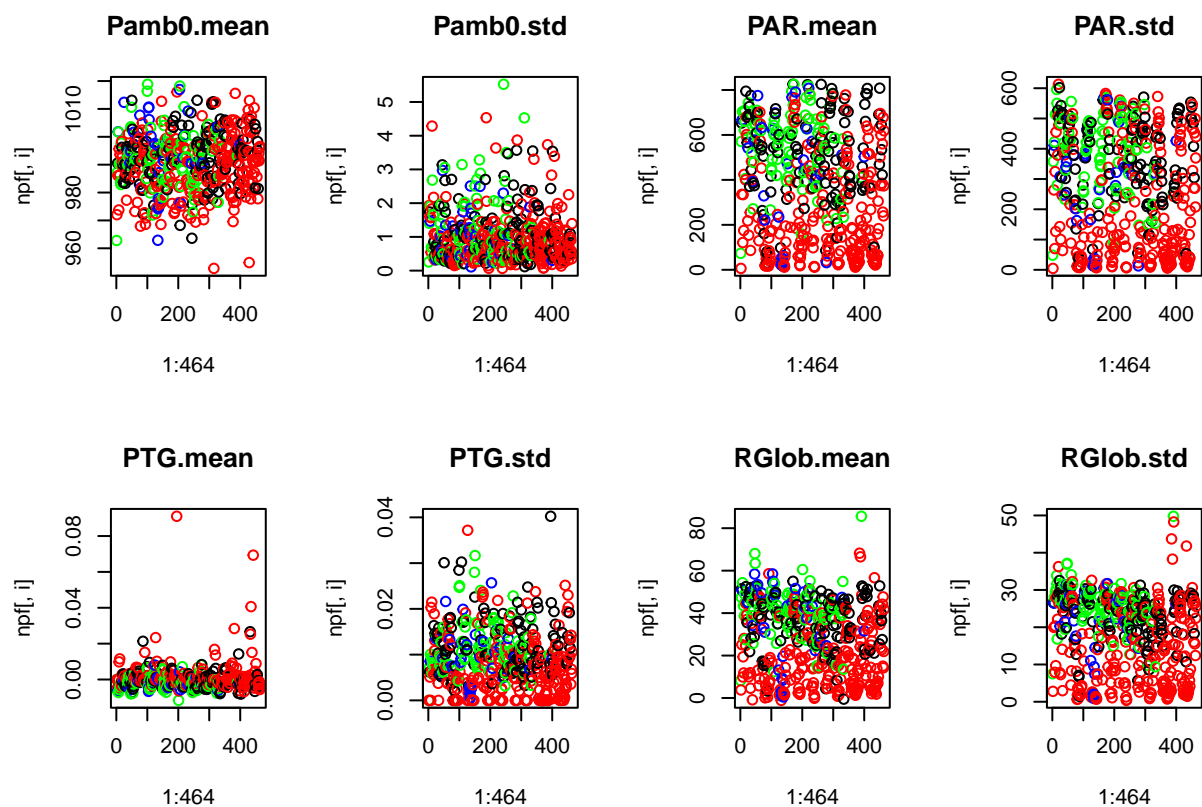


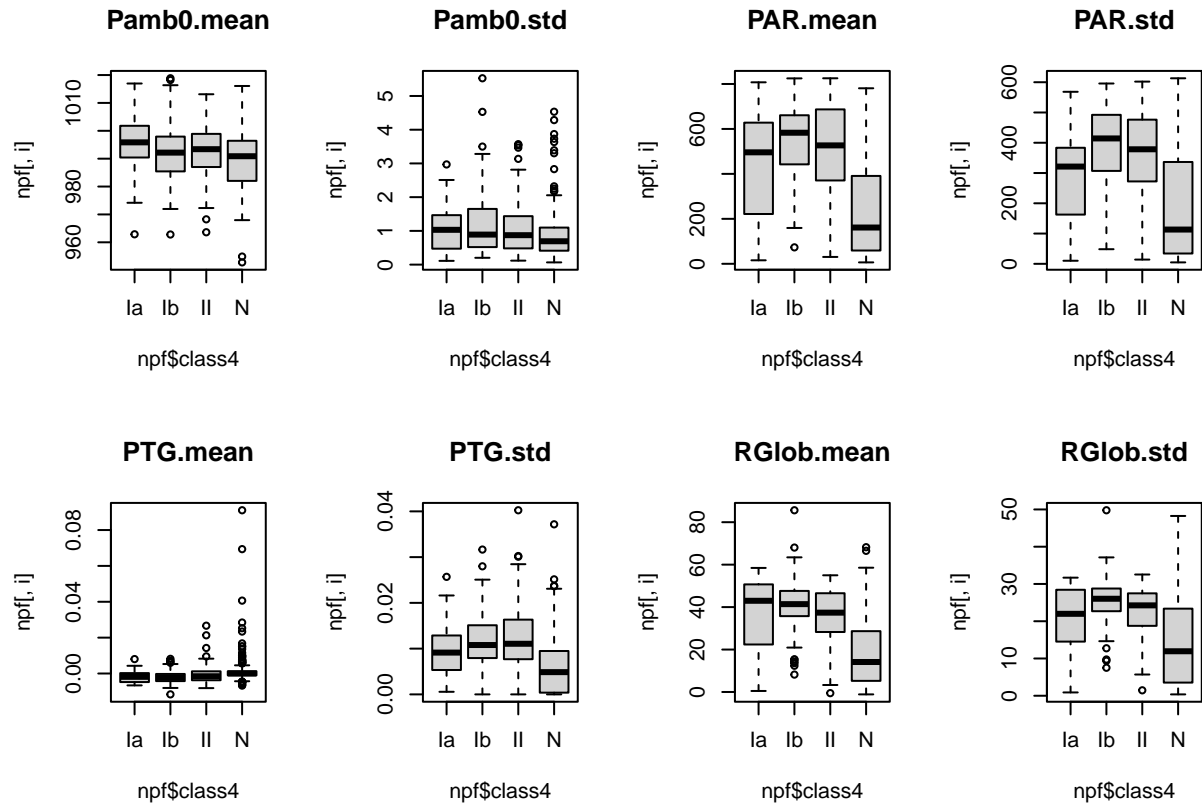


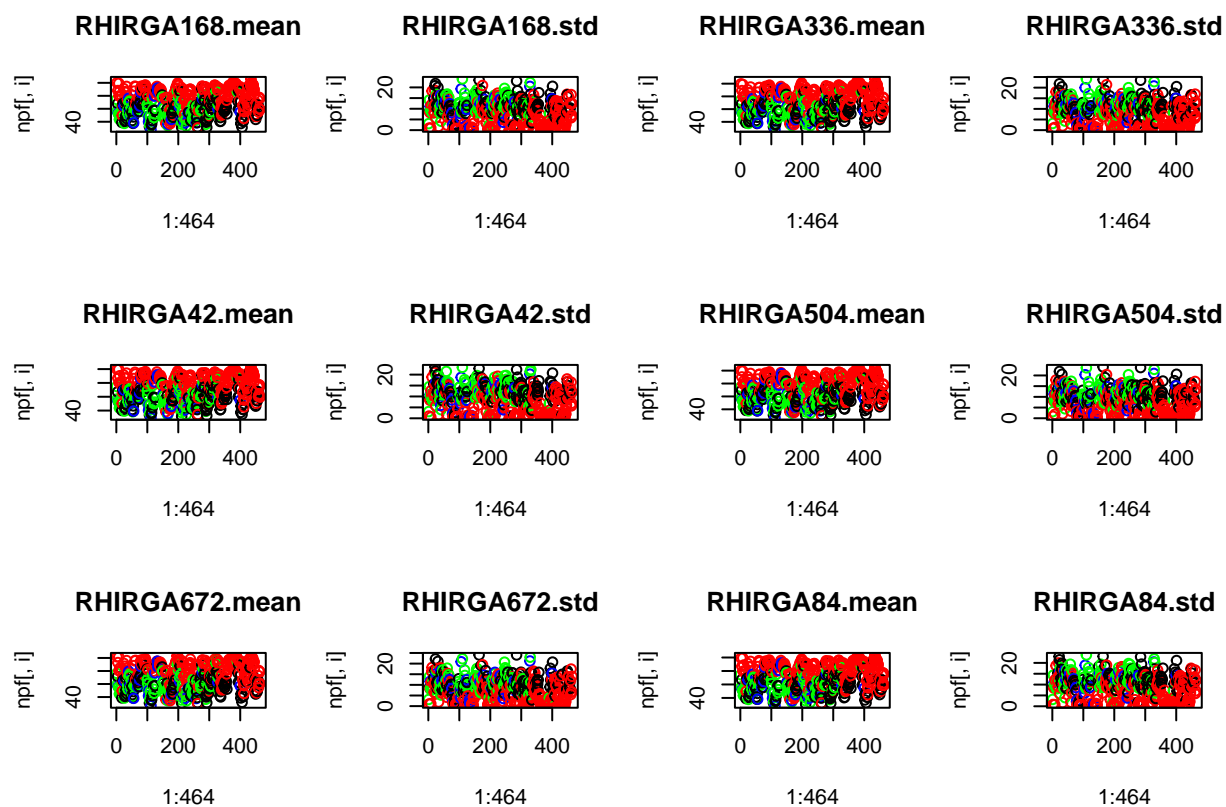


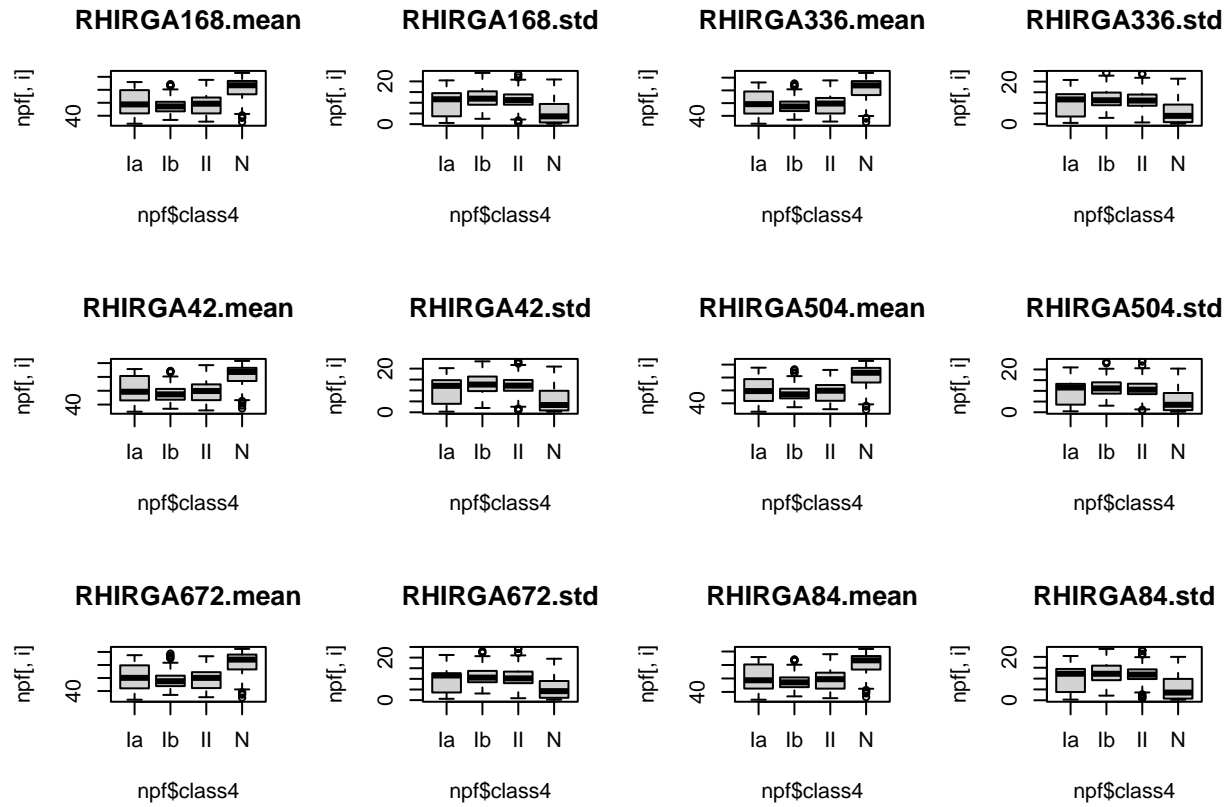


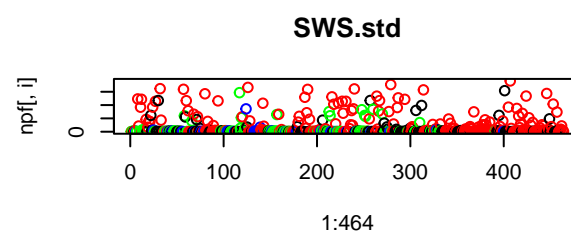
