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 phenomenona 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
##   CO2168.mean      CO2168.std        CO2336.mean      CO2336.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
##    CO242.mean      CO242.std        CO2504.mean      CO2504.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        H2O168.mean       H2O168.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
##   H2O336.mean       H2O336.std       H2O42.mean       H2O42.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
##   H2O504.mean       H2O504.std        H2O672.mean       H2O672.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
##    H2O84.mean       H2O84.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
##    NO168.mean         NO168.std         NO336.mean         NO336.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
##    NO42.mean           NO42.std         NO504.mean         NO504.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
##    NO672.mean         NO672.std          NO84.mean           NO84.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
##   NOx168.mean       NOx168.std       NOx336.mean       NOx336.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
##    NOx42.mean         NOx42.std         NOx504.mean        NOx504.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
##   NOx672.mean       NOx672.std        NOx84.mean        NOx84.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
##    O3168.mean       O3168.std         O342.mean        O342.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
##    O3504.mean       O3504.std        O3672.mean       O3672.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
##   SO2168.mean        SO2168.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
```

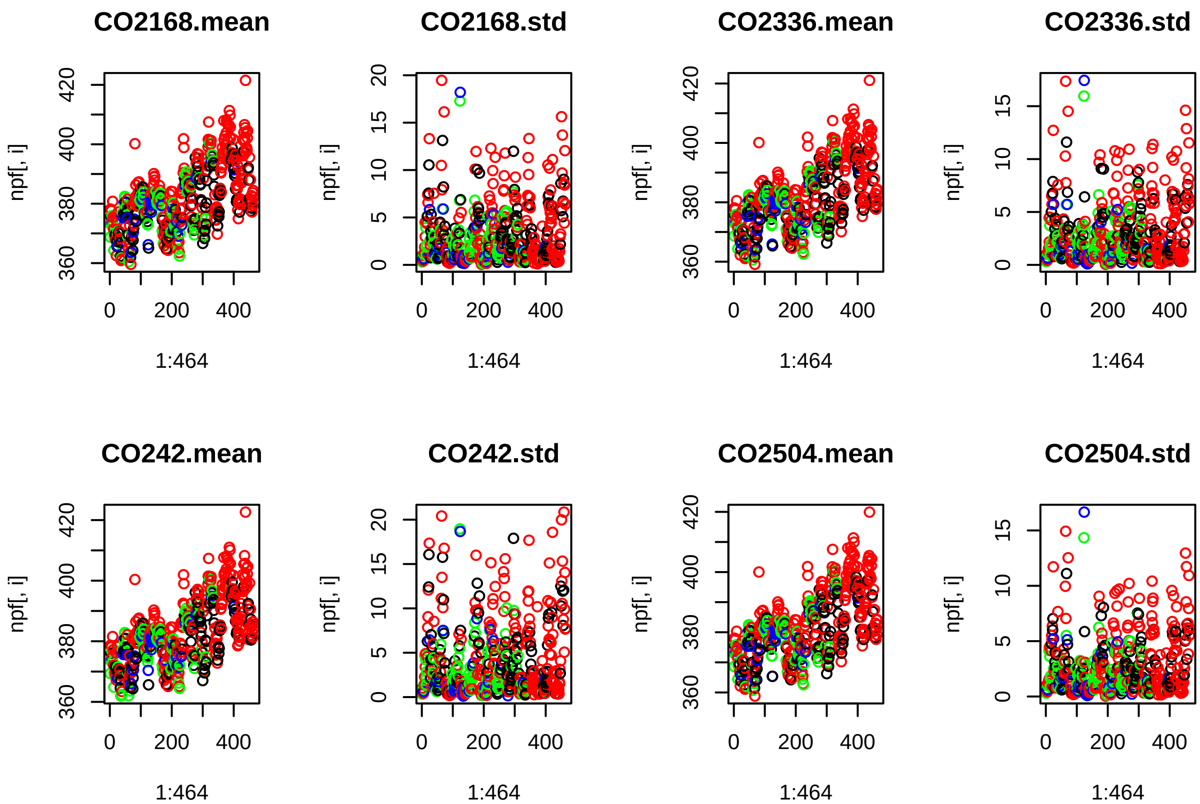
```
##  Min.   :-24.778   Min.   :0.04589   Min.   :-24.883   Min.   :0.05069
##  1st Qu.: -1.530   1st Qu.:0.72766   1st Qu.: -1.510   1st Qu.:0.75975
##  Median :  6.402   Median :1.80772   Median :  6.621   Median :1.98491
##  Mean   :  5.681   Mean   :1.79699   Mean   :  5.752   Mean   :1.95714
##  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
##
##
##
```

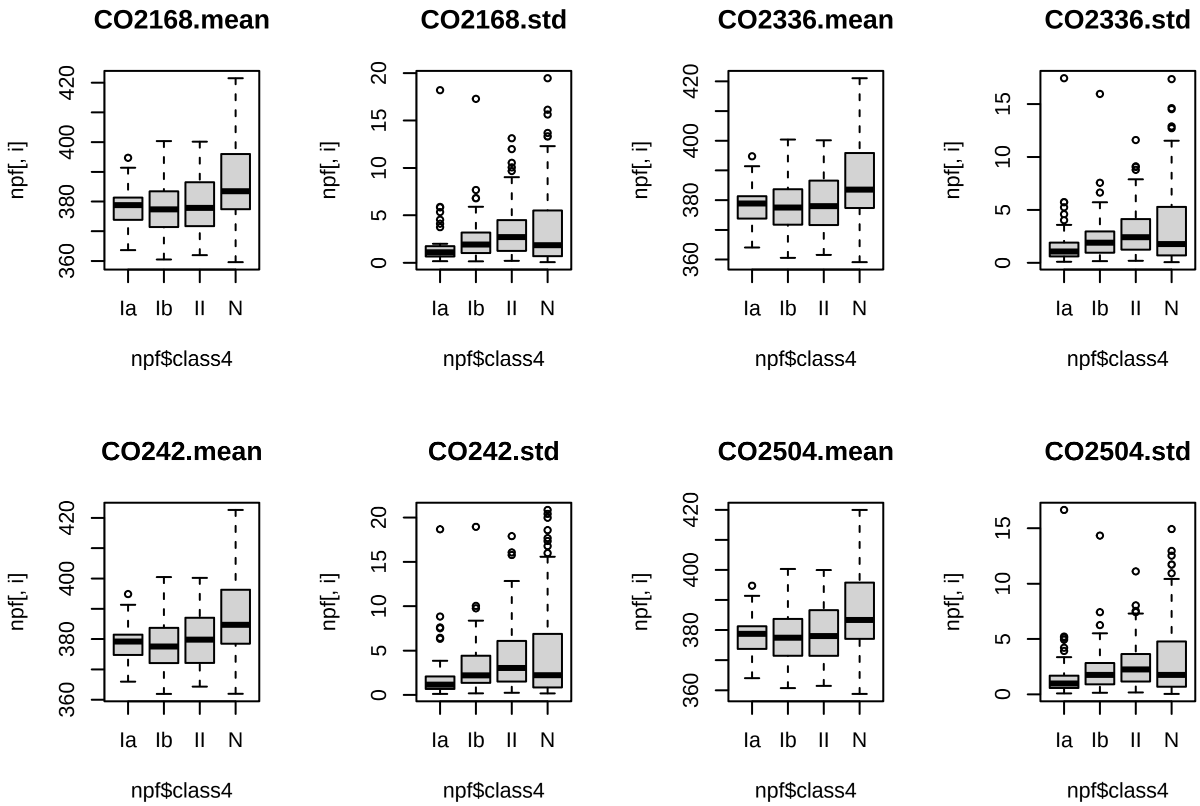
Of particular interest here is that the variable "partlybad" seems to have only observations of type "FALSE". As a result, we can remove it from the dataset as it gives no extra information. We can also remove the variable id, as the order of the observations is not of interest in our analysis. And on 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.

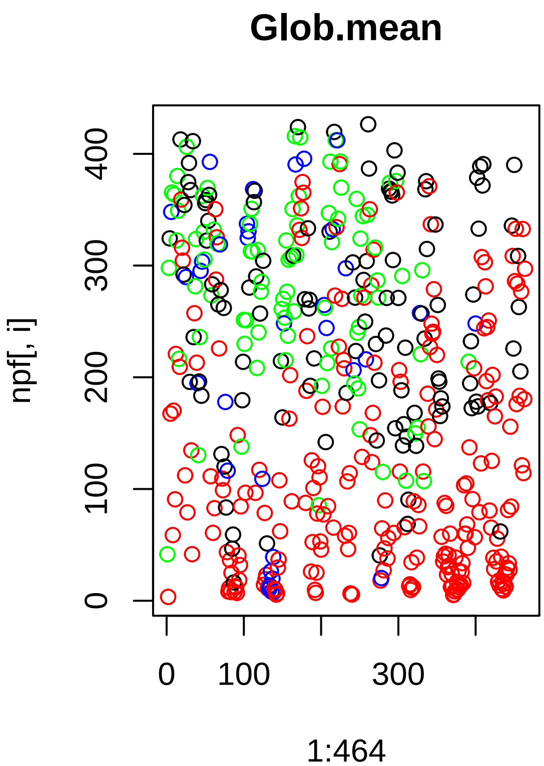
Now we are left with our variable of interest, as well as 100 explanatory variables.

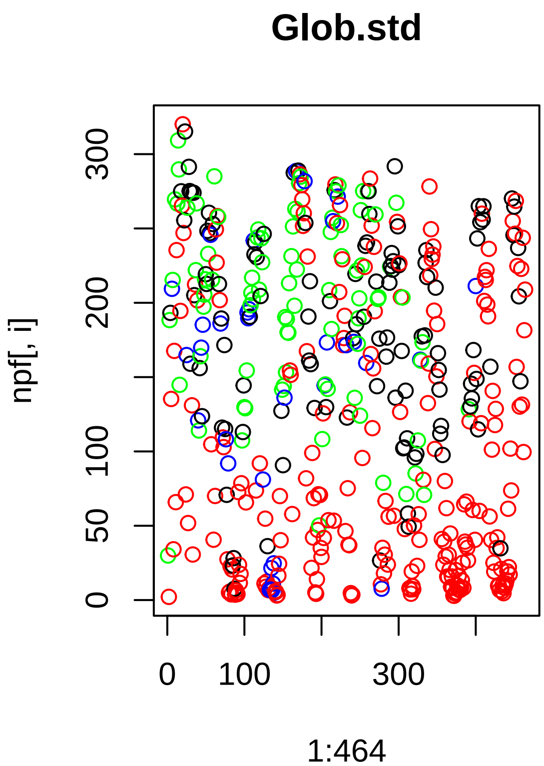
%Mitä teemme tälle, haluammeko viitata tähän visualisointien ja nimien suhteen vai onko ideaalia, että teemme omat visualisointimme, jotka esittelemme tekstissä? % (Sara) Ainakin jos tehdään omat visualisoinnit, mielestäni tämän voi poistaa. Visualisointien kanssa kuitenkin miettisin, että mitä todella 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 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.

