DATA11002 Introduction to Machine Learning 2021

Term Project Final Report

Predicting NPF events

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1. Introduction

In this report, we are studying New Particle Formation (NPF) and predicting NPF events based on training data gathered at the Hyytiälä forestry field station SMEAR II mast on different days in the years 2000-2011.

NPF is an event of particle formation from micro-particles, found in air, to new molecular particles. It is known to affect climate, air quality and thus human and animal health, but the particle formation process is quite complex and not fully known.

Therefore, we are using machine learning methods and libraries to help predicting NPF phenomena based on multiple variables found in training data. The interesting question is: When and under which conditions do NPF events occur, and what kind of events could they be? This is also closely related to weather forecasting.

The training data, npf_train.csv, contained observed NPF data and exactly 100 feature columns presenting physical characteristics. In fact, there were 50 measured variables in total, and for each of the variables, computed mean and std values.

The measurements have been gathered during various days and times between sunrise and sunset. The test data, npf_test_hidden.csv, is similar to the training data, but the classes are unknown and thus need to be predicted.

The class variable class4 (because of 4 different classes) could be either nonevent or one of the three events: II. Ia or Ib.

The label nonevent means that no NPF event occurred, otherwise some of the three events occurred.

Event classes were separated into classes II and I, the latter into two additional classes Ia and Ib. Class II meant that the confidence level of NPF growth and formation rates was low. Classes belonging to I had high confidence level. Class Ia meant strong NPF events, while Ib included other events.

Eventually, I decided to use Gaussian Naive Bayes (NB, or GNB vs. Bernoulli BNB) classifier to predict NPF events based on testing data, npf_test_hidden.csv. The "hidden" means that the testing data did not include the class labels.

This project was done using R with R Markdown and Git as version control. The computations as well as tables in this report were performed with R, and the text mostly with R Markdown. The used IDE was RStudio. There exist small displayed chunks of code, but the code is mostly not echoed. It can be found from the Git repo.

In the following sections, I will present the data pre-processing, machine learning methods used, training of the model, discussing and results of the project.