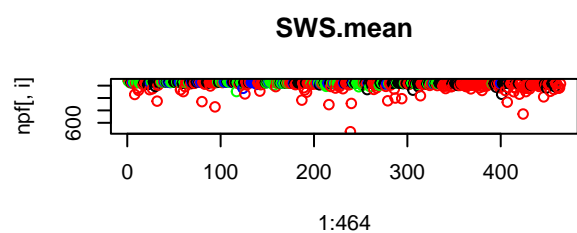
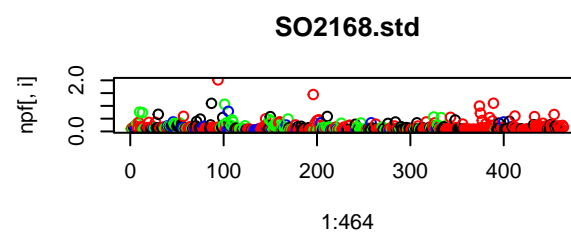
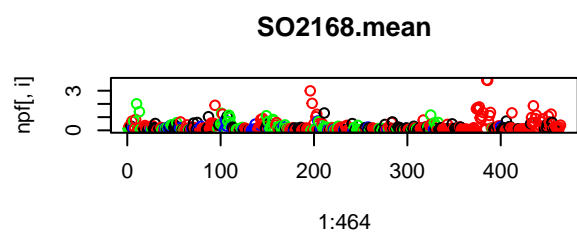
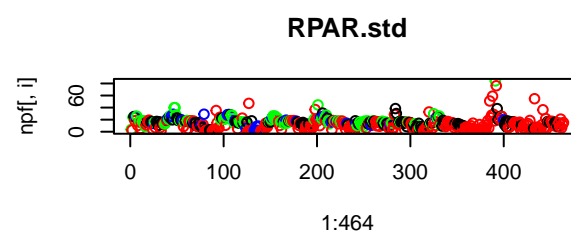
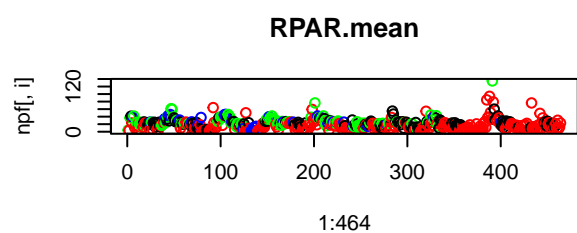