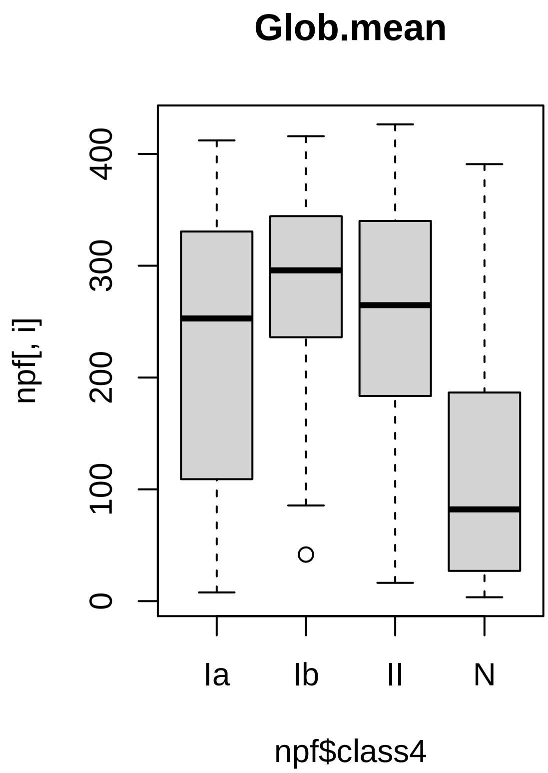
Let's next visualize some our explanatory variables via boxplots and scatterplots to get a deeper understanding of them. For the sake of simplicity, these visualizations grouped by the phenomena being measured. In order to also prelminarily look at how these variables behave in relation to new particle 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:

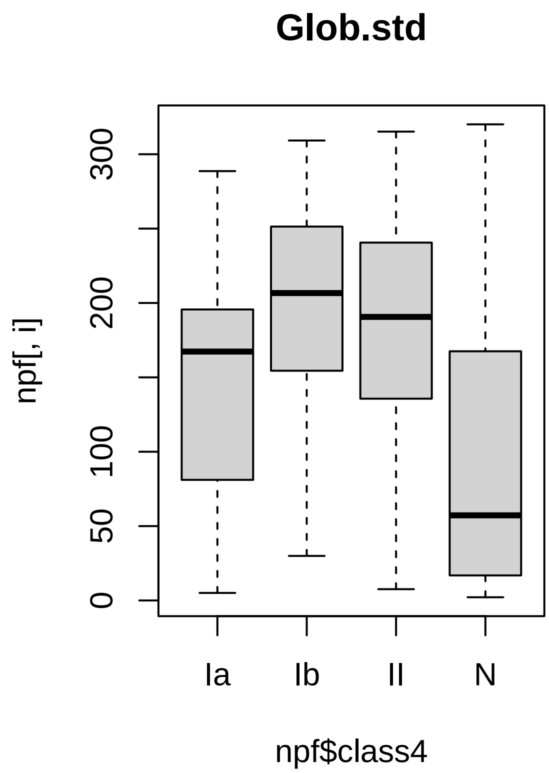


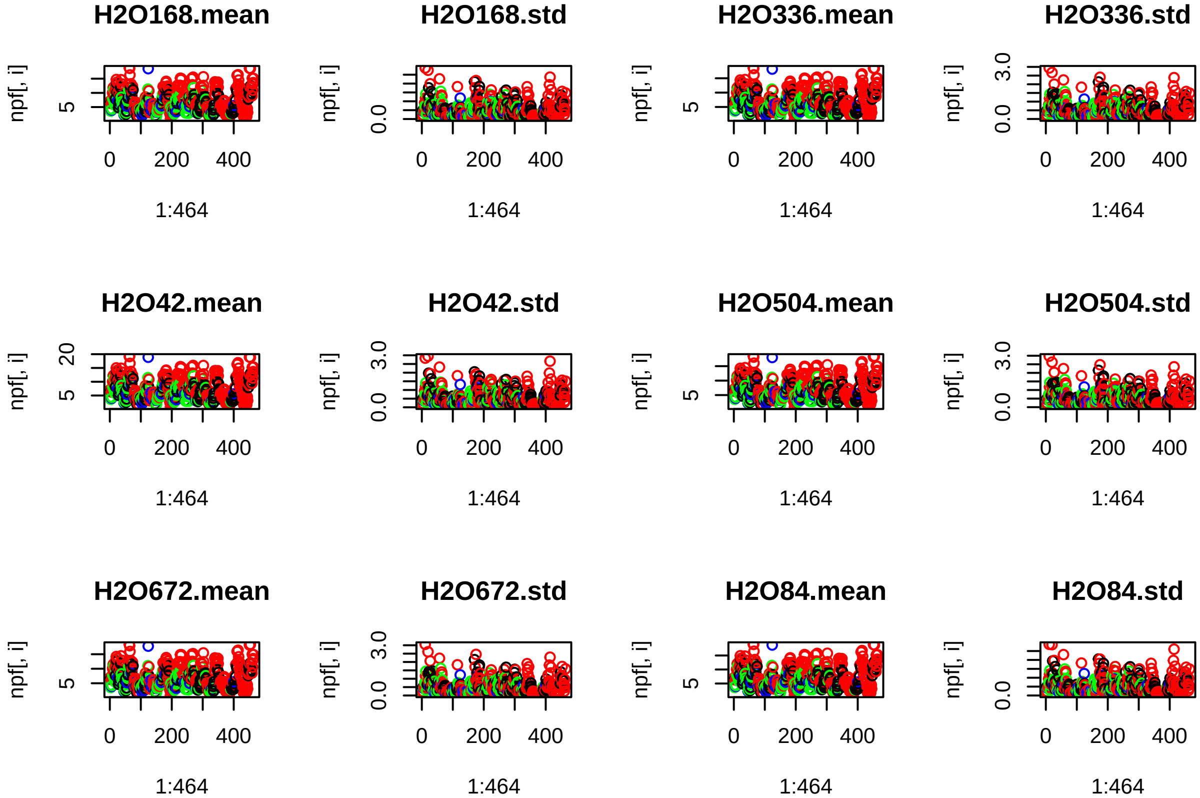

CO2168.mean
CO2168.std
CO2336.mean
CO2336.std
CO242.mean
CO242.std
CO2504.mean
CO2504.std
npf[, i]
npf$class4
Ia
Ib
II
N

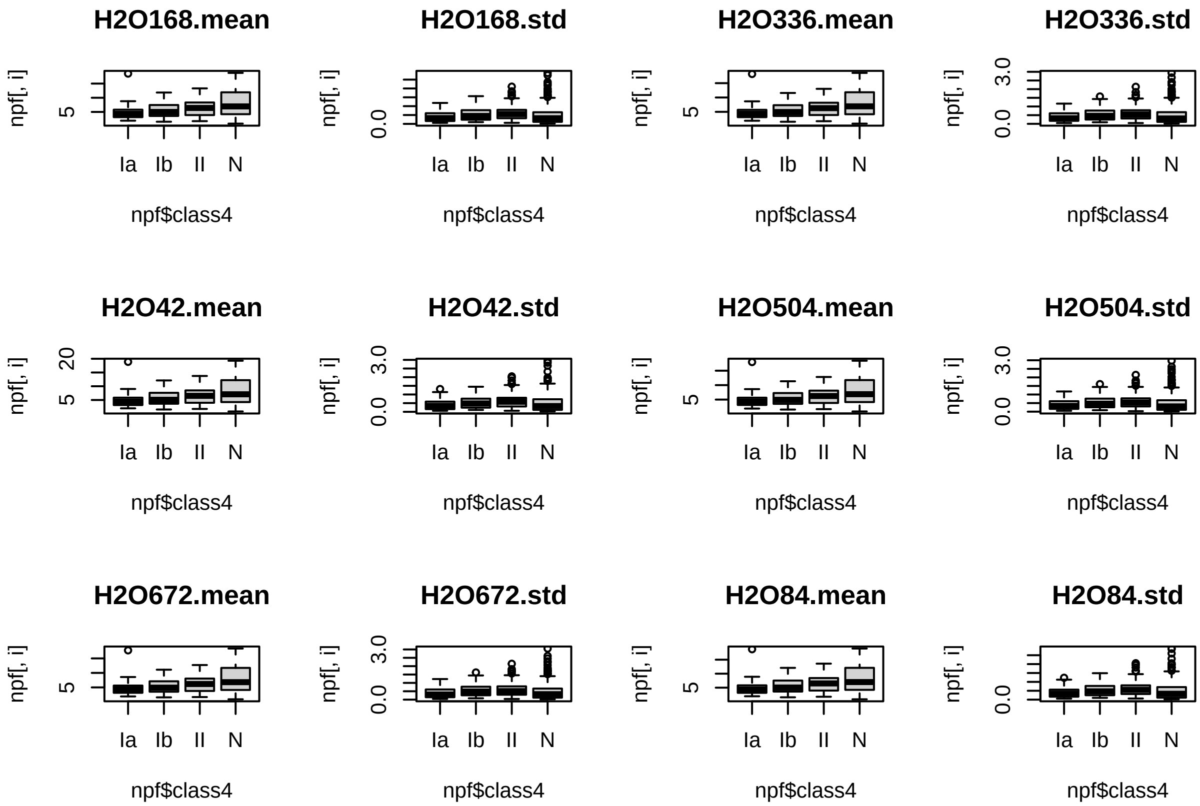

Glob.mean
npf[, i]
0
100
200
300
400
0
100
300
1:464

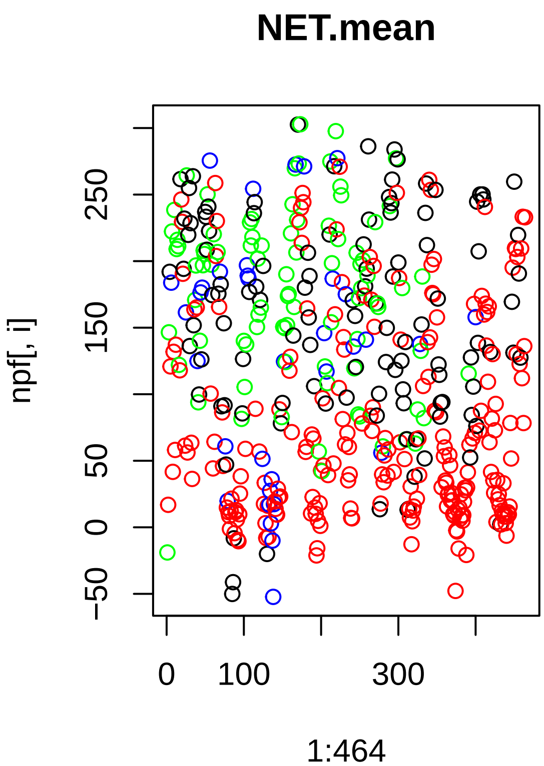

Glob.std
npf[, i]
0
50
100
200
300
0
100
300
1:464

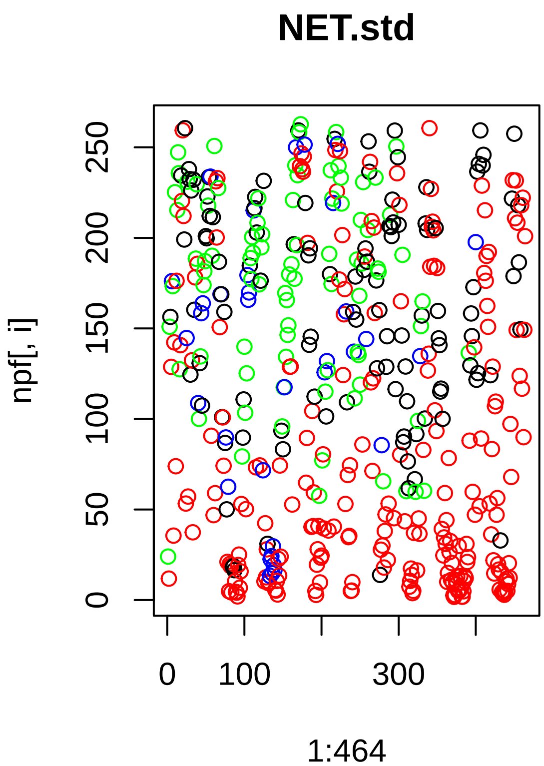

Glob.mean
npf[, i]
0
100
200
300
400
Ia
Ib
II
N
npf$class4

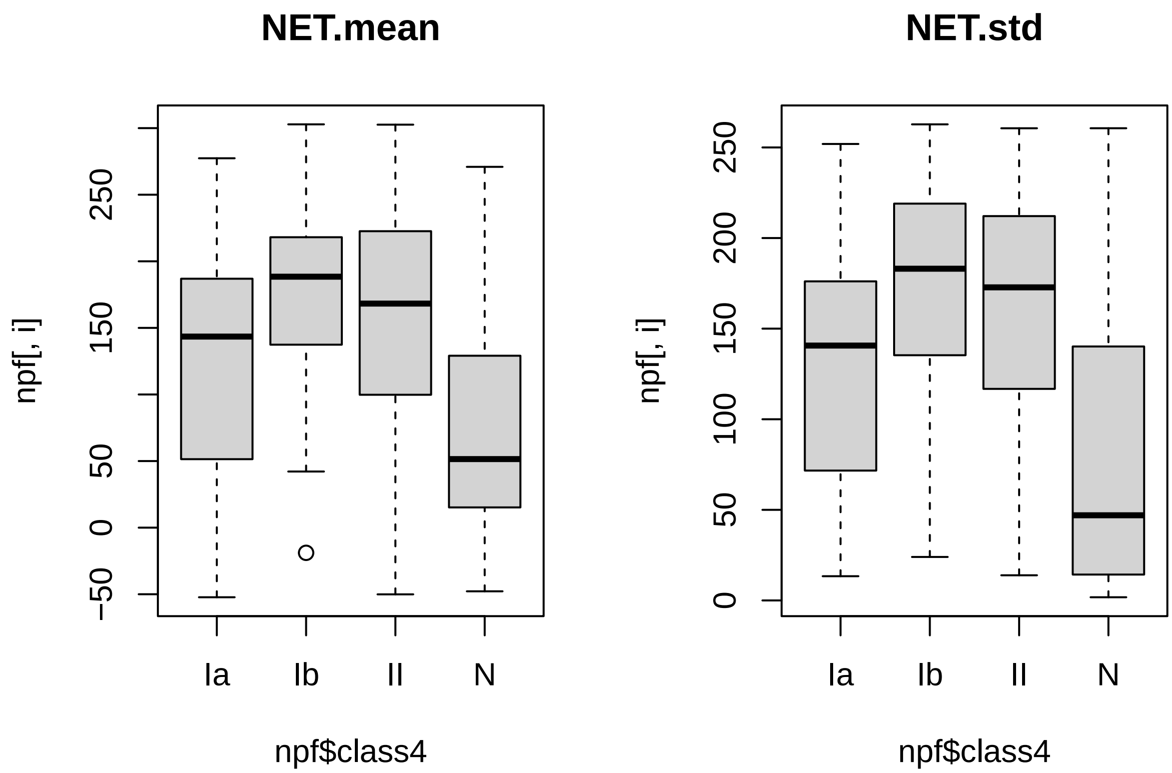

Glob.std
npf[, i]
0
50
100
200
300
Ia
Ib
II
N
npf$class4

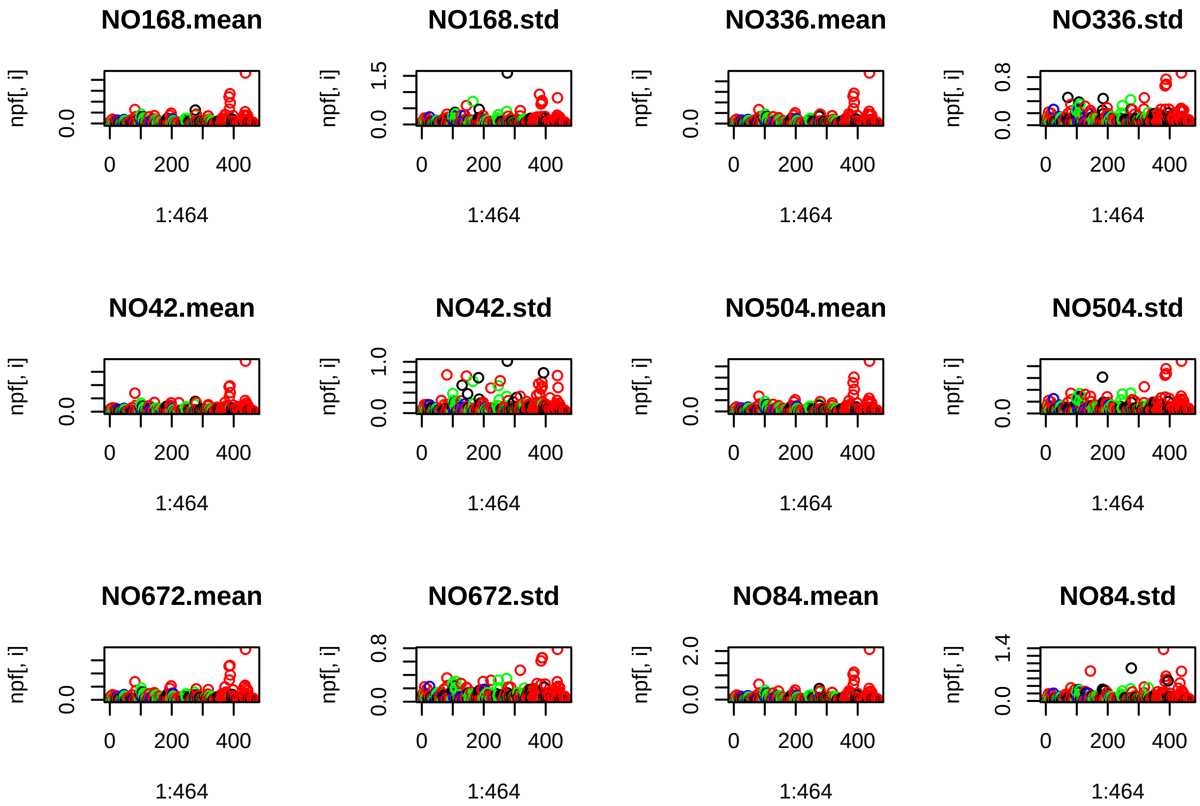

H2O168.mean
H2O168.std
H2O336.mean
H2O336.std
H2O42.mean
H2O42.std
H2O504.mean
H2O504.std
H2O672.mean
H2O672.std
H2O84.mean
H2O84.std
npf[, i]
1:464
0
200
400
5
20
0.0
3.0

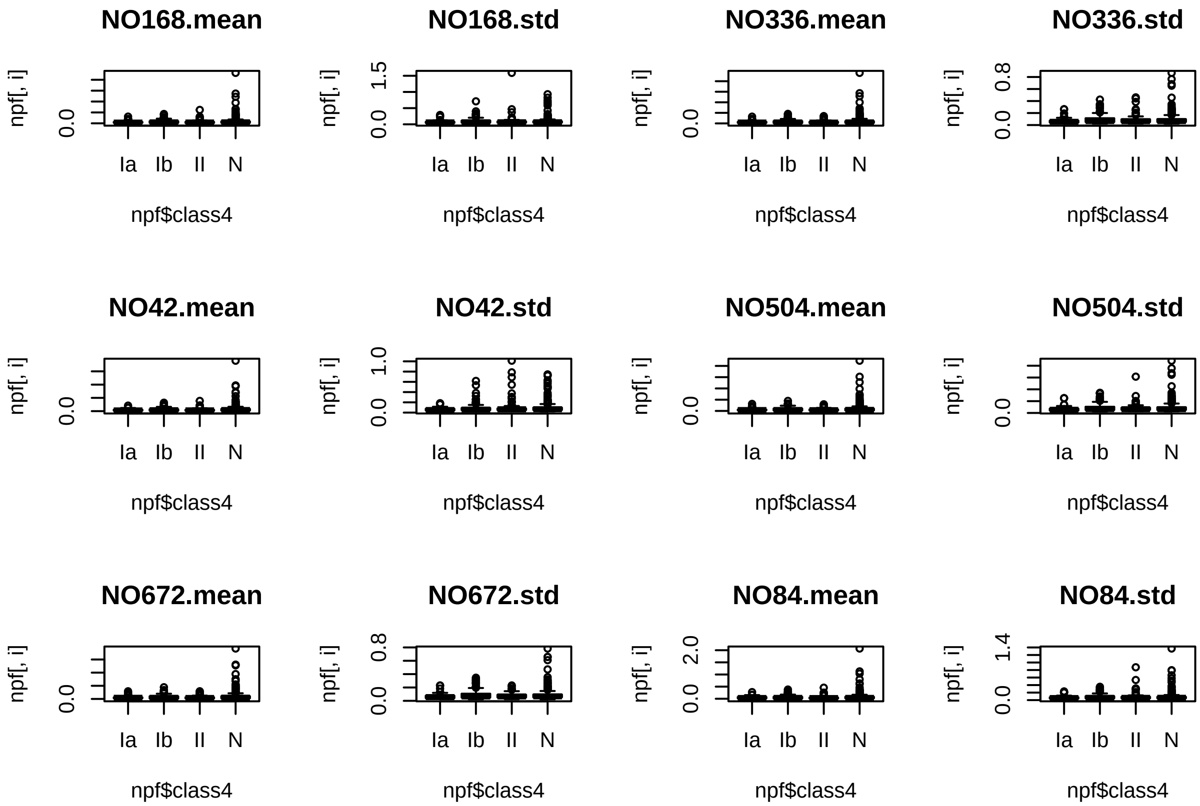

H2O168.mean
H2O168.std
H2O336.mean
H2O336.std
H2O42.mean
H2O42.std
H2O504.mean
H2O504.std
H2O672.mean
H2O672.std
H2O84.mean
H2O84.std