2. Data analysis and pre-processing

The training data, npf_train.csv, included 104 columns and 458 observations in total. The test data, npf_test_hidden.csv, included 965 unclassified observations. There were columns id, date, class4, partlybad and 100 other feature variables measured. The datasets were quite clean and did not need much pre-processing. This shows how the data looked like. This is the first observation.

```
class4 partlybad CO2168.mean CO2168.std CO2336.mean
## 1
     1 2000-01-01 nonevent
                                FALSE
                                          384.462
                                                     2.284996
                                                                 384.1645
     C02336.std C0242.mean C0242.std C02504.mean C02504.std Glob.mean Glob.std
##
## 1
       2.135062
                  385.2747
                            2.211695
                                        383.8851
                                                    1.955198 19.24551 11.90955
##
     H20168.mean H20168.std H20336.mean H20336.std H2042.mean
                                                               H2042.std
## 1
        2.278154 0.05150523
                                  2.272 0.05187726
                                                      2.316406 0.05165106
##
     H20504.mean H20504.std H20672.mean H20672.std H2084.mean H2084.std NET.mean
        2.262308 0.05589525
                               2.272769 0.06414115
                                                      2.289062 0.05368097 13.96418
## 1
##
      NET.std NO168.mean NO168.std NO336.mean NO336.std NO42.mean
## 1 11.05117 0.07953846 0.07122655 0.08446154 0.06803103
                                                           0.054375 0.04730432
     NO504.mean NO504.std NO672.mean NO672.std NO84.mean
                                                              NO84.std NOx168.mean
  1 0.08553846 0.07874069 0.06476923 0.05520155
                                                    0.07125 0.06390717
##
     NOx168.std NOx336.mean NOx336.std NOx42.mean NOx42.std NOx504.mean NOx504.std
## 1 0.7728003
                   2.136923
                             0.7141536
                                         2.071875 0.6294565
                                                                2.078769
                                                                          0.6251687
##
     NOx672.mean NOx672.std NOx84.mean NOx84.std O3168.mean O3168.std O342.mean
## 1
                  0.5824053
                              2.085781
                                        0.663547
                                                    20.29892
                                                             2.258243
##
     0342.std 03504.mean 03504.std 03672.mean 03672.std 0384.mean 0384.std
## 1 2.231756
                20.79462
                           1.88802
                                     21.31831 1.976654
                                                          20.11359 2.273609
##
     Pamb0.mean Pamb0.std PAR.mean PAR.std
                                               PTG.mean
                                                             PTG.std RGlob.mean
       999.8595 0.1664669 20.66235 13.77842 0.003560372 0.005574335
## 1
                                                                       7.169164
##
     RGlob.std RHIRGA168.mean RHIRGA168.std RHIRGA336.mean RHIRGA336.std
## 1
     4.595515
                     98.33385
                                   1.127238
                                                  99.06662
                                                                 1.324536
##
     RHIRGA42.mean RHIRGA42.std RHIRGA504.mean RHIRGA504.std RHIRGA672.mean
## 1
          96.47422
                       1.333359
                                      98.88585
                                                     1.375835
                                                                    101.0309
     RHIRGA672.std RHIRGA84.mean RHIRGA84.std RPAR.mean RPAR.std S02168.mean
##
          1.650608
                                                                     1.070769
## 1
                        96.99047
                                     1.117522
                                              8.864799 5.279957
     SO2168.std SWS.mean
                         SWS.std T168.mean T168.std T42.mean
     0.1919416 924.8636 12.33769 -12.66211 0.3762745 -12.20161 0.3752439
##
     T504.mean T504.std T672.mean T672.std T84.mean
                                                          T84.std UV A.mean
## 1 -12.80858 0.4363618 -13.01647 0.5256979 -12.42297 0.3763239
      UV A.std UV B.mean
                            UV_B.std
                                       CS.mean
## 1 0.8569483 0.02643777 0.01461688 0.0033739 0.0007332531
```

I decided to drop out columns id, date and partlybad from both train and test data, because id and date did not have any impact on the results, and the value of partlybad was always FALSE. The class4 column indicated the observed class, and it was one of these: II, Ia, Ib, nonevent.

The binary classification task was to identify nonevent and event classes, ie. II, Ia, Ib. The hidden test data was similar to training data, but did not contain the class values. I replaced the NA values with a placeholder nonevent. I factored the training data classes as II, Ia, Ib, nonevent.