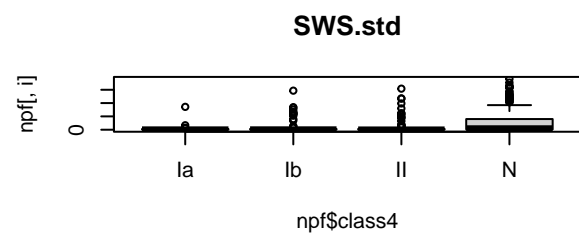
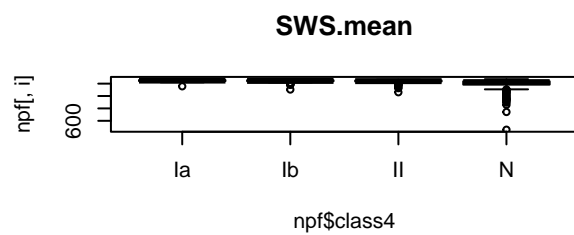
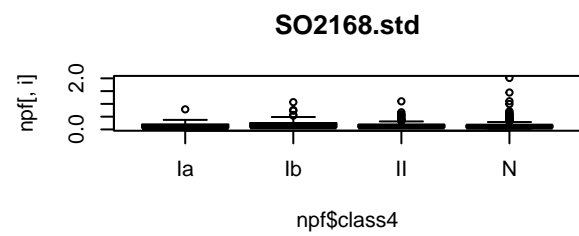
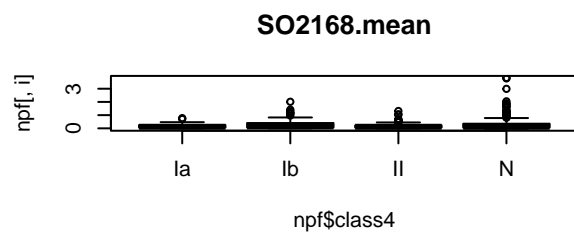
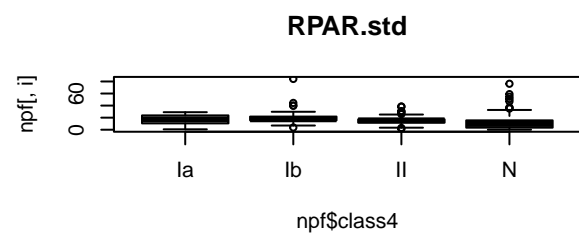
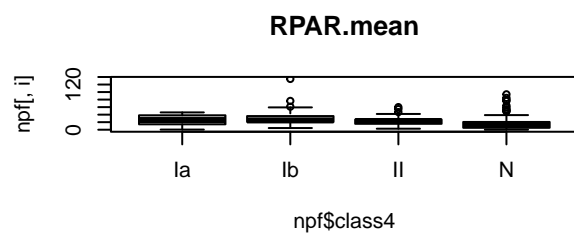