npf[, i]
5
0.0
3.0
20
Ia
Ib
II
N
npf$class4

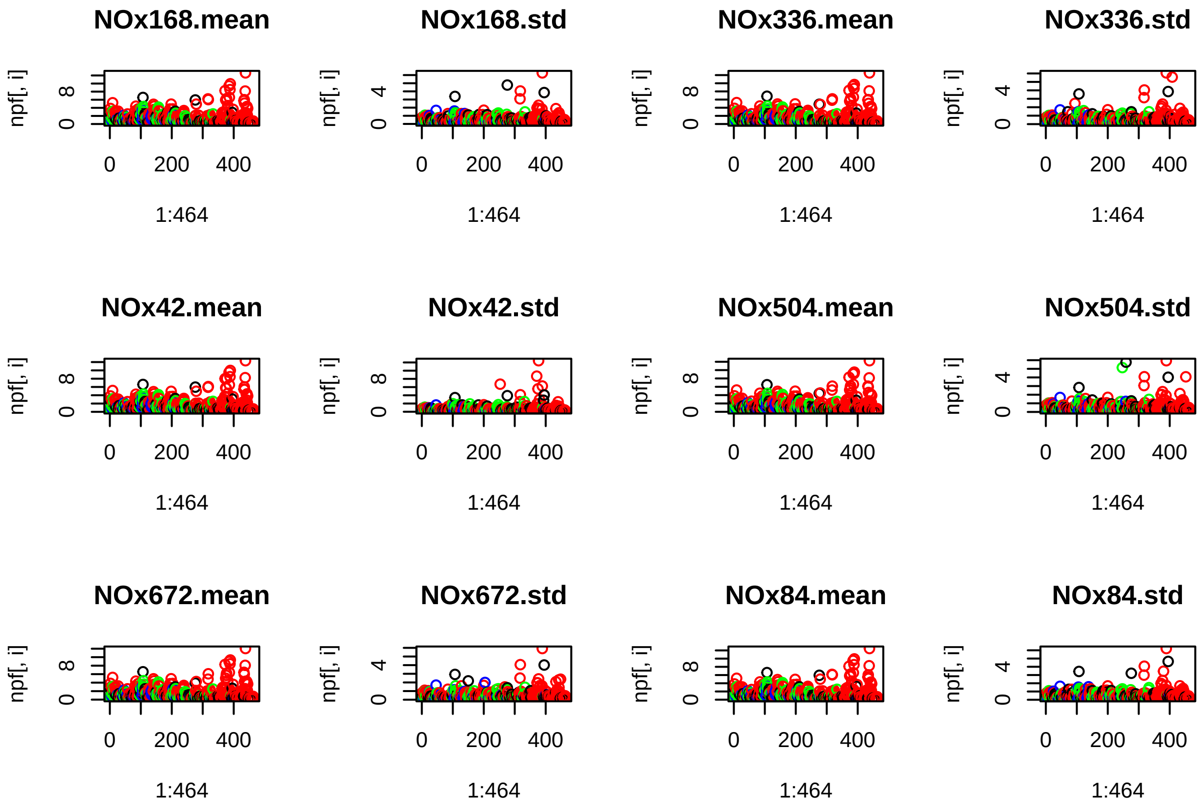

NET.mean
npf[, i]
−50
0
50
150
250
0
100
300
1:464

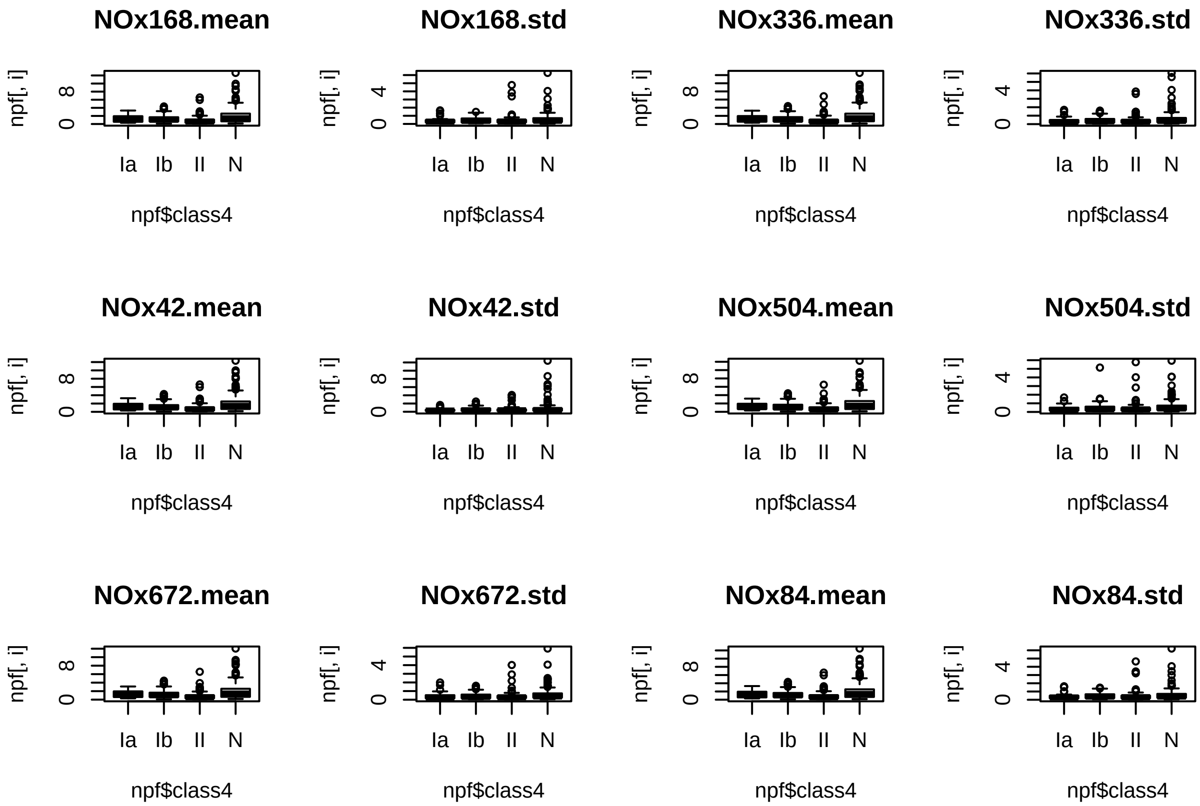

NET.std
npf[, i]
0
50
100
150
200
250
0
100
300
1:464

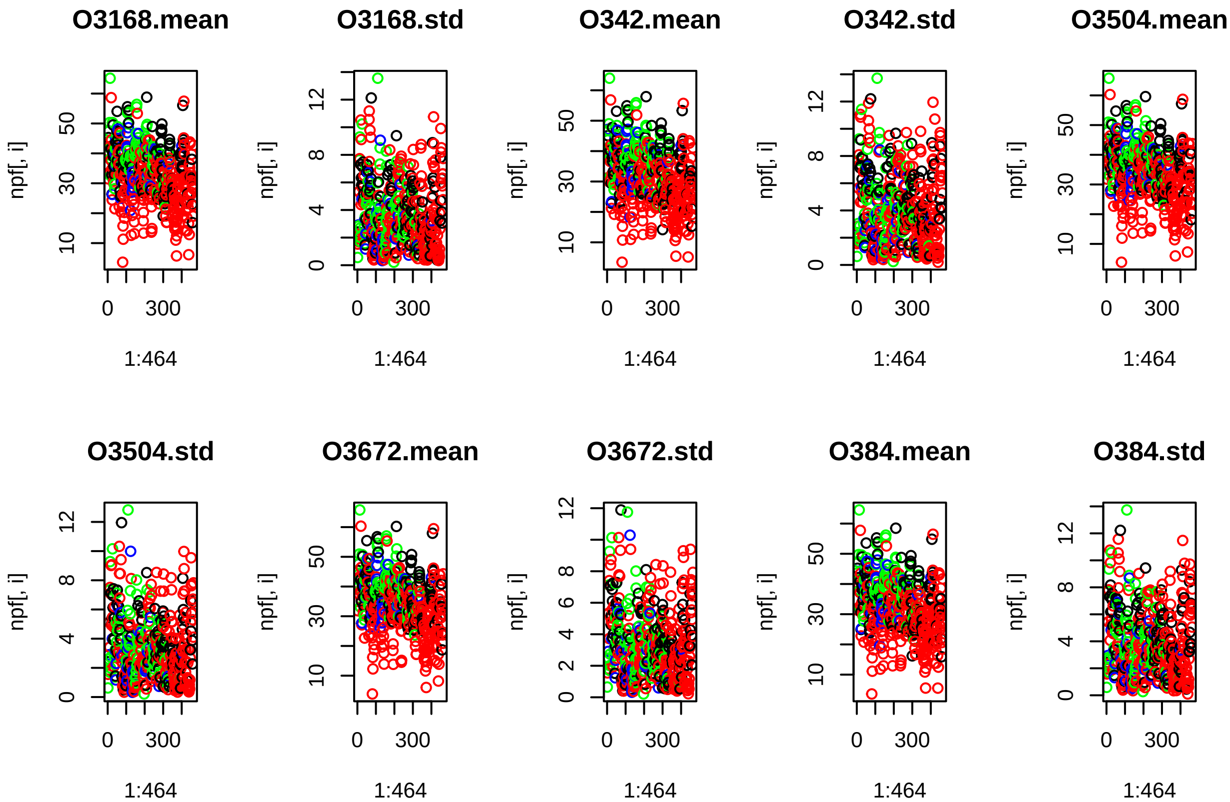

NET.mean
npf[, i]
−50
0
50
150
250
Ia
Ib
II
N
npf$class4
NET.std
npf[, i]
0
50
100
150
200
250
Ia
Ib
II
N
npf$class4

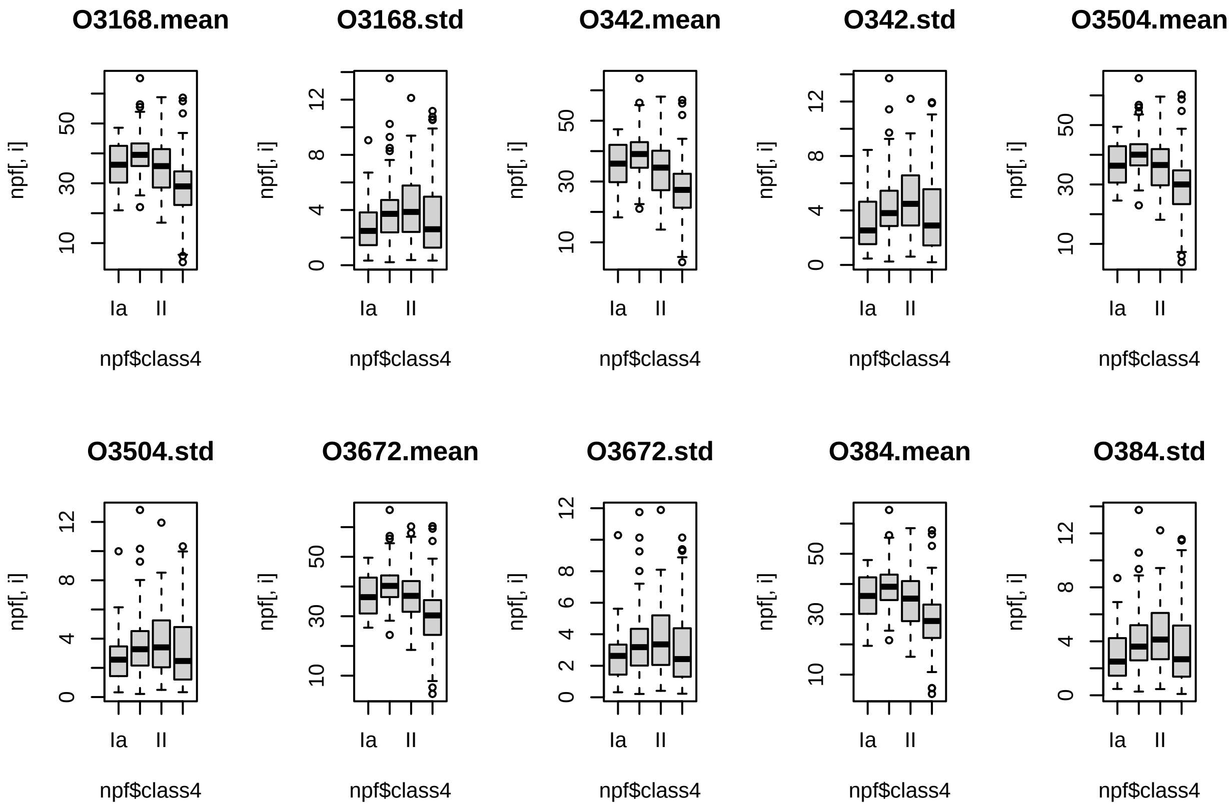

NO168.mean
NO168.std
NO336.mean
NO336.std
NO42.mean
NO42.std
NO504.mean
NO504.std
NO672.mean
NO672.std
NO84.mean
NO84.std
npf[, i]
1:464
0
200
400
0.0
1.5
0.8
1.0
2.0
1.4

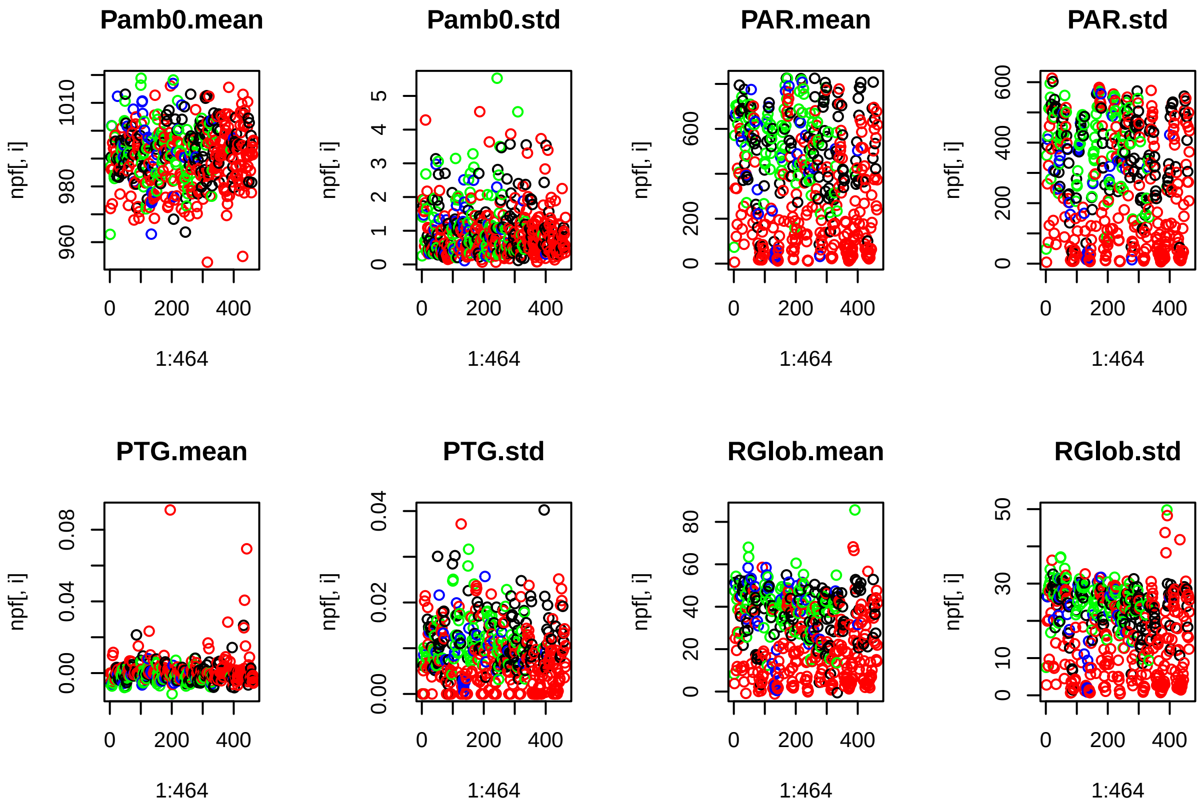

NO168.mean
NO168.std
NO336.mean
NO336.std
NO42.mean
NO42.std
NO504.mean
NO504.std
NO672.mean
NO672.std
NO84.mean
NO84.std
npf[, i]
npf$class4
Ia
Ib
II
N
0.0
1.5
0.8
1.0
2.0
1.4

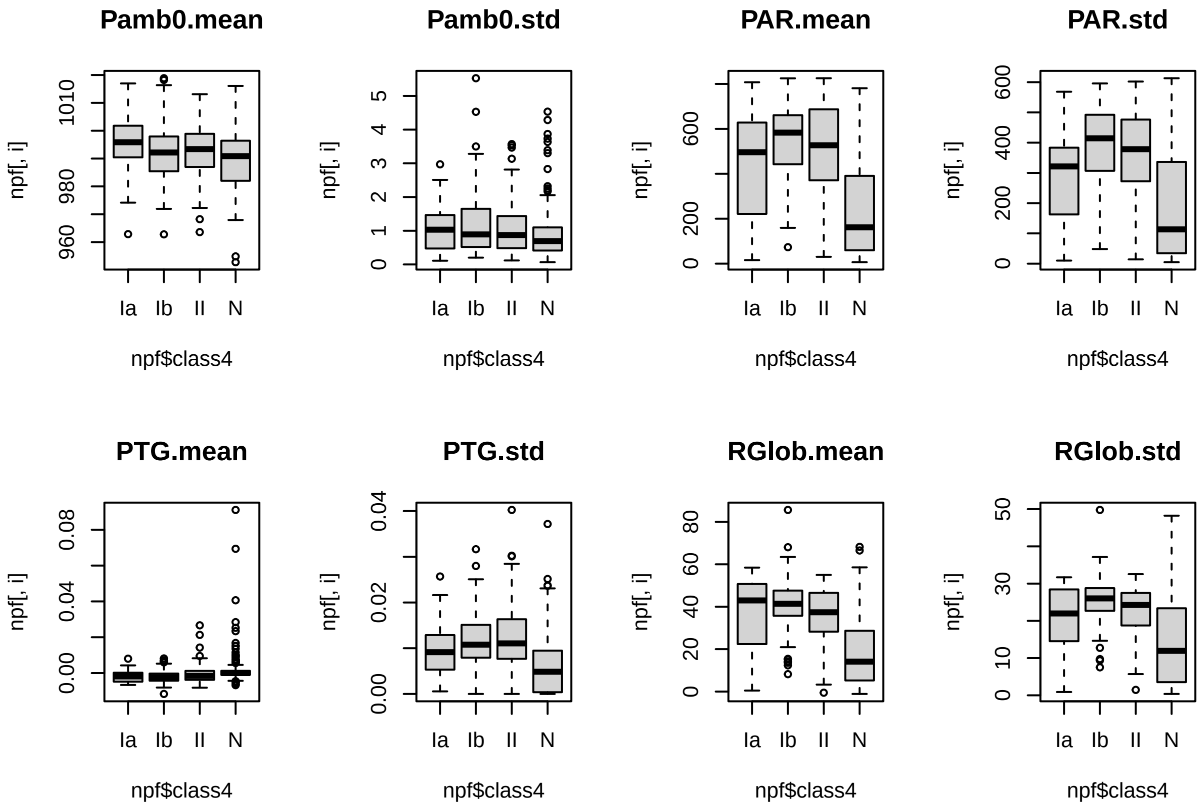

NOx168.mean
NOx168.std
NOx336.mean
NOx336.std
NOx42.mean
NOx42.std
NOx504.mean
NOx504.std
NOx672.mean
NOx672.std
NOx84.mean
NOx84.std
npf[, i]
1:464
0
200
400
0
8
4

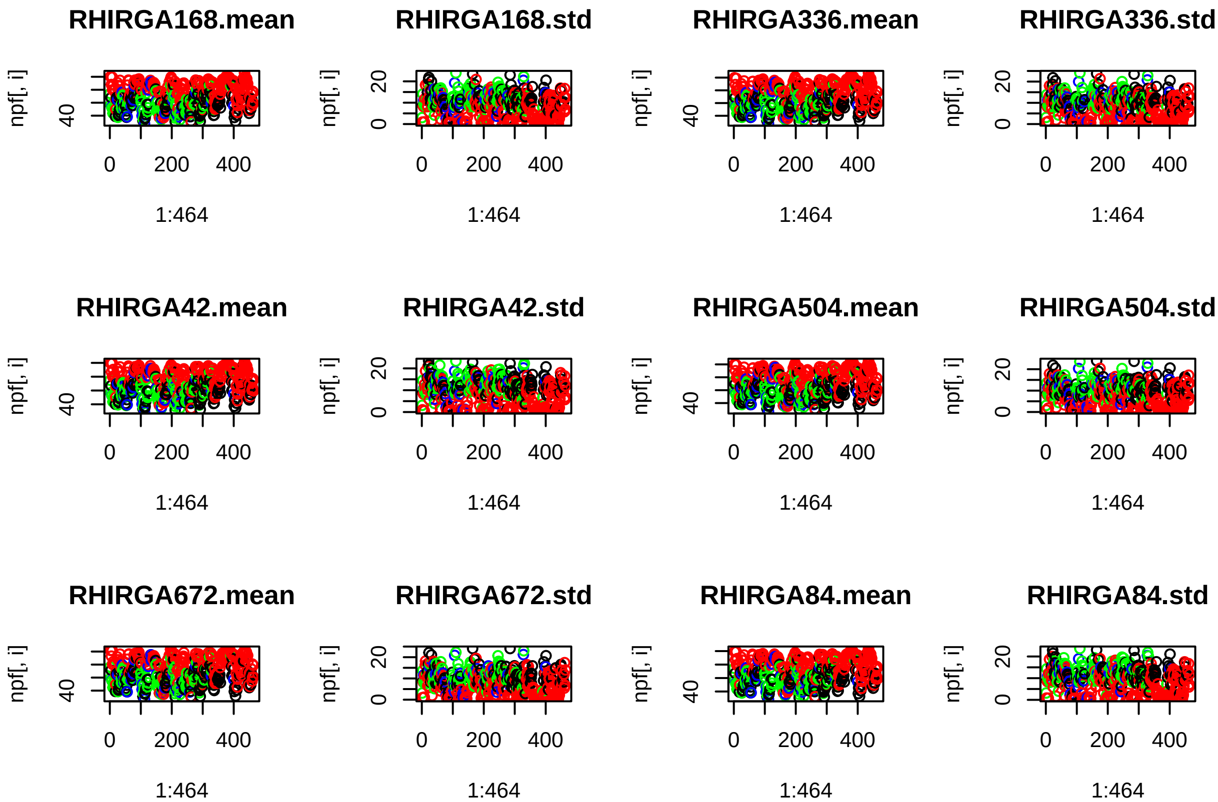

NOx168.mean
NOx168.std
NOx336.mean
NOx336.std
NOx42.mean
NOx42.std
NOx504.mean
NOx504.std
NOx672.mean
NOx672.std
NOx84.mean
NOx84.std
npf[, i]
npf$class4
Ia Ib II N
0 8
0 4

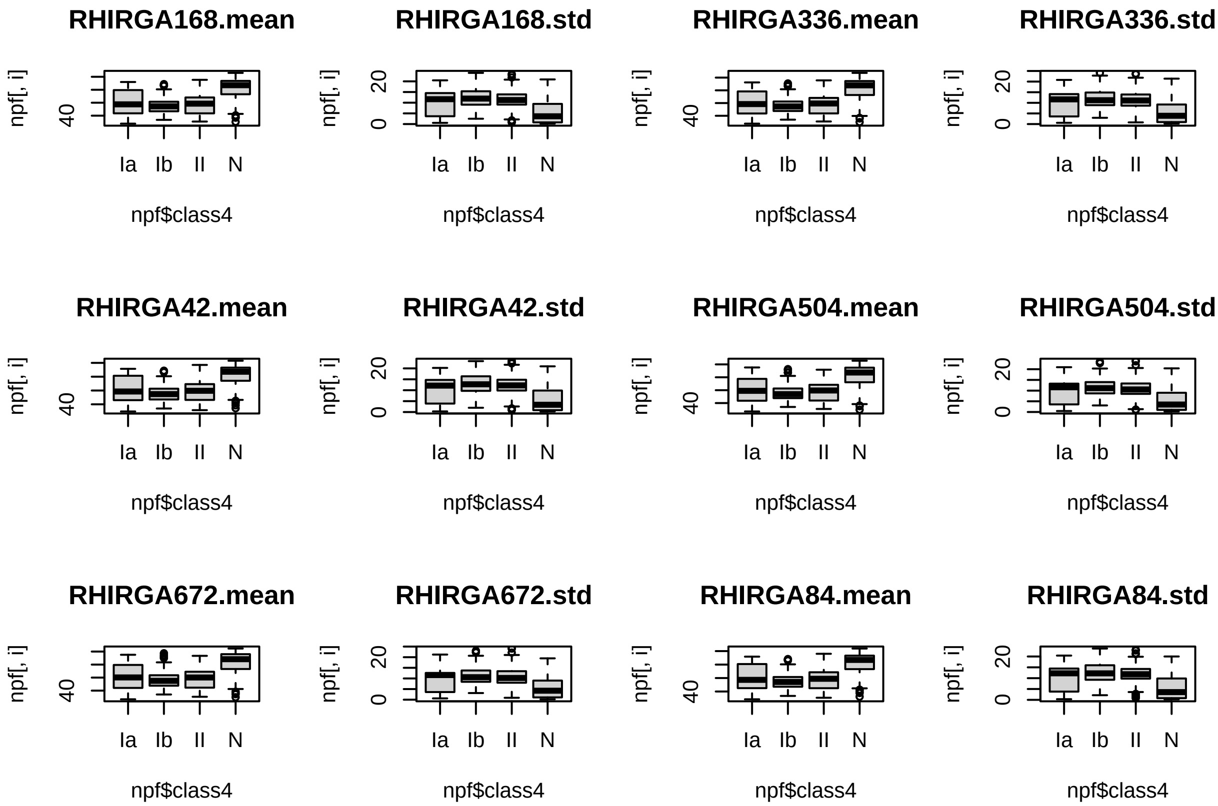

O3168.mean
O3168.std
O342.mean
O342.std
O3504.mean
O3504.std
O3672.mean
O3672.std
O384.mean
O384.std
npf[, i]
1:464
0
300

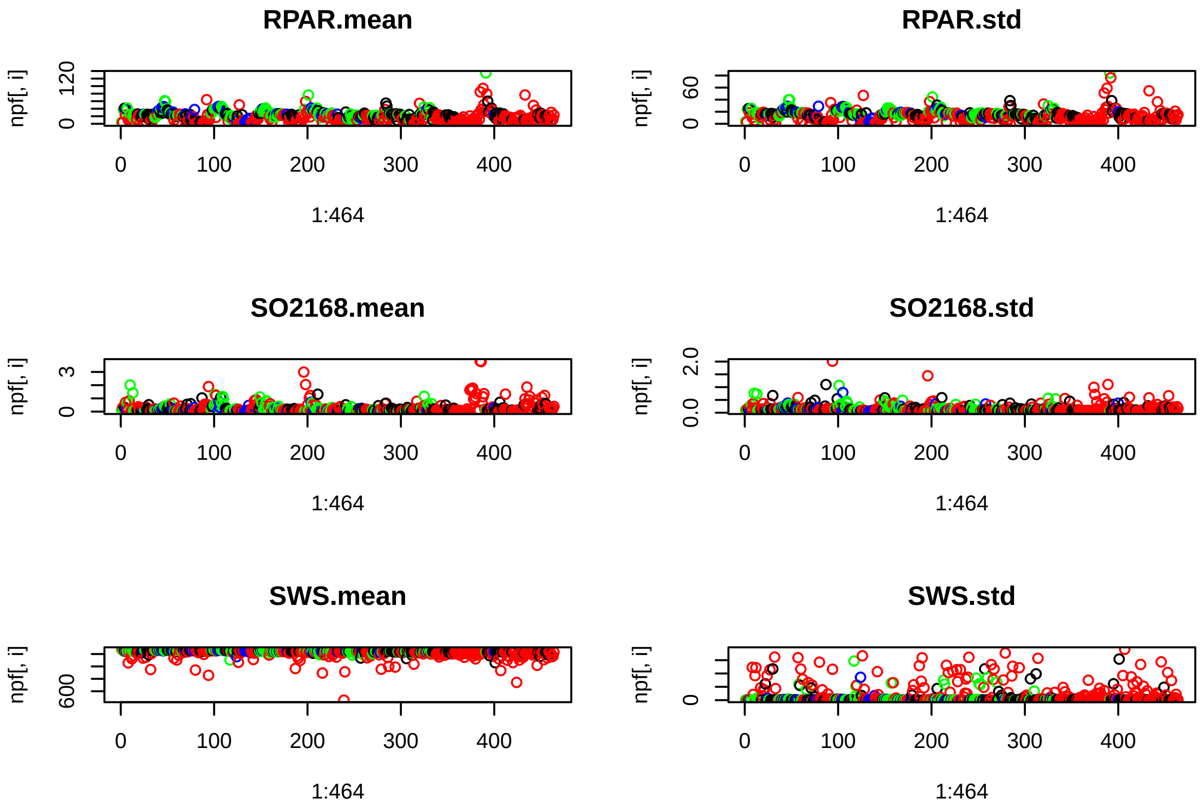

O3168.mean
O3168.std
O342.mean
O342.std
O3504.mean
O3504.std
O3672.mean