class non.n	neachass non.s	scclassII.mea	nclassII.sd	classIa.mea	mlassIa.sd	classIb.mea	mlassIb.sd
CO2168.mean383.3257592	12.0163656	379.781655	89.6374969	377.3983620	07.9319611	377.5385938	88.5728401
CO2168.std 3.8076389	3.7136048	3.4647404			3.3126275	3.3173097	3.0186016
CO2336.mean383.3010772		379.835508				377.6037099	
CO2336.std 3.5851381	3.4501180	3.2415884		1.7707188	3.1835412	3.1055142	2.7644834
CO242.mean 384.3454936				378.054553		378.4111268	
CO242.std 4.5978001	4.4815486	4.2714589		2.1576477		4.2127625	4.3486898
CO2504.mean383.1770183				377.4236330		377.5267348	
CO2504.std 3.4192060	3.1583781	2.9971388		1.6631054		2.8382270	2.4519342
Glob.mean 124.1843709						3 4 73.8362652	
Glob.std 100.3933153						5 197.614956	
H2O168.mean 8.3952240	4.2909264	6.6839081		4.7256178		6.1144060	2.7852484
H2O168.std 0.5305522	0.4666248	0.6812579		0.3949500		0.6062125	0.3944818
H2O336.mean 8.3234504	4.2414113	6.6003523		4.6750551		6.0381327	2.7308122
H2O336.std 0.5293356	0.4655487	0.6725026		0.3950264		0.6076353	0.3960382
H2O42.mean 8.5241697	4.3895086	6.8414829		4.8100257		6.2500283	2.8805575
H2O42.std 0.5447998	0.4825249	0.7035039		0.4007320		0.2500283 0.6189761	0.3851627
H2O504.mean 8.2824671	4.2084802	6.5496678		4.6486063	2.9945831		2.7011730
H2O504.std 0.5274781	0.4679204	0.6699628		0.3928798		0.6094654	0.3996900
H2O672.mean 8.2507405	4.1830761	6.5114863		4.6267247		5.9550852	2.6803969
H2O672.std 0.5299801				0.3879299		0.6088883	
	0.4680479 4.3504865	0.6695066 6.7679388		4.7685026		6.1851300	0.4012817
		0.6954969		0.3943370		0.1851300 0.6118577	2.8420338 0.3918308
H2O84.std 0.5398556 NET.mean 80.5261547	$0.4769061 \\ 74.3785508$					0.0116577 9171.690150'	
NET.std 87.6830282	78.6126033					9172.493228	
NO168.mean 0.0832628 NO168.std 0.0868361	$\begin{array}{c} 0.1178991 \\ 0.0701328 \end{array}$	0.0486565 0.0762156		0.0840824 0.0756751	0.1708901 0.0743735	0.0618202 0.1103664	0.0845130 0.1480846
NO336.mean 0.0891754	0.0701328 0.1240921	0.0702130 0.0505879		0.0730731		0.0630157	0.1480840 0.0884501
NO336.std 0.0903346	0.1240921 0.0772049	0.0800398	0.0558533		0.1823832	0.0865659	0.0334301 0.0772434
NO42.mean 0.0708654	0.0772049 0.0952515	0.0300338 0.0372286		0.0679048	0.1414973	0.0305059 0.0495214	0.0668548
NO42.std 0.0985503	0.0332913 0.1232974	0.0372230 0.0735775		0.0079546 0.0749556	0.0684068	0.0433214	0.1676579
NO504.mean 0.0886274	0.1232974 0.1226654	0.0490583	0.0415577		0.1906810	0.1125454 0.0615647	0.1070579
NO504.mean 0.0000274 NO504.std 0.0905429	0.1220034 0.0839672	0.0490503 0.0763539	0.0300430		0.0805113	0.0839574	0.0689388
NO672.mean 0.0871272	0.0033012 0.1183312	0.0482930		0.0906560	0.0803113 0.1928020	0.0599156	0.0845935
NO672.mean 0.0871272 NO672.std 0.0914093	0.1183312 0.0878955	0.0482950 0.0744356	0.0374997		0.1928020 0.0788534	0.0399130 0.0850076	0.0345935 0.0706539
NO84.mean 0.0696912	0.0378933 0.1038470	0.0744350 0.0393163		0.0730297 0.0749010		0.0525418	0.0760259
NO84.std 0.0797140	0.1038470 0.0603073	0.0393103 0.0729624		0.0749010 0.0751914	0.1339954 0.0719955		0.0700239
NOx168.mean 1.8006764	1.6301601	0.0729024 0.8619501		1.4469960		1.0933323	0.1100099 0.8587382
NOx168.std 0.5197397	0.4535324	0.4625667		0.3706119		0.4621600	0.3910069
NOx336.mean 1.7959607	1.6180526	0.4025007 0.8485011		1.4394845		1.0824423	0.8536414
		0.3930678		0.3676035		0.4216894	
	0.5687775						0.3590915
NOx42.mean 1.8093522	$\begin{array}{c} 1.6224146 \\ 0.7791902 \end{array}$	0.8625380 0.4397016		$1.4401144 \\ 0.3895916$		$1.1101887 \\ 0.6164194$	0.8502164
NOx42.std 0.6384147							0.8641324
NOx504.mean 1.7811794	$\begin{array}{c} 1.5945210 \\ 0.6577056 \end{array}$	0.8390183		1.4176531		1.0648497	0.8472283
NOx504.std 0.5897877		0.4328458		0.3526593		0.4132702	0.3432988
NOx672.mean 1.7631446	1.5703224	$\begin{array}{c} 0.8313492 \\ 0.3815342 \end{array}$		$\begin{array}{c} 1.4099343 \\ 0.3555551 \end{array}$		$1.0594163 \\ 0.4136651$	0.8493411
NOx672.std 0.5487984 NOx84.mean 1.7905142	0.5379051	0.8608148				1.0974465	0.3522673
	1.6296561			1.4411304			0.8517585
	0.4434093	0.4490562		0.3744475		0.4846042	0.4074471
O3168 std 3 5200114	8.7015444					38.1966494	
O3168.std 3.5209114	2.3207539	4.0125807		3.1157460		4.0468967	2.3752102
O342.mean 27.7531718	8.5799124	55.9105184	8.1800544	34.7040199	9.0125137	37.1545134	9.0931088