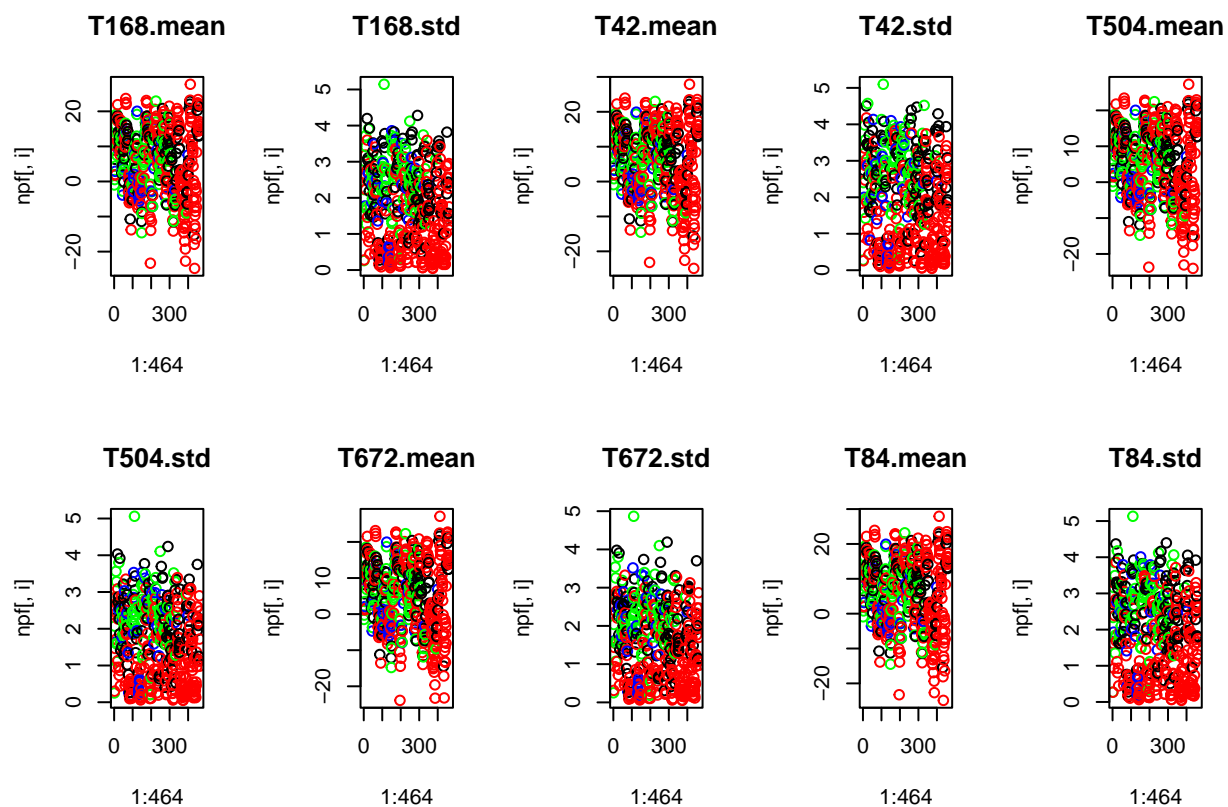


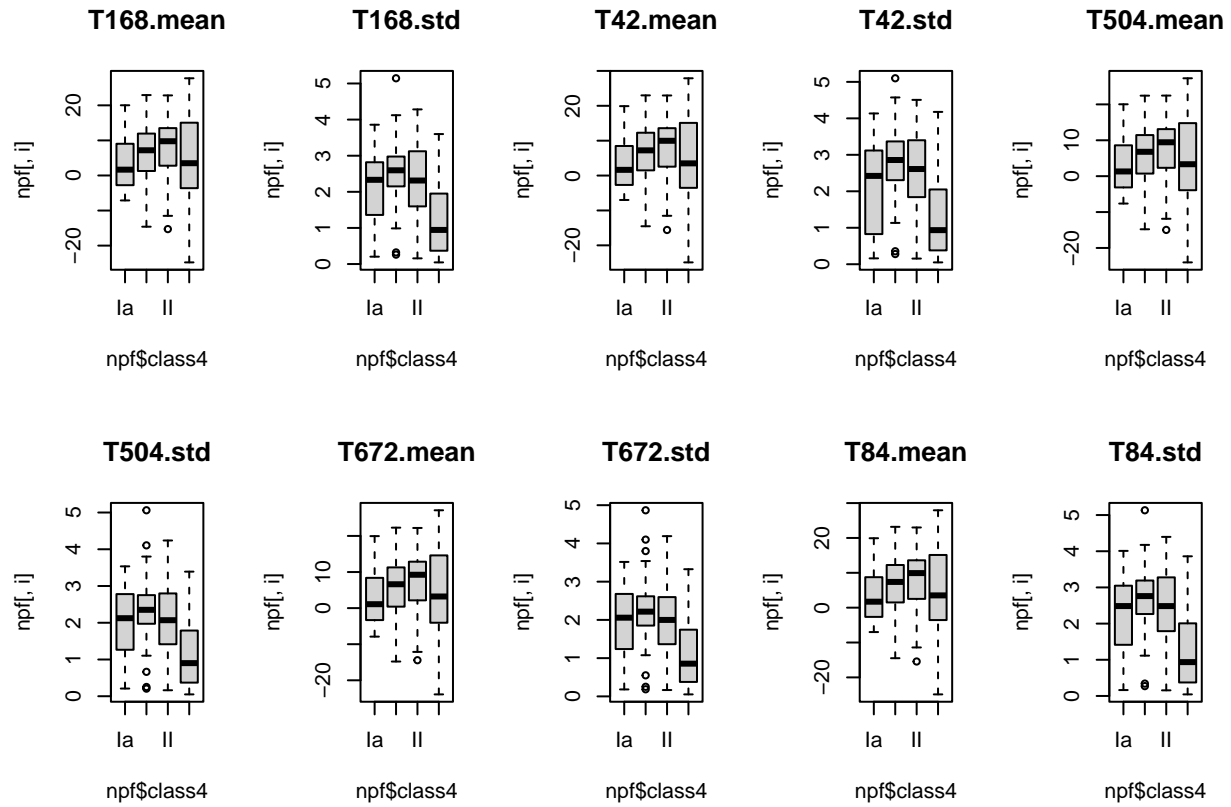




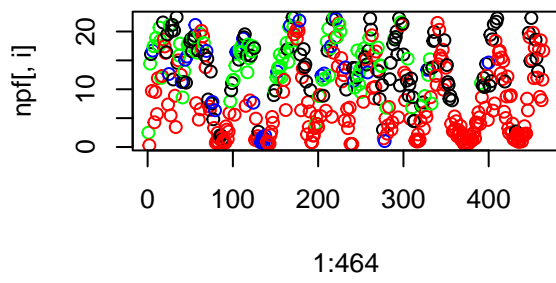




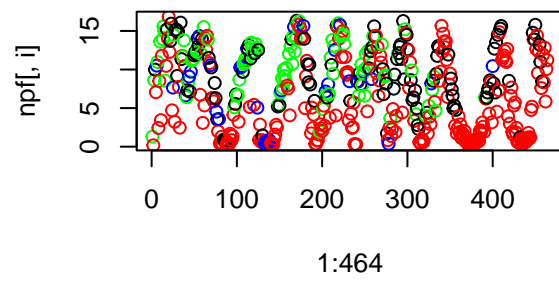




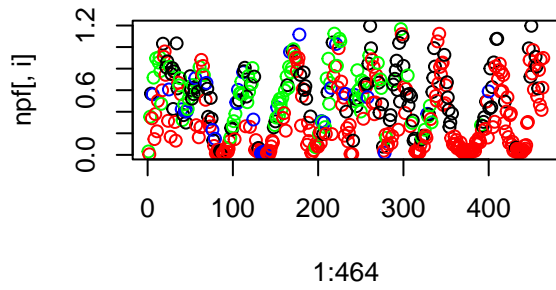
**UV\_A.mean**



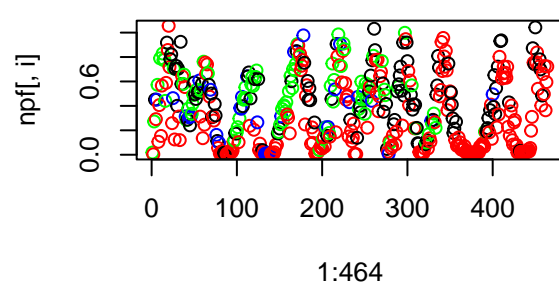
**UV\_A.std**

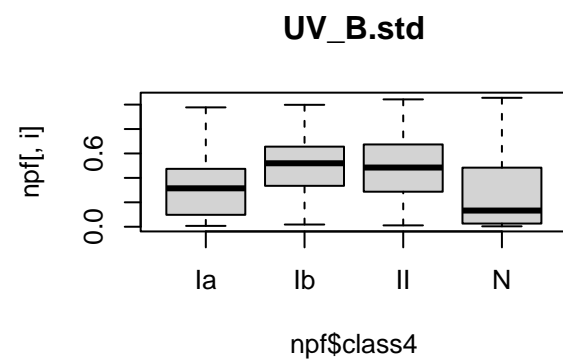
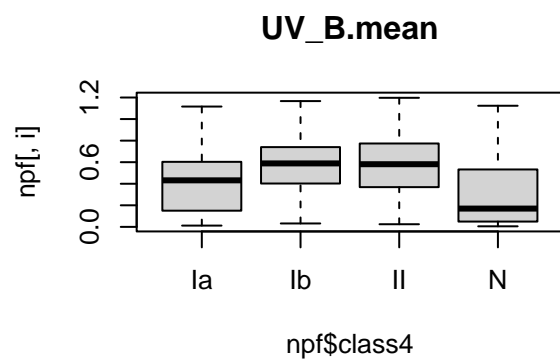
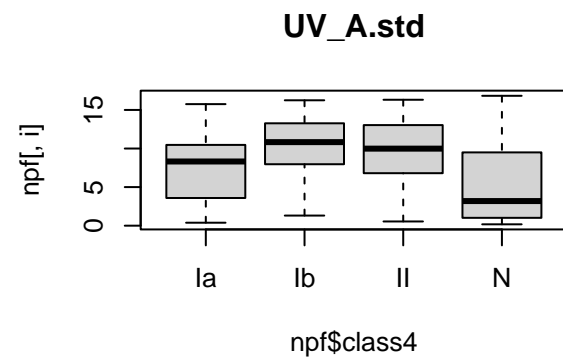
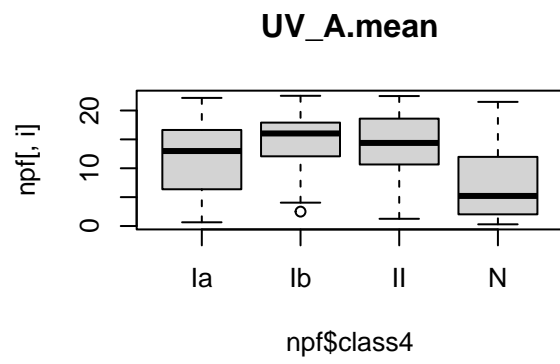


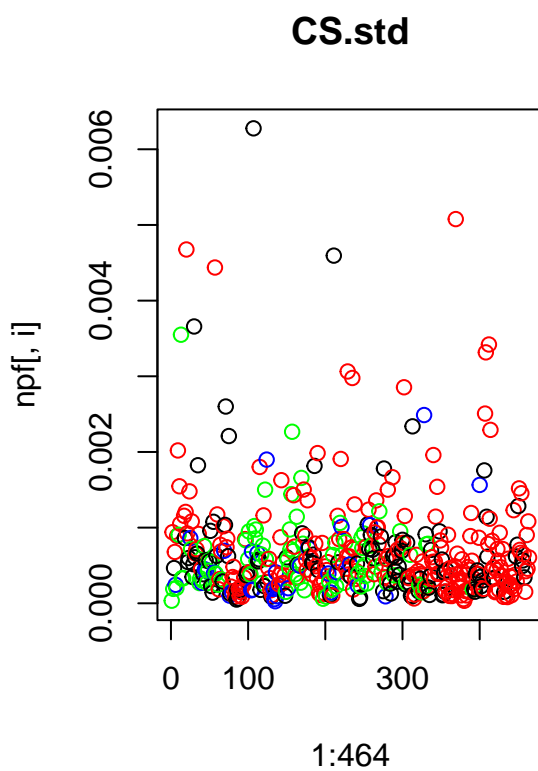
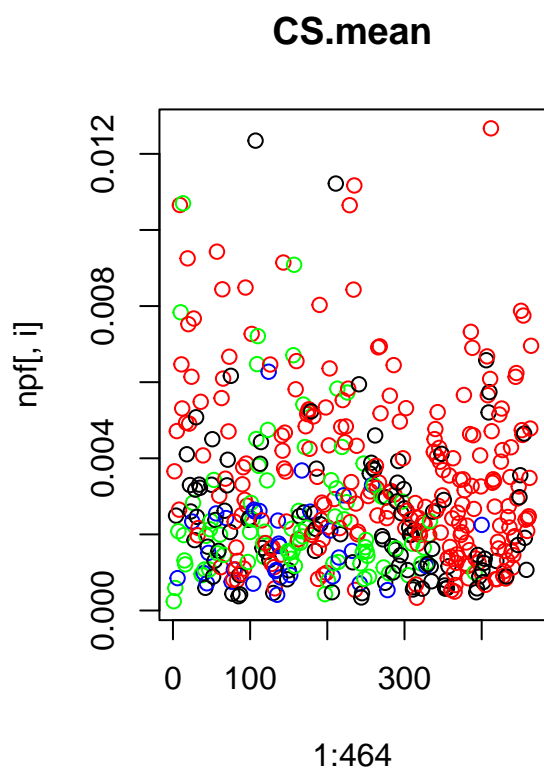
**UV\_B.mean**