O3672.std
O384.mean
O384.std
npf[, i]
Ia
II
npf$class4

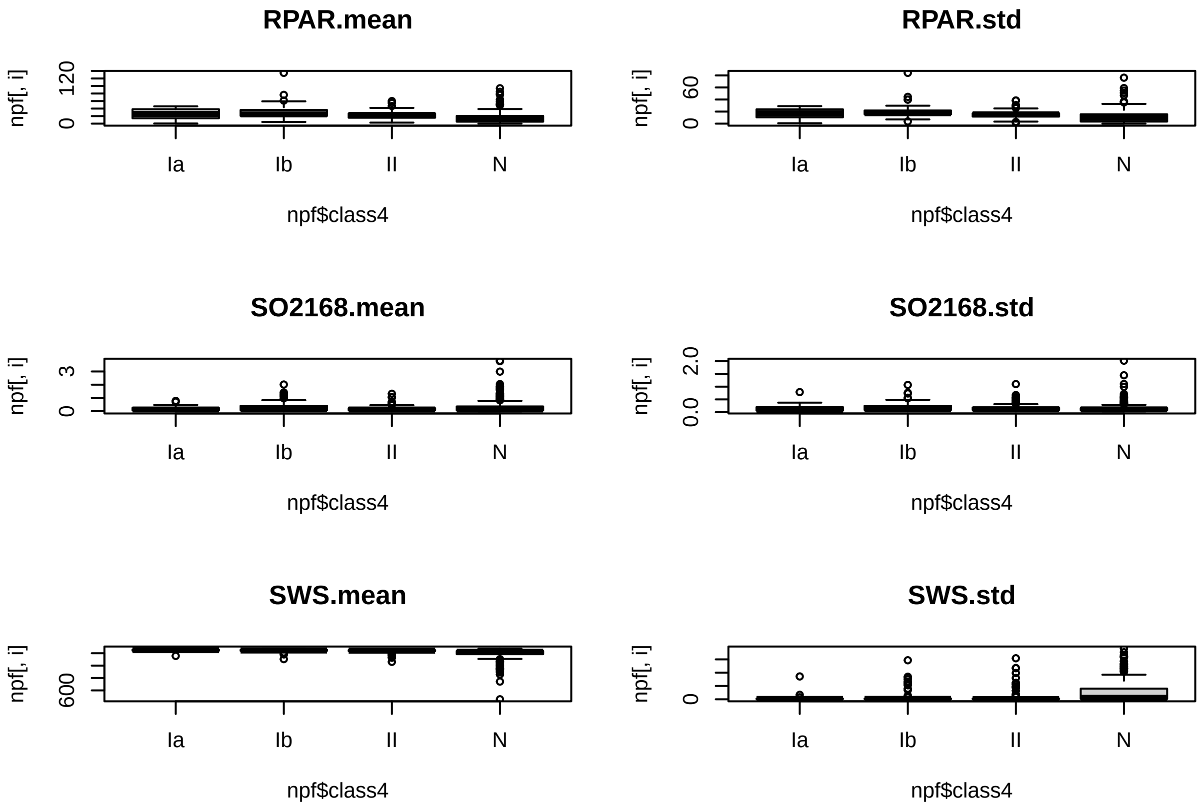

Pamb0.mean
Pamb0.std
PAR.mean
PAR.std
PTG.mean
PTG.std
RGlob.mean
RGlob.std
npf[, i]
1:464

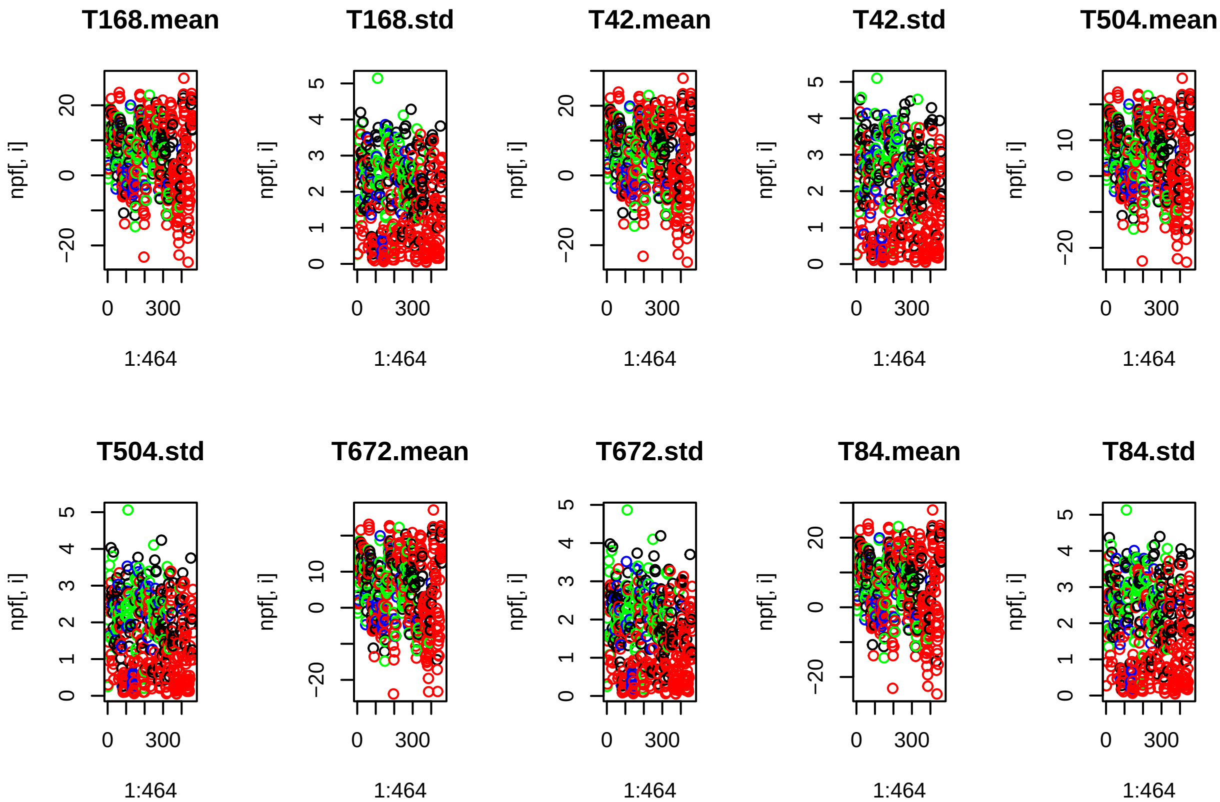

Pamb0.mean
Pamb0.std
PAR.mean
PAR.std
PTG.mean
PTG.std
RGlob.mean
RGlob.std
npf[, i]
npf$class4
Ia
Ib
II
N

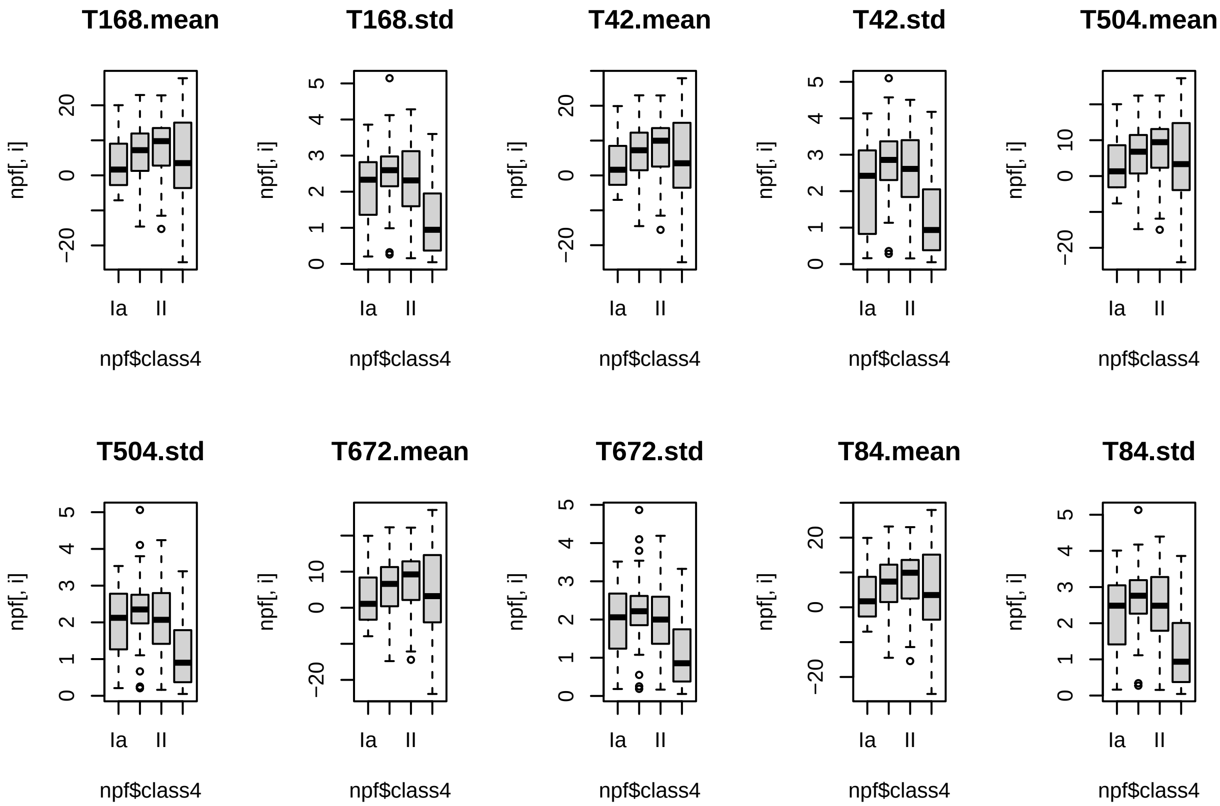

RHIRGA168.mean
RHIRGA168.std
RHIRGA336.mean
RHIRGA336.std
RHIRGA42.mean
RHIRGA42.std
RHIRGA504.mean
RHIRGA504.std
RHIRGA672.mean
RHIRGA672.std
RHIRGA84.mean
RHIRGA84.std
npf[, i]
1:464
0
200
400
40
20

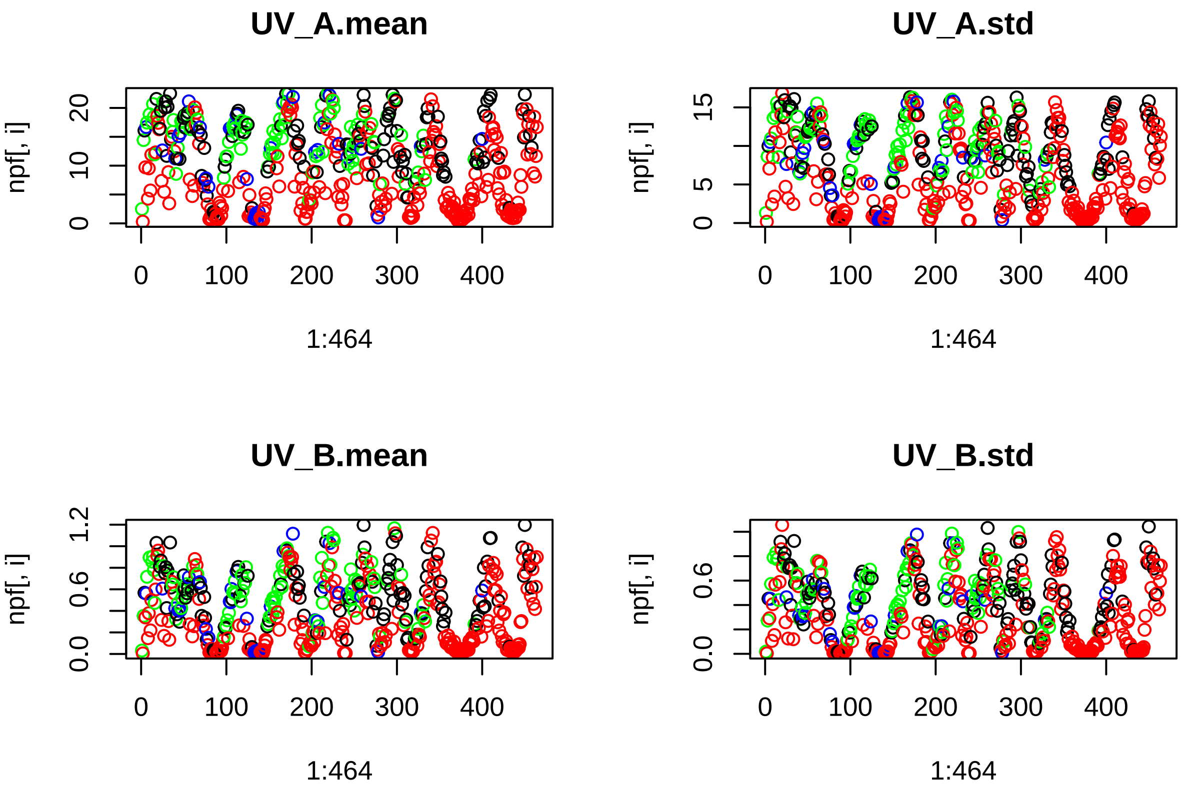

RHIRGA168.mean
RHIRGA168.std
RHIRGA336.mean
RHIRGA336.std
RHIRGA42.mean
RHIRGA42.std
RHIRGA504.mean
RHIRGA504.std
RHIRGA672.mean
RHIRGA672.std
RHIRGA84.mean
RHIRGA84.std
npf[, i]
40
20
0
Ia
Ib
II
N
npf$class4

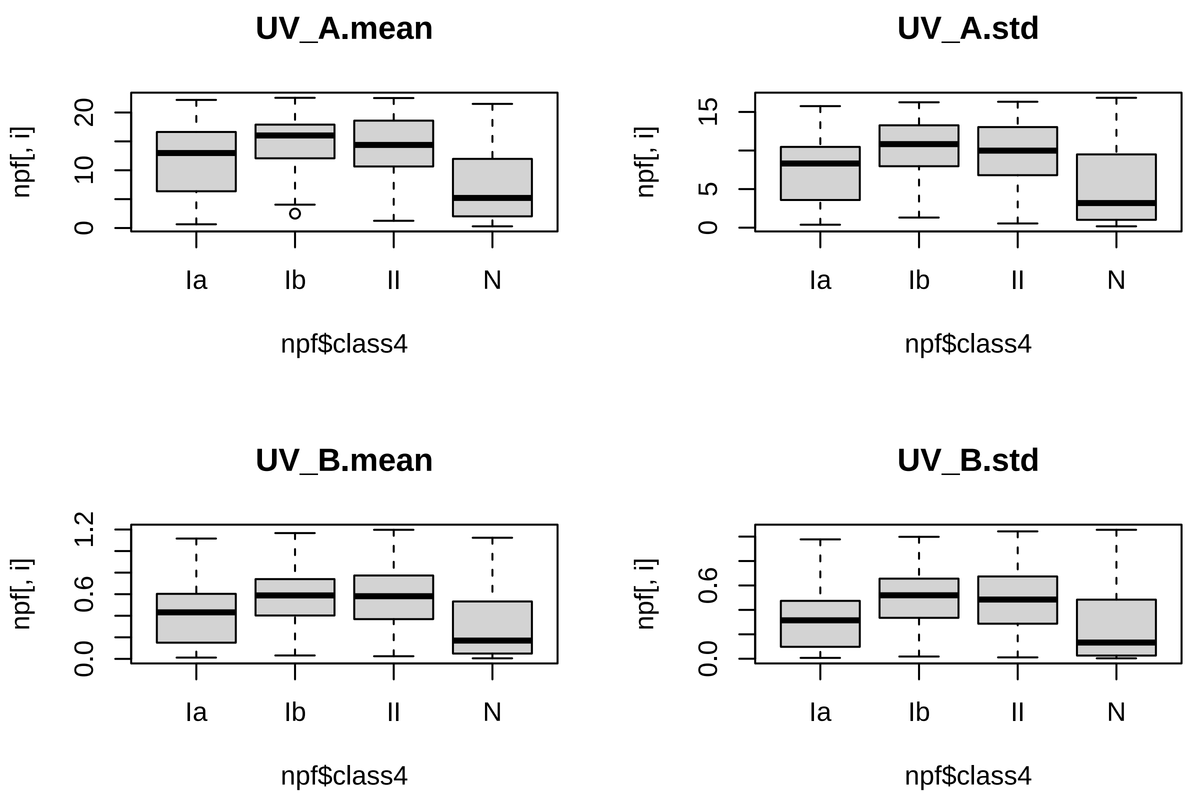

RPAR.mean
npf[, i]
0
120
0
100
200
300
400
1:464
RPAR.std
npf[, i]
0
60
0
100
200
300
400
1:464
SO2168.mean
npf[, i]
0
3
0
100
200
300
400
1:464
SO2168.std
npf[, i]
0.0
2.0
0
100
200
300
400
1:464
SWS.mean
npf[, i]
600
0
100
200
300
400
1:464
SWS.std
npf[, i]
0
0
100
200
300
400
1:464

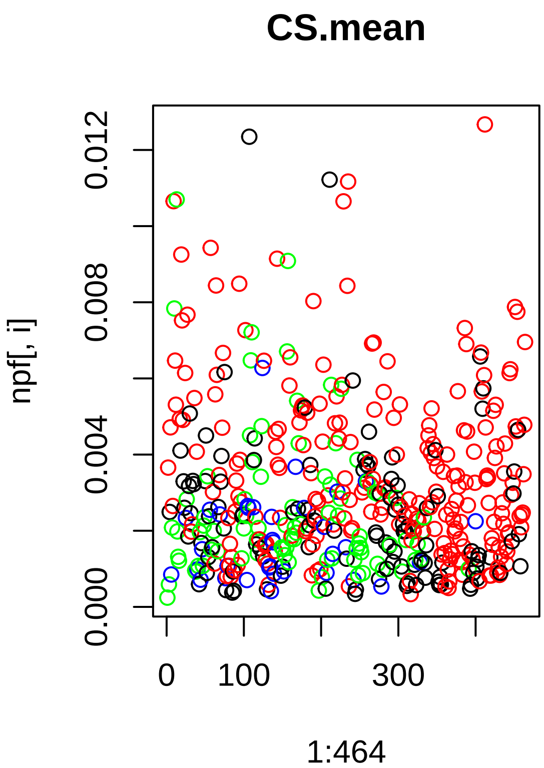

RPAR.mean
npf[, i]
0
120
Ia
Ib
II
N
npf$class4
RPAR.std
npf[, i]
0
60
Ia
Ib
II
N
npf$class4
SO2168.mean
npf[, i]
0
3
Ia
Ib
II
N
npf$class4
SO2168.std
npf[, i]
0.0
2.0
Ia
Ib
II
N
npf$class4
SWS.mean
npf[, i]
600
Ia
Ib
II
N
npf$class4
SWS.std
npf[, i]
0
Ia
Ib
II
N
npf$class4

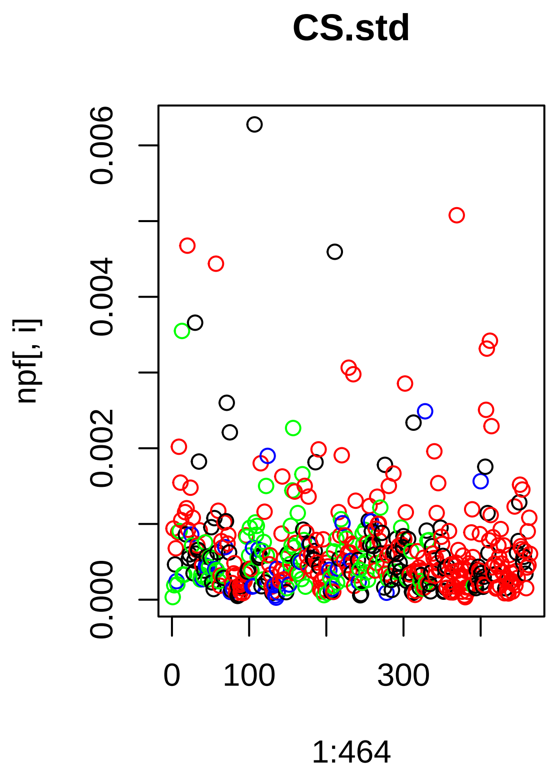

T168.mean