	1	1	11 TT	1 77 1	1 T	1 7 1	1 T1	
	class_non.m	ieachass_non.	sœlassII.mea	nclassII.sd	classla.mea	nclassla.sd	class1b.mea	mlass1b.sd
O342.std	3.9320093	2.5715429	4.5629995		3.4300530	2.2983362	4.5916329	2.6110586
O3504.mean	29.9223688	8.7826482	38.1124111	7.6215776	36.1765368	9.4885172	38.9206969	7.4458559
O3504.std	3.3379269	2.1808745	3.6198586	2.0168362	2.9581700	2.1895254	3.6856651	2.1572885
O3672.mean	30.2570159	8.8153168	38.4638542	7.5423407	36.4179137	9.4671344	39.1708386	7.4083422
O3672.std	3.2974286	2.1320519	3.4793625	1.8999729	2.8855798	2.2111996	3.5270694	2.0859228
O384.mean	28.2950117	8.6449395	36.4847757	8.0918533	35.2079586	9.5844538	37.6702692	7.8834566
O384.std	3.6818176	2.4325495	4.2321932	2.3653424	3.1852934	2.1710969	4.2537071	2.4787015
${\bf Pamb 0. mean}$	989.5739182	10.4595733	992.434422	17.5447690	993.083107	512.7955733	3 993.8398014	49.2653530
Pamb0.std	0.9036629	0.7414164	1.1832659	0.8141691	1.0277771	0.6889135	1.1659888	0.8041929
PAR.mean	252.1034293	219.836291	0521.825264	7189.138226	3 2 15.749190	2262.77427	3 6 33.1584717	7184.637852
PAR.std	201.6516309	180.623172	4387.977789	5139.014894	4 0 286.6517870	0191.622924	18 86.993314	4139.2281508
PTG.mean	0.0013185	0.0072903	_	0.0047814	-	0.0053309	-	0.0031918
			0.0005988		0.0007118		0.0016611	
PTG.std	0.0067485	0.0064188	0.0120327	0.0058381		0.0069848	0.0115483	0.0054228
RGlob.mean		14.4447614	36.2972617					11.9587230
RGlob.std	13.7137875		23.9939113					
RHIRGA168.			57.2879848					
RHIRGA168.		4.7117565	11.6976471				12.1942132	
RHIRGA336.			57.4444120					
RHIRGA336.		4.6981200	11.4247132				11.9648446	
RHIRGA42.n			58.4772003				956.8580399	
RHIRGA42.s		5.0783234	12.4831364				13.0917220	
RHIRGA504.			57.3573156				15.0317220	
RHIRGA504.		4.6848747	11.1521853				11.5776651	
RHIRGA672.			57.8459091					
RHIRGA672.		4.6333869	10.9344953				11.2599693	
RHIRGA84.n			57.6708747					
RHIRGA84.s			12.1984752				12.7443155	
RPAR.mean		4.9777942	22.5765995				24.4094019	
	10.5616485							
RPAR.std		8.7993333					16.9022109	
SO2168.mean		0.4872757	0.1926844		0.1695263		0.2362119	0.3058720
SO2168.std	0.1529806	0.1386084	0.1577387	0.1276472			0.1684688	0.1246219
SWS.mean	901.2928793		915.222233					
SWS.std	28.9825589		16.4777475				5 12.6442312	
T168.mean	6.0779466		8.5962921		2.8687104		7.6928053	8.0038911
	1.3599286	0.9772331					2.4789441	
T42.mean	6.1653770		8.6499311		2.9865494		7.7541718	8.0064785
T42.std	1.4646568	1.1112941	2.6472802		2.1859501		2.7393903	1.0755007
T504.mean	5.8160029		8.2703335		2.5531536		7.3368535	8.0393041
T504.std	1.2650820	0.9053966	2.1760562		1.8472449		2.2836336	0.9179909
T672.mean	5.6329681		8.0609689		2.3391703		7.1069544	8.0400739
T672.std	1.2171312	0.8754616	2.0874301		1.7835714		2.1963858	0.8942363
T84.mean	6.1500669		8.6976018		2.9538699		7.8076448	8.0135334
T84.std	1.4406672	1.0637270	2.5498165		2.1481955		2.6451795	1.0221479
$UV_A.mean$	7.6842886	6.1089685					14.7907621	
UV A.std	5.6597847	4.8468768	10.3911167	3.9771654	7.5590838	5.1088458	10.3899427	3.9910193
	0.2050000	0.3044106	0.6028462	0.2732618	0.4214711	0.2929315	0.5940769	0.2781953
UV_B.mean	0.3258228	0.3044100						
	0.3238228 0.2887586	0.3044100 0.2824756	0.5214276		0.3465650	0.2574466	0.5066760	0.2556018
$UV_B.mean$				0.2522659			$\begin{array}{c} 0.5066760 \\ 0.0024524 \end{array}$	$\begin{array}{c} 0.2556018 \\ 0.0016285 \end{array}$