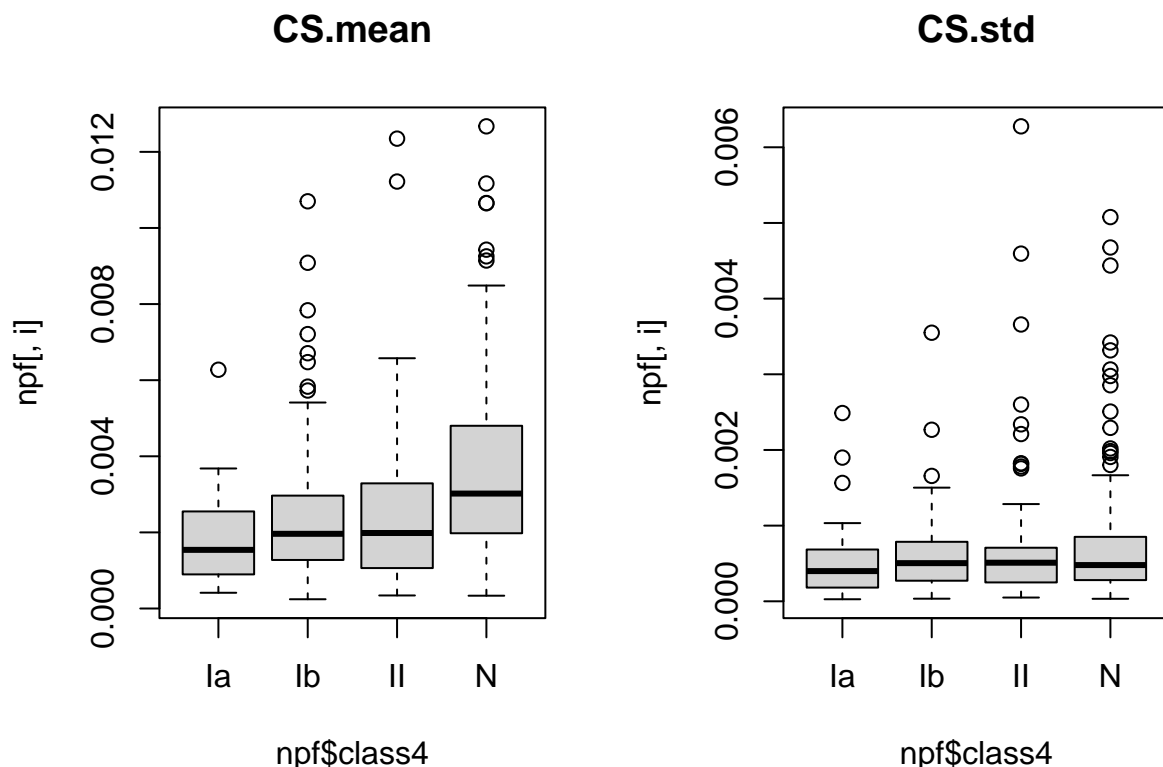


**UV\_B.std**









In particular we notice that with several of the variables the boxplots for the nonevent group observations differ more from the observations for days with NPF events than the boxplots for the different NPF event groups both in terms of smaller or higher values but also spanning larger intervals (although this can partially be caused by there being observations within this group). Another notable thing is that the measurements of the same variables at different heights behave very similarly, which imply correlation between them (we take a more detailed look into this in the section *Correlation between parameters*). We also notice a few interesting sets of variables, such as nitrogen monoxide (measurements NO), potential temperature gradient (measurements PTG), rain indicator signal (measurements SWS), sulphur dioxide concentration (measurements SO2) and (measurements CS), which seem to mostly have very small standard deviations. This would imply that the shifts during the day in relation to the corresponding mean observations are on average very small.

Let's also observe correlations between our explanatory variables by themselves and the variable we're attempting to predict. As there is no natural way of turning the four-class multinomial variable into a numeric form (because the different classes don't have a clear direction in which they rise or fall), let's observe how the explanatory variables correlate with the variable "class" instead. This should help us get a preliminary sense of what explanatory variables might describe our variable of interest the best.

##	C02168.mean	C02168.std	C02336.mean	C02336.std	C0242.mean
##	-0.30626777	-0.09596773	-0.30271045	-0.10806722	-0.32985917
##	C0242.std	C02504.mean	C02504.std	Glob.mean	Glob.std
##	-0.08793757	-0.29887003	-0.11393071	0.56928615	0.48236139
##	H20168.mean	H20168.std	H20336.mean	H20336.std	H2042.mean
##	-0.27790050	0.05382782	-0.28144835	0.05359948	-0.27131753
##	H2042.std	H20504.mean	H20504.std	H20672.mean	H20672.std
##	0.04299127	-0.28349790	0.05559773	-0.28529105	0.04823407
##	H2084.mean	H2084.std	NET.mean	NET.std	N0168.mean

```

##      -0.27456743      0.04349242      0.48609505      0.49417773      -0.12711787
##      N0168.std      N0336.mean      N0336.std      N042.mean      N042.std
##      -0.02889094      -0.13899494      -0.06847844      -0.15285335      -0.04893791
##      N0504.mean      N0504.std      N0672.mean      N0672.std      N084.mean
##      -0.14272836      -0.07816737      -0.15283971      -0.10621825      -0.12969448
##      N084.std      N0x168.mean      N0x168.std      N0x336.mean      N0x336.std
##      -0.07182797      -0.27466662      -0.08621634      -0.27903932      -0.13286528
##      N0x42.mean      N0x42.std      N0x504.mean      N0x504.std      N0x672.mean
##      -0.27633195      -0.10229014      -0.28264902      -0.10067518      -0.28437084
##      N0x672.std      N0x84.mean      N0x84.std      O3168.mean      O3168.std
##      -0.13807492      -0.27065623      -0.08856140      0.46504624      0.10349253
##      O342.mean      O342.std      O3504.mean      O3504.std      O3672.mean
##      0.46498198      0.11189109      0.46028886      0.06857651      0.45846357
##      O3672.std      O384.mean      O384.std      Pamb0.mean      Pamb0.std
##      0.05833510      0.46599615      0.11090869      0.16284163      0.15887982
##      PAR.mean      PAR.std      PTG.mean      PTG.std      RGlob.mean
##      0.54942511      0.46556287      -0.20133638      0.40030049      0.55973492
##      RGlob.std      RHIRGA168.mean      RHIRGA168.std      RHIRGA336.mean      RHIRGA336.std
##      0.47701430      -0.62724876      0.53196348      -0.62334360      0.52157036
##      RHIRGA42.mean      RHIRGA42.std      RHIRGA504.mean      RHIRGA504.std      RHIRGA672.mean
##      -0.63030377      0.54032646      -0.62093390      0.51271466      -0.61695967
##      RHIRGA672.std      RHIRGA84.mean      RHIRGA84.std      RPAR.mean      RPAR.std
##      0.49239697      -0.63023535      0.53490698      0.35123511      0.31087959
##      S02168.mean      S02168.std      SWS.mean      SWS.std      T168.mean
##      -0.10607274      0.02183685      0.33076219      -0.26767867      0.09695338
##      T168.std      T42.mean      T42.std      T504.mean      T504.std
##      0.51372072      0.09537137      0.52006333      0.09221095      0.50047378
##      T672.mean      T672.std      T84.mean      T84.std      UV_A.mean
##      0.09038205      0.49176171      0.09791565      0.52080878      0.51594601
##      UV_A.std      UV_B.mean      UV_B.std      CS.mean      CS.std
##      0.44214769      0.39813283      0.34950884      -0.28010884      -0.05254049
##      class2
##      1.00000000

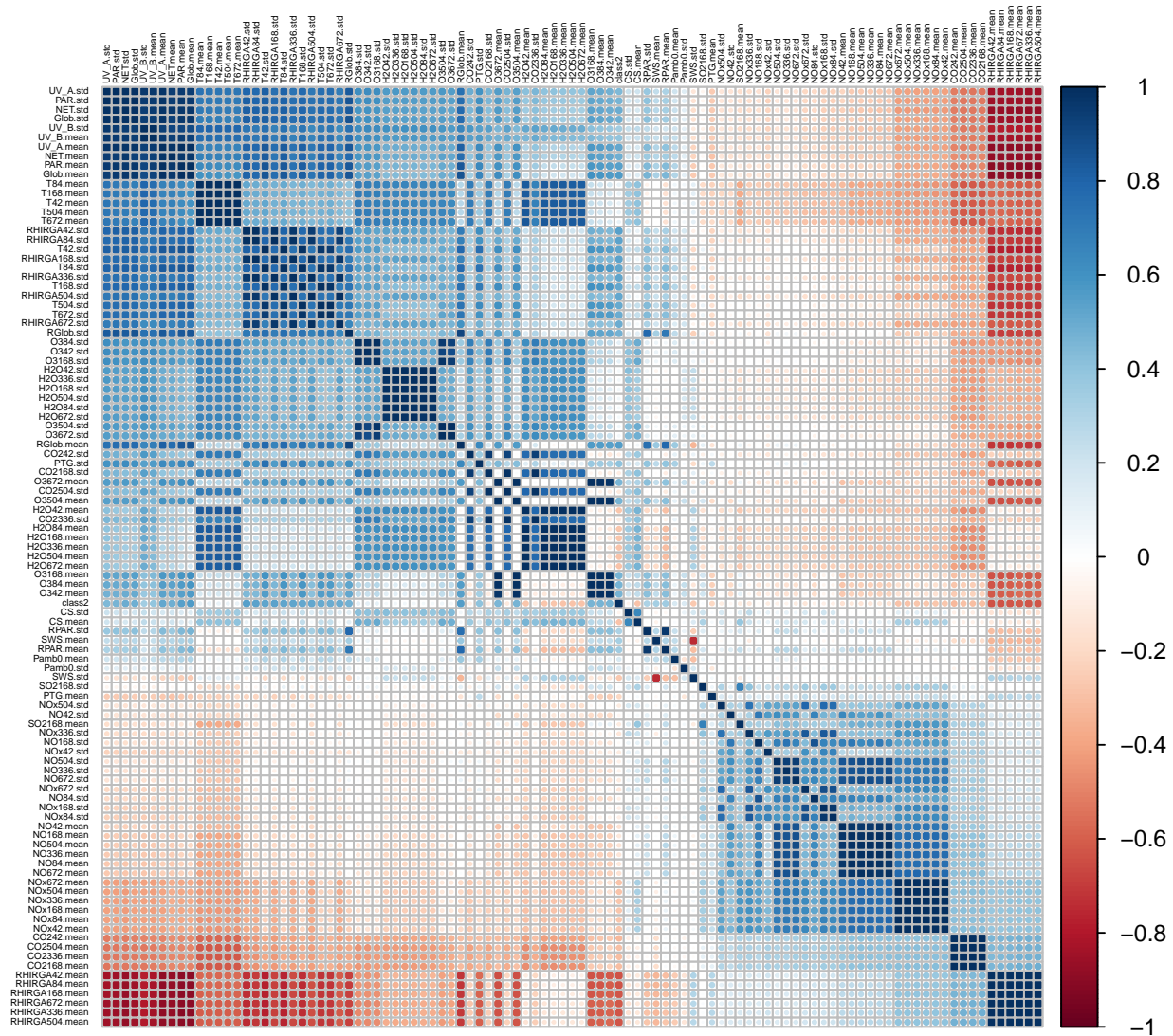
```