T168.std
T42.mean
T42.std
T504.mean
T504.std
T672.mean
T672.std
T84.mean
T84.std
npf[, i]
1:464

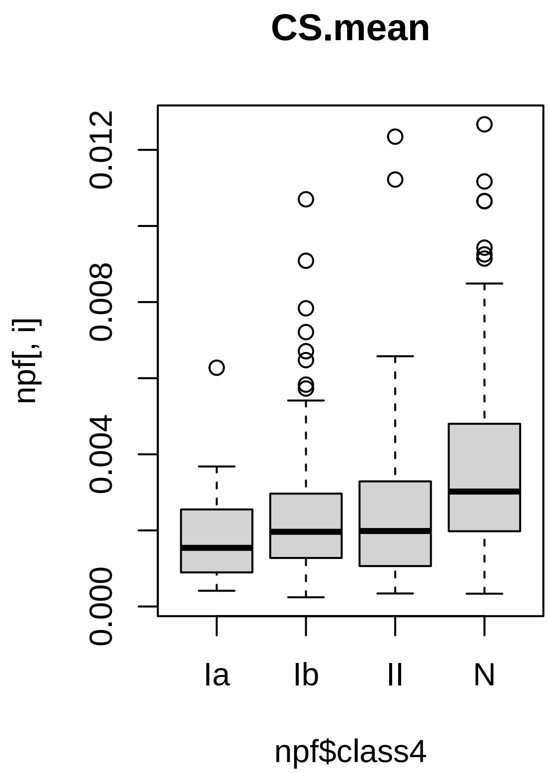

T168.mean
T168.std
T42.mean
T42.std
T504.mean
T504.std
T672.mean
T672.std
T84.mean
T84.std
npf[, i]
npf$class4
Ia
II

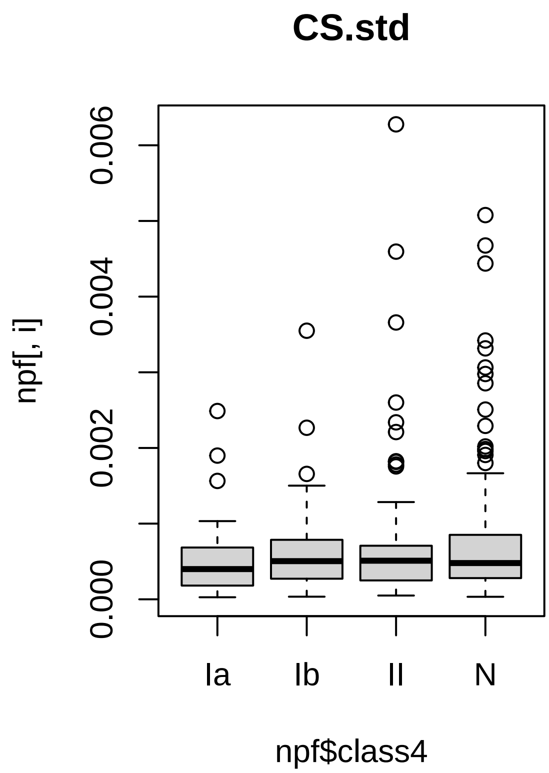

UV_A.mean
npf[, i]
0
10
20
0
100
200
300
400
1:464
UV_A.std
npf[, i]
0
5
15
0
100
200
300
400
1:464
UV_B.mean
npf[, i]
0.0
0.6
1.2
0
100
200
300
400
1:464
UV_B.std
npf[, i]
0.0
0.6
0
100
200
300
400
1:464


UV_A.mean
UV_A.std
UV_B.mean
UV_B.std
npf[, i]
npf$class4
Ia
Ib
II
N
0
10
20
5
15
0.0
0.6
1.2


CS.mean
npf[, i]
0.000
0.004
0.008
0.012
0
100
300
1:464


CS.std
npf[, i]
0.000
0.002
0.004
0.006
0
100
300
1:464





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.

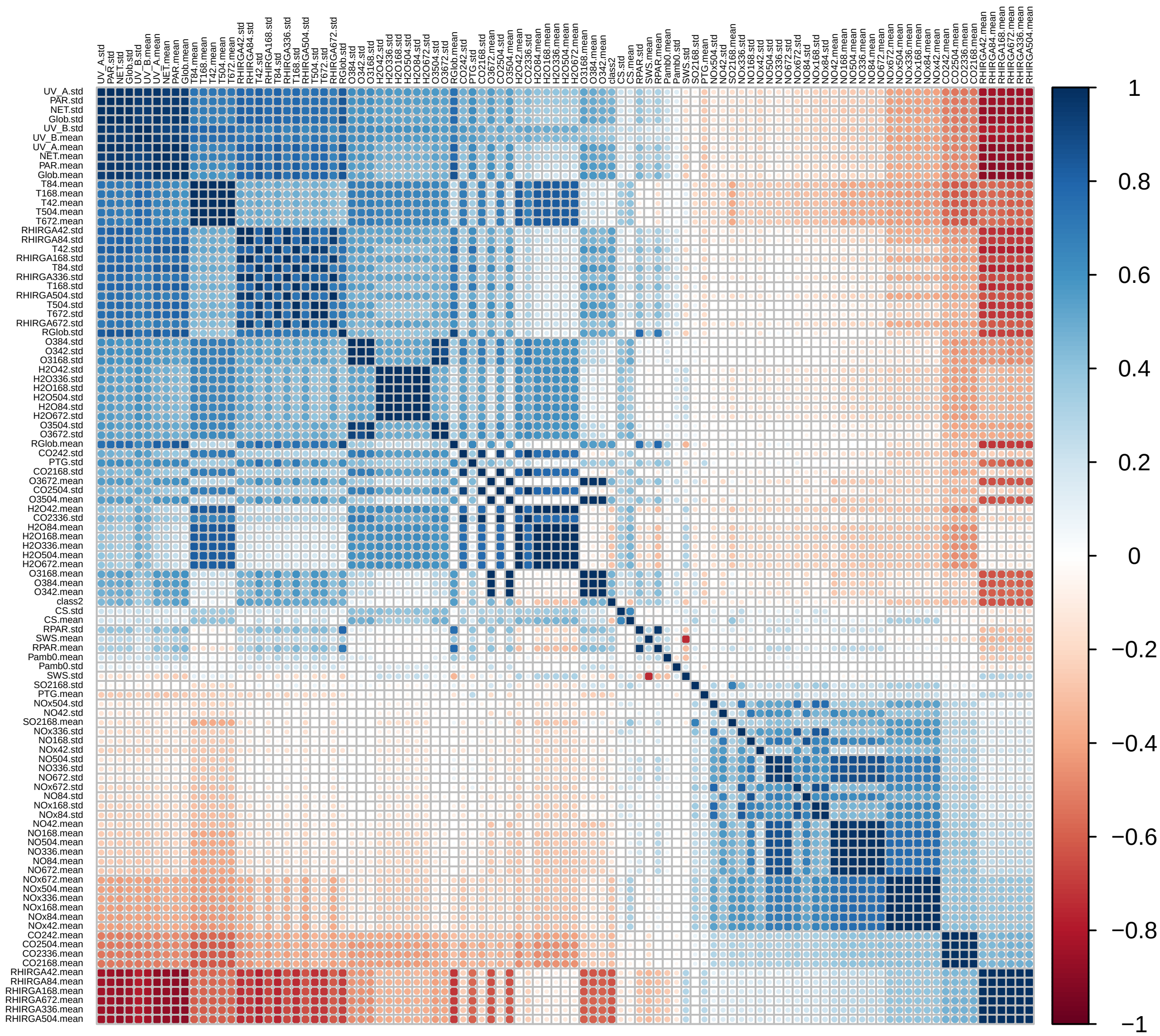
```
##    CO2168.mean     CO2168.std    CO2336.mean     CO2336.std     CO242.mean
##    -0.30626777    -0.09596773    -0.30271045    -0.10806722    -0.32985917
##      CO242.std    CO2504.mean     CO2504.std      Glob.mean       Glob.std
##    -0.08793757    -0.29887003    -0.11393071     0.56928615     0.48236139
##    H2O168.mean     H2O168.std    H2O336.mean     H2O336.std     H2O42.mean
##    -0.27790050     0.05382782    -0.28144835     0.05359948    -0.27131753
##      H2O42.std    H2O504.mean     H2O504.std    H2O672.mean     H2O672.std
##     0.04299127    -0.28349790     0.05559773    -0.28529105     0.04823407
##     H2O84.mean      H2O84.std       NET.mean        NET.std     NO168.mean
```