We notice that there are some undefined measurements, but they do not have a large impact. Laplace smoothing of 1 was used for the data. The estimated class probabilities for training data:

nb_class

##

nonevent II Ia Ib ## 0.49783550 0.25541126 0.06493506 0.18181818

3. Machine learning methods and steps

I applied Gaussian NB classifier to compute the class probabilities for all rows of testing data. The variables were considered as conditionally independent (because of that is the pre-assumption), even though some of them might have a relationship, smaller or larger correlation.

The variables were studied and only a subset of the variables were used. There were some challenges choosing the variables. The classifier predicted the probabilities of each class for each row. The row was identified as nonevent, if the probability was higher than the nb_class probability for that class.

The formula of NB Gaussian density was

$$\frac{e^{(-(x-\mu)^2/(2*\sigma^2))}}{\sqrt{2*\pi*\sigma^2}}\tag{1}$$

I used some small coefficient adjustments and modifications for the multiclass classification problem. The multiclass problem was, of course, more challenging than the binary classification problem because of more events to be predicted.

The predicted probabilities were compared step by step, with different coefficients. The target was to produce reasonable prediction probabilities for the classes.

After having identified the class as nonevent or event, the event class had to be predicted, if it was not nonevent. I compared the probabilities of different predicted events with NB classifier and chose suitable coefficients for predicting the event classes. I guessed that the accuracy of the binary classification could be 0.73.

Regarding the different classification sub-tasks, the main target was to build a reasonably performing binary classifier. Building a more accurate event class classifier was not as important, although the higher accuracy, the better.