Based on this, we might at least preliminarily be interested in measurements of solar radiation (measurements Glob), net radiation (measurements Net),  $O^3$  (measurements O3), potential temperature gradient in C/m (measurements PTG), reflected solar radiation (measurements RGlob), temperature (measurements T)m type-A UV radiation (measurements UV\_A) and measurements RHIRGA (which perhaps refer to some kind of relative humidity) as explanatory variables.

## Correlation between parameters

The correlation between the predictors and the value to be predicted is a very natural starting point when it comes to correlation analysis. It is also possible that the predictors themselves are correlated. Many classifiers are affected by high correlation, i.e. *collinearity* between variables. In regression models, for example, it can be difficult to differentiate between the individual effects of collinear variables on the response.





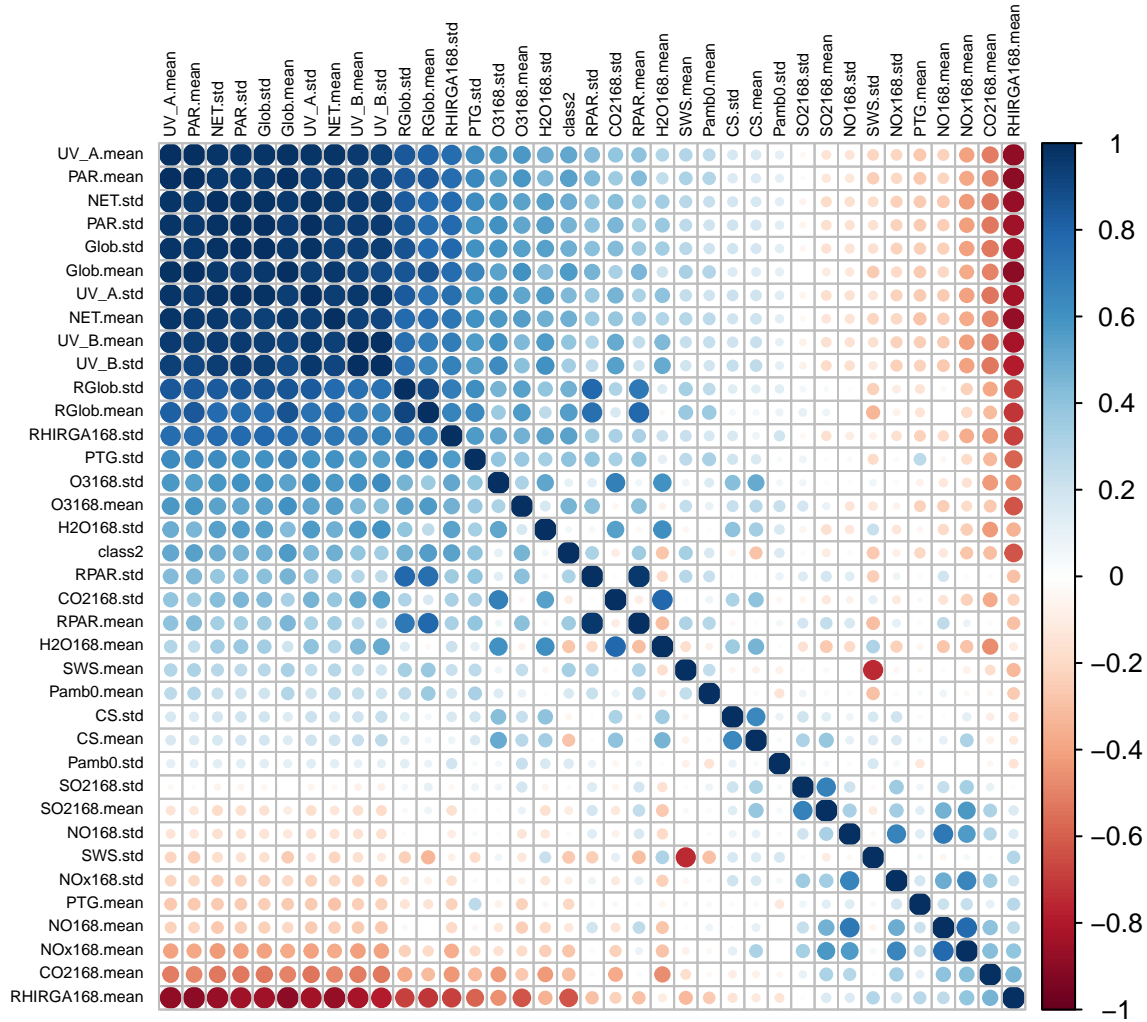
As expected, the correlation plot shows that many of the variables describing the same phenomenon at different heights are correlated, as are variables related to radiation. For many classifiers, highly correlated parameters are problematic, and for this reason we would like to drop some of the most highly correlated columns from the dataset.

We know that many of the parameters are measurements of the same thing at different heights. For example, water vapour concentration (H2O) has been measured at heights 4.2m, 8.4m, 16.8m, 33.6m, 50.4m and 67.2m. As can be seen from the table below, the correlation coefficients between the daily means of water vapour concentration at different heights are essentially 1.

