Adverse Reaction Classification and Clusters of the COVID-19 Vaccine: Potential Clinical Prediction Tool

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Our application project clusters and classifies COVID-19 vaccine adverse reactions. The purpose of the project is having a detailed understanding of the common types of adverse reactions and identifying which adverse reactions are in need of immediate care. This project suggests a two-step approach. First, using an unsupervised machine learning algorithm (clustering) to segment adverse reactions into groups. This will give us the most common symptoms for each group. Second, using symptoms, along with additional patient information (gender, age, allergies) and vaccine manufacturer information, we will predict the need of urgent medical care by using fatalities and hospital visits.

The dataset is provided by the Vaccine Adverse Event Reporting System VAERS and contains reports about adverse events that may be associated with COVID-19 vaccines. The database we chose was the dataset provided for the current year 2021, considering that our goal is to explore reactions due to Covid vaccines. The data contains reports processed as of 3/26/2021.

Dataset Source: VAERS - Vaccine Adverse Event Reporting System. Data Retrieve on 4/8/2021
https://vaers.hhs.gov/data/datasets.html

Clean each dataset

In [1]:
```python
import pandas as pd
import numpy as np

all_data =  pd.read_csv('2021VAERSDATA.csv', sep=",", encoding = "ISO-8859-1")
symptoms_data = pd.read_csv('2021VAERSSYMPTOMS.csv', sep=",", encoding = "ISO-8859-1")
vax_data = pd.read_csv('2021VAERSVAX.csv', sep=",", encoding = "ISO-8859-1")

print('Main Dataset Size:', all_data.shape)
print('Symptoms Dataset Size:', symptoms_data.shape)
print('Vaccine Info Dataset Size:', vax_data.shape)
```

```
Main Dataset Size: (40348, 35)
Symptoms Dataset Size: (56533, 11)
Vaccine Info Dataset Size: (40937, 8)
```

```
C:\Users\andre\anaconda3\lib\site-packages\IPython\core\interactiveshell.py:3146: DtypeW
arning: Columns (7,12,23) have mixed types.Specify dtype option on import or set low_mem
ory=False.
  has_raised = await self.run_ast_nodes(code_ast.body, cell_name,
```

1. all_data dataset

This dataset contains data like gender, age, and other useful features.

In [2]:
```
all_data.head()
```

Out[2]:

	VAERS_ID	RECVDATE	STATE	AGE_YRS	CAGE_YR	CAGE_MO	SEX	RPT_DATE	SYMPTOM_TEXT	DIE
0	916600	01/01/2021	TX	33.0	33.0	NaN	F	NaN	Right side of epiglottis swelled up and hinder...	Na
1	916601	01/01/2021	CA	73.0	73.0	NaN	F	NaN	Approximately 30 min post vaccination administ...	Na
2	916602	01/01/2021	WA	23.0	23.0	NaN	F	NaN	About 15 minutes after receiving the vaccine, ...	Na
3	916603	01/01/2021	WA	58.0	58.0	NaN	F	NaN	extreme fatigue, dizziness,. could not lift my...	Na
4	916604	01/01/2021	TX	47.0	47.0	NaN	F	NaN	Injection site swelling, redness, warm to the ...	Na

5 rows × 35 columns

In [3]:
```
#Find duplicates
all_data.duplicated().any()
```

Out[3]:
```
False
```

In [4]:
```
#Find duplicates of 'VAERS_