The first 15 estimated classes and probabilities were:

head(df, 15)

```
##
## 1
          0.73
## 2
        class4
                   0.727504450479219
## 3
            Ιa
                   0.080463843559317
      nonevent
## 5
            Ib
                   0.990897111743513
## 6
            II
                   0.991238939899939
## 7
                   0.120253990842419
      nonevent
## 8
                   0.978951849227886
            II
      nonevent 0.000677548460571997
## 9
## 10 nonevent
                0.00245307701477748
## 11
            TT
                   0.926588565138545
## 12
            II
                   0.539002979107427
## 13 nonevent
                0.00085019262958641
## 14 nonevent
                   0.497539389391826
## 15
                   0.790420964630693
```

The first row contains the guessed accuracy, and the second row labels for the classes and probabilities: class4 and p.

After that, each row contains the predicted class and prediction probability for the class being an event class, for each data row in the test data. So if the probability **p** is 0.3, the probability of a **non-event** would be 0.7.

This whole data frame was exported as a csv file answers.csv. That file contains all the predicted results.

4. Summary and discussing

The predicted class distributions for testing data for classes nonevent, II, Ia, Ib:

```
## [1] 0.4611399
```

[1] 0.2683938

[1] 0.09948187

[1] 0.1709845

These probabilities were quite close to the probabilities in training data.

It turned out that my binary accuracy (predicting event vs. nonevent) was about 0.795, actually higher than the guessed 0.73. The margin of error was quite small: about 0.065. In addition, the multiaccuracy (predicting the correct class) was around 0.585, meaning that the model could have performed better, but at least it predicted almost 3 out of 5 classes correctly. As expected, it was more difficult to predict event classes than to predict binary classes (i.e. event vs. non-event).

The perplexity turned out to be 1.65, meaning that it was placed between 1 and 2, the perplexities of "perfect" and dummy random classifiers. The perfect classifier would predict the class always correct, and dummy classifier would assign probability 0.5 to both binary classes.

Regarding the methods, I considered using also cross-validation, Random Forest, logistic regression, kNN and SVM. I ended up in using NB, because of the pros of it. They are that the model is highly scalable and simple generative classifier, it can usually be trained efficiently in supervised learning, and it often requires only a small number of training data.

The downsides of using NB in this project were that all the variables were not independent and normally distributed. Those are the assumptions, but by leaving the correlated and not normally distributed variables out, the assumption is still holding and the classifier performed reasonably.

One of the features of NB is that it can be making strong assumptions based on the data, because it is a "naive" model. However, that can also be advantageous, but not every time.

As a hindsight, different subset of the feature variables could have been used. One option would have been to use e.g. only mean values instead of std values, or other variables based on the correlations.

After making some tweaks, I got the NB classifier to predict reasonable results, but there were initially some problems with the class distributions. I learned a lot about the effectiviness and usability of NB classifier.

5. Self-grading

"At the end of the course, you will be asked to give your project deliverables (final report, presentation, and challenge submission) an integer grade on a scale from 0 (fail) to 5 (excellent)".

I am giving these grades to my deliverables:

- Challenge submission: 3. This looked as it should, and was returned in time. The accuracy could have been a bit better, but there are no large problems with it. This showed understanding of the topic and was suitable for the problem. The challenge was based on the model.
- Presentation: 0. Unfortunately, I didn't have time with this.
- Final report: 3. The level of final report was about the same as in challenge submission. Nothing relevant was missing, and this showed some deeper understanding of the topic as well as critical analyzing. The readability should be ok. However, the report could have been a bit more comprehensive, and more machine learning methods could have been used. All in all, the topics and research questions were answered in sufficient manner.

The average grade of these deliverables is 2, so I will give myself a grade 2 of this project in total. The minimal requirements are satisfied; the presentation was not defined as a minimal requirement anywhere. But unfortunately, that drops the grade with a number. The work mostly follows the instructions given.

6. References

Articles

 $\rm https://iopscience.iop.org/article/10.1088/1748-9326/aadf3c$

https://www.who.int/health-topics/air-pollution

http://www.borenv.net/BER/archive/pdfs/ber10/ber10-323.pdf

 $\rm https://acp.copernicus.org/articles/18/9597/2018/$

Git repo

https://github.com/hartzka/iml21