Table 1: Correlation (H2O)

	H2O168.mean	H2O336.mean	H2O42.mean	H2O504.mean	H2O672.mean	H2O84.mean
H2O168.mean	1.0000000	0.9998966	0.9997062	0.9997158	0.9994631	0.9998894
H2O336.mean	0.9998966	1.0000000	0.9993506	0.9999302	0.9997498	0.9996330
H2O42.mean	0.9997062	0.9993506	1.0000000	0.9990202	0.9986416	0.9999330
H2O504.mean	0.9997158	0.9999302	0.9990202	1.0000000	0.9998589	0.9993631
H2O672.mean	0.9994631	0.9997498	0.9986416	0.9998589	1.0000000	0.9990316
H2O84.mean	0.9998894	0.9996330	0.9999330	0.9993631	0.9990316	1.0000000

Hence we discard most of the measurements of H2O and other variables for which we have multiple highly correlating measurements, both the means and the standard deviations. We keep the parameters measured at 16.8 meters as for some parameters, the measurements have only been measured at that height. This rather crude method of discarding data leaves us with 38 unique columns. The figure below describes the correlation coefficients between the remaining parameters.



The correlation plot for the remaining parameter shows us that the remaining highly correlated parameters are all radiation-related.

## Classifier

### Description of considered machine learning approaches

In order to use a model that describes the process that creates the data the best, we attempted to use several different kinds of models to assess the data. After defining each of these models, we would assess which of the models we used performed best and use said model in our predictions.

Specifically, the two measures we used to assess the quality of each model were its accuracy and perplexity. We defined accuracy as simply the relative amount of values the model predicted correctly, expressed mathematically for variables of interest  $y_i$  and related predictions  $\hat{y}_i$  as  $\frac{\sum_{i=1}^n I(y_i = \hat{y}_i)}{n}$ . This measures whether the model defines the labels correctly. All values naturally receive values within interval  $[0, 1]$  and higher values imply better results.

Perplexity instead expresses the relative confidence in those predictions. The models we use give estimated probabilities  $\hat{p}(\hat{y}_i = y)$  that the datapoints  $\hat{y}_i$  we're predicting receive specific values  $y$ . Thus, if the model is descriptive of the phenomena which create the dataset, it would seem reasonable that for the actual realized values  $y$  the measure  $\hat{p}(\hat{y}_i = y)$  would be relatively high. Thus its logarithmic transformation  $\log(\hat{p}(\hat{y}_i = y))$  would also be able to receive high values, and similarly  $-\log(\hat{p}(\hat{y}_i = y))$  and  $e^{\log(\hat{p}(\hat{y}_i = y))}$  would receive small values. Thus we can use as a corresponding overall measure for the dataset the measurement  $e^{-\frac{\sum_{i=1}^n \log(\hat{p}(\hat{y}_i = y_i))}{n}}$  where  $y_i$  are realized values of the observations we're attempting to assess through  $\hat{y}_i$ . As  $\hat{p}(y_i = y) \in [0, 1]$  for all  $\log(\hat{p}(y_i = y)) \leq 0$  for all  $y$ . Thus, all values of our general perplexity measure are within interval  $[1, \infty)$  and smaller values are preferred.

However, it is not sufficient to simply define the model on the training dataset and assess accuracy and perplexity on said training dataset as this would woefully inflate the accuracy assessment and deflate the perplexity assessment of the model on a general dataset. We instead attempted to assess accuracy and perplexity through cross-validation methods, specifically leave-one-out cross-validation (loo-cv). The idea behind loo-cv is that for each observation in the training dataset, a model is trained based on all other observations in the dataset. This new model is then used to predict the training dataset value that was left out of defining the model. With this method, we receive based on observations of explanatory variables both predicted values and estimates of probabilities for specific events for each measurement in a way that didn't include the observations in both defining the model training and assessing its quality. Thus, we can use these measures in our accuracy and perplexity calculations to better assess how the model using all the observations in the training dataset behaves on a completely separate test dataset.

Next, let's discuss some of the models we considered

### Logistic regression

Logistic regression models can be used for binomial variables as well as for multinomial variables under specific assumptions. The idea of logistic regression in a binary case is that our variable of interest  $Y$  is binomially distributed with parameter  $q \in [0, 1]$  representing probability that  $Y$  receives one of the values (this is somewhat irrelevant as the corresponding parameter for the other value would simply be  $1 - q$ ). Now, with explanatory variables  $X$  we assume that these  $X$  influence the parameter  $p$  for each observation, meaning  $p(Y|X) = q(X)^Y (1 - q(X))^{1-Y}$  is a binomial probability with parameter  $q(X)$  being of form  $\sigma(\sum \lambda_i X_i)$  for values of individual explanatory variables  $X_i$  and coefficients  $\lambda_i$  and link function  $\sigma : \mathbb{R} \rightarrow [0, 1]$ . Thus we can estimate a logistic regression by finding parameters  $\lambda_i$  that maximize the likelihood function  $\prod p(Y_i|X)$ .

Notable benefits of the logistic regression model include that as a discriminative model it eventually reaches a lower asymptotic variance than comparable generative models. On top of this, compared to for example comparable support vector classifiers, on average logistic regression models fare better under situations where the classes are not easily separable by explanatory variables.

However, possible shortcomings of the logistic regression model include assumptions of linearity in relation to the explanatory variables and the parameter (which we could attempt to correct but with such a collection of explanatory variables, this at least can't be applied immediately), assumptions of for link function that are required to define coefficients, and especially with high-dimensional models, multicollinearity can become a notable problem.

In our model, we used specifically the logistic link function, implying  $\sigma(x) = \frac{e^x}{e^x + 1}$ , although we acknowledge that other choices such as the probit link could have also been viable options. In order to curb issues related to multicollinearity, we first limited ourselves to the dataset with observations measured at multiples only observed at 16.8 meters. After this, we reduced the set of explanatory variables further via variance inflation factors. Variance inflation factors (VIFs) can be calculated for each explanatory variable in a model through assessing linear models for each of the explanatory variables. The VIF for explanatory variable  $X_i$  is defined as  $\frac{1}{1-R_i^2}$  where  $R_i^2$  is the amount of variance of  $X_i$  explained through a linear model by the other explanatory variables. Thus, these values express how much the explanatory variable in question can be described by a linear combination of the other explanatory variables. Thus, particularly high VIFs imply multicollinearity being present in the model.

As removing one explanatory variable effects the VIFs of all other variables, we chose to implement an iterative process to remove variables based on VIFs. After defining a logistic regression model with all explanatory variables, we calculated the VIFs, assessed which variable had the highest VIF, removed both this variable and the other variable describing the same set of observations (if a mean variable had the highest VIF, we would also remove the corresponding standard deviation and if a standard deviation variable had the highest VIF, we would also remove the corresponding mean variable). We decided to do this as it felt imprudent to choose to not include one descriptor of an observation in the baseline model which we're assessing while including the other one. After this, we would repeat the process until the highest VIF value for a variable was less than 10. The choice of the limit was based on descriptions in the course material.

After this, we had a remaining set of 18 explanatory variables, which we modelled using logistic regression. After checking the coefficients, there were still variables for which the likelihood ratio tests gave relatively high p-values for hypotheses involving non-zero coefficients. In order to deal with this, we set those coefficients equal to zero and assessed the model with the remaining explanatory variables. Through this, we received a simpler model with explanatory variables.

## Lasso regression

Lasso regression has obvious links to logistic regression but it includes a penalty term which punishes models with high values of coefficients. In comparable linear regression minimizing squared error, the minimizable function is the sum of the squared error terms and  $\sum_{i=1}^n \gamma |\lambda_i|$  where  $\gamma > 0$ . We similarly as in logistic regression assess coefficients for a model that describes parameter  $q$  of a binomial model that minimizes this function.

One of the benefits of lasso regression is that including this penalty term in the optimization process leads to simpler models with fewer explanatory variables, as also lower-dimensional models lead are preferred. Thus, the lasso model in and of itself can remove variables which are highly correlated with other variables from the model and thus at least alleviate multicollinearity within the model. However, the selection between possible correlated variables can apparently be rather random and thus not perhaps fully descriptive of the data-generating process.

In terms of our modelling, we decided to use lasso instead of a comparable method called ridge regression, which uses penalty term  $\sum_{i=1}^n \gamma \lambda_i^2$ . The reason for this is that we preferred to make a simpler model with fewer explanatory variables rather than ridge regression, which tends to not reduce the dimension of the model but rather simply give similar coefficients to all correlated explanatory variables. We attempted to assess the value of  $\gamma$  which would minimize loo cross-validated misclassification rate with the function `cv.glmnet`. After defining this value, we calculated cross-validated accuracy (which should be equivalent to what was calculated by `cv.glmnet`) as well as the cross-validated perplexity.

## Generative models

In logistic regression models, we directly model  $p(Y|X)$ , i.e. the conditional distribution of the response  $Y$  given the predictors  $X$ . Generative models offer a less direct approach, where the focus is in modeling  $p(X|Y)$  and using these estimates to estimate  $p(Y|X)$  for each possible class  $k$  with Bayes' theorem:

$$p(Y = k|X) = \frac{\pi_k p(X|Y = k)}{\sum_i \pi_i p(X|Y = i)}.$$

Here  $\pi_k$  is an estimate of the prior probability that a random observation comes from the  $k$ th class, in our case computed as the fraction of the observations in the training dataset that are in the  $k$ th class.

While the general approach is the same for all generative models, they differ in how they estimate  $p(X|Y)$ . In a dataset with  $p$  predictors, estimating  $p(X|Y)$  amounts to estimating a  $p$ -dimensional density function for an observation in the  $k$ th class. The task is challenging, as we must consider the distribution of each predictor on its own *and* the joint distribution of the predictors. Different models make different assumptions that mitigate the difficulty.

### Linear Discriminant Analysis

A linear discriminant analysis (LDA) classifier assumes that all  $p$  predictors  $X = (X_1, \dots, X_p)$  are drawn from a multivariate Gaussian distribution. This means that each predictor follows a normal distribution  $N(\mu_k, \Sigma)$  where  $\mu_k$  is the class-specific mean and  $\text{Cov}(X) = \Sigma$  the covariance matrix of  $X$ , and there is some correlation between each pair of predictors. The estimate of  $p(X|Y)$  is

$$p(X|Y) = \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}} \exp \left( -\frac{1}{2} (x - \mu_k)^T \Sigma^{-1} (x - \mu_k) \right)$$

meaning that the classifier assigns an observation  $X$  to the class for which

$$\delta_k(x) = x^T \Sigma^{-1} \mu_k - \frac{1}{2} \mu_k^T \Sigma^{-1} \mu_k + \log \pi_k$$

is maximized. The covariance matrix being the same for all classes is a defining feature of linear discriminant analysis. The assumption makes the model linear and reduces the number of parameters to estimate. This reduces the flexibility and hence lowers the variance of the model. Lower variance can mean that the model performs well, but if the assumption is not reflected in the data, bias can be high and overall performance suffers due to the bias-variance trade-off.

For linear discriminant analysis to work, it is important to have enough observations with regards to the number of predictors, as performance suffers greatly as the number of predictors approaches the number of observations.

In our modeling, we used the function `lda` from the library *MASS*. We tested the performance of the model on the dataset with observations measured at multiples only observed at 16.8 meters.

### Quadratic Discriminant Analysis

The assumption that the covariance matrix is shared for all classes is quite strict. Allowing each class to have its own covariance matrix brings us to quadratic discriminant analysis (QDA). The observations are still assumed to be drawn from a multivariate Gaussian distribution with a class-specific mean vector, so otherwise the assumptions remain the same as in LDA. Each predictor now follows a normal distribution  $N(\mu_k, \Sigma_k)$ . The expression to be maximized is

$$\delta_k(x) = x^T \Sigma_k^{-1} \mu_k - \frac{1}{2} x^T \Sigma_k^{-1} x - \frac{1}{2} \mu_k^T \Sigma_k^{-1} \mu_k - \frac{1}{2} \log |\Sigma_k| + \log \pi_k.$$

Generally, quadratic discriminant analysis is expected to perform better than linear discriminant analysis on large data sets, but as in linear discriminant analysis, the number of predictors must be small enough to

produce decent results. Quadratic discriminant analysis is also recommended when the assumption that all classes share a covariance matrix is clearly unfounded.

In our approach, we used the *qda* function from the *MASS* library, and as with linear discriminant analysis, tested the performance of the model on both the original dataset and the dataset with observations measured at multiples only observed at 16.8 meters.

## Naive Bayes

A naive Bayes classifier makes no assumptions on the distribution of the observations, and instead assumes that within the  $k$ th class, the  $p$  predictors are independent. In other words, the assumption is that there is no association between the predictors, and therefore no joint distribution to consider. With this, the posterior probability can be computed as

$$p(Y = k|X) = \frac{\pi_k p(X_1|Y = k) \cdots p(X_p|Y = k)}{\sum_i \pi_i p(X_1|Y = i) \cdots p(X_p|Y = i)}.$$

In a naive Bayes model, there are a few possible ways to estimate  $p(X|Y)$ . For quantitative predictors such as ours, we assume that within each class, the  $j$ th predictor is drawn from a univariate normal distribution, i.e.  $X_j|Y = k \approx N(\mu_{jk}, \sigma_j^2 k)$ . The assumption of independence between predictors is often not realistic, but the model can perform well nonetheless. This is especially true for small datasets, since estimating a joint distribution requires a large amount of data.

## Support Vector Classifiers

The idea of the binary support vector classifier is based on the notion of finding within a  $p$ -dimensional problem a  $(p - 1)$ -dimensional hyperplane  $\lambda_0 + \sum \lambda_i x_i = 0$  to divide the set of explanatory variables. Now, for this hyperplane, we can divide our observations into two groups, those values for which  $\lambda_0 + \sum_{i=1}^m \lambda_j x_i > 0$  and those values for which  $\lambda_0 + \sum \lambda_i x_i < 0$ . Thus, this can function as a model through which we can predict binary variables such as our variable of interest.

However, defining such hyperplanes can be slightly difficult as all values might not be separable by a hyperplane or the hyperplane that separates values can overfit to training data. Thus, we define a soft-margin classifier, which has the benefits of letting some values be misclassified or be closer to the hyperplane than a strict maximal margin classifier would define, which leads to a more robust model that fits most of the training dataset better.

In order to define this, we need to find the optimal hyperplane to separate the observations. This optimization problem is an optimization problem of  $M$  in relation to coefficients  $\lambda_i$  and slack variables  $\epsilon$  within inequation  $y_i(\lambda_0 + \sum_{j=1}^m \lambda_j x_{ij}) \geq M(1 - \epsilon_i)$  with limitations  $\sum_{j=1}^m \lambda_j^2 = 1$ ,  $\epsilon_i \geq 0$  and  $\sum_{i=1}^n \epsilon_i \leq C$  for tuning parameter  $C$ .

As in our optimization the data only depends on the inner products of the explanatory variables and the values of the variable of interest, we can use different generalizations of inner products to gain different kinds of models. Thus with different choices of kernels we can model different kinds of data.

Other benefits of using support vector classifiers include that they have been proven to behave well in several different applications and that it has been shown that on average support vector classifiers perform better than logistic regression models in problems where the classes are well-separated. However, the model can vary quite notably based on the tuning parameter  $C$  as this parameter affects the amount of observations that violate the margin and thus increases or decreases the amount of support vectors that influence the model.

For our model, we chose to run a 10-fold cross validation on a set of tuning parameters  $C$  to assess which kernel performed best and chose to model the value based on that. In these preliminary assessments, we assessed the radial and linear kernels had the best performance of the ones available in the R package *e1071*. For these kernels, we ran loo-cross validation to assess the value of tuning parameter  $C$  and calculated for said tuning parameter loo-cross-validated accuracy and perplexity. Eventually, the radial kernel had slightly

better accuracy but the linear kernel had lower perplexity and as a result, we chose to use the linear kernel in our model

**Chosen classifier, pros and cons of this particular classifier for this application**

**Results**

**Classifier performance (numerical)**

**Insights, conclusions, discussion etc.**