```
##    -0.27456743     0.04349242     0.48609505     0.49417773    -0.12711787
##      NO168.std     NO336.mean      NO336.std      NO42.mean       NO42.std
##    -0.02889094    -0.13899494    -0.06847844    -0.15285335    -0.04893791
##     NO504.mean      NO504.std     NO672.mean      NO672.std      NO84.mean
##    -0.14272836    -0.07816737    -0.15283971    -0.10621825    -0.12969448
##       NO84.std    NOx168.mean     NOx168.std    NOx336.mean     NOx336.std
##    -0.07182797    -0.27466662    -0.08621634    -0.27903932    -0.13286528
##     NOx42.mean      NOx42.std    NOx504.mean     NOx504.std    NOx672.mean
##    -0.27633195    -0.10229014    -0.28264902    -0.10067518    -0.28437084
##     NOx672.std     NOx84.mean      NOx84.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
##    SO2168.mean     SO2168.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 as 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.



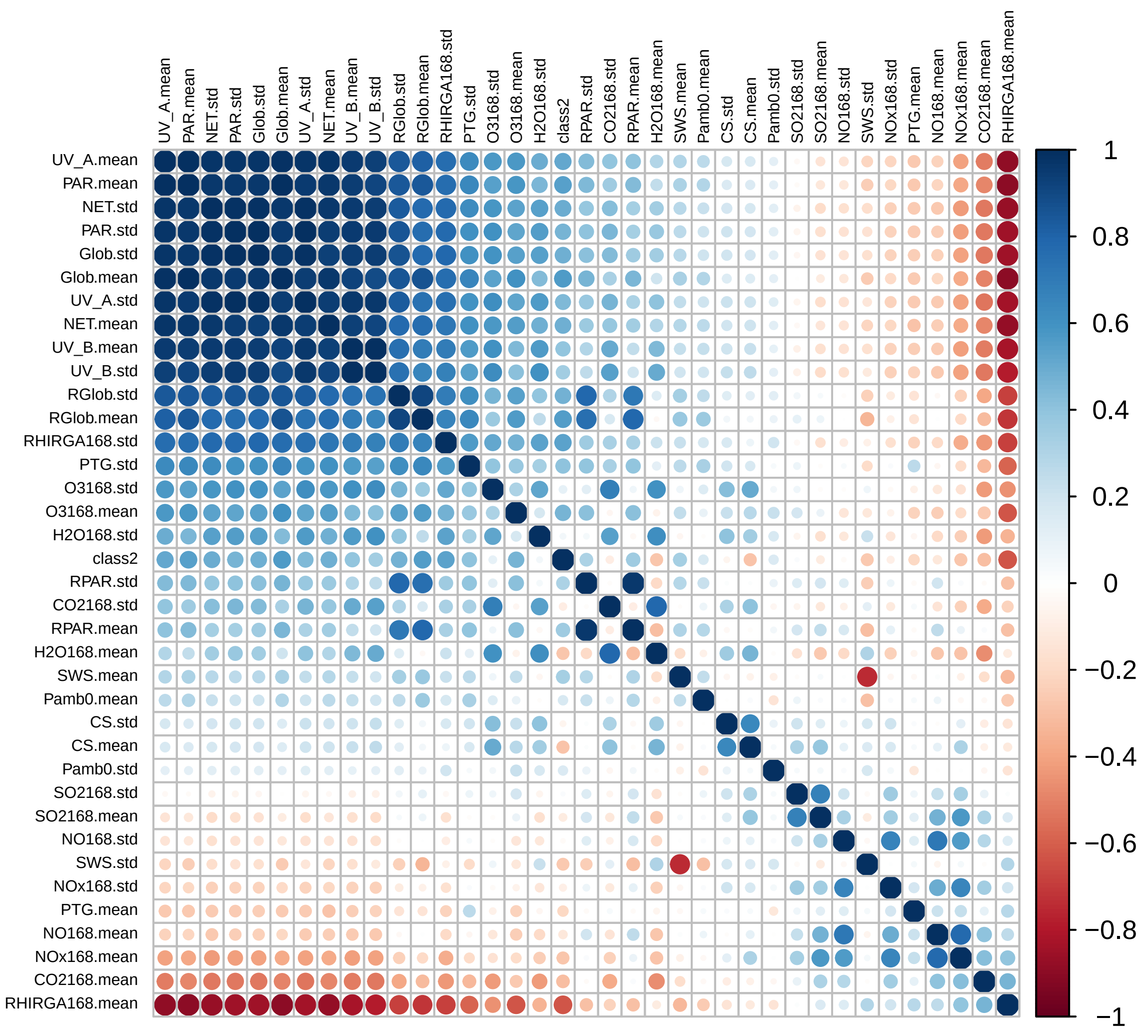
As expected, the correlation plot shows that many of the variables describing the same phenomenon at different heights are correlated, as are variables related to radiation. For many classifiers, highly correlated parameters are problematic, and for this reason we would like to drop some of the most 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 (H20) 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 (H20)

	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 hihgly 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 receieve 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

ogistic 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 receieves 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 λ_i and link function $\sigma : \mathbb{R} \to [0, 1]$. Thus we can estimate a logistic regression by finding parameters λ_i that maximize the likelihood function $\prod p(Y_i|X)$.

Notable benefits of the logistic regression model include %tähän pitää vielä kirjoittaa lisää

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 γ 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 kth class, in our case computed as the fraction of the observations in the training dataset that are in the kth class. While this general approach is the same for all generative models, they differ in how they estimate $p(X|Y)$.

Linear Discriminant Analysis (LDA)

A linear discriminant analysis classifier assumes that all p predictors $X = (X_1, \ldots, X_p)$ are drawn from a multivariate Gaussian distribution. This means that each predictor follows a normal distribution $N(\mu_k, \Sigma)$ where μ_k is the class-specific mean and $\mathrm{Cov}(X) = \Sigma$ the covariance matrix of X, and there is some correlation between each pair of predictors. The covariance matrix is assumed to be the same for all classes. 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 to the class for which

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

is maximized. In our modeling, we used the function *lda* from the package *MASS*. As the training dataset we used the dataset with observations measured at multiples only observed at 16.8 meters.

Quadratic Disriminant Analysis

The

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

Results

Classifier performance (numerical)

Insights, conclusions, discussion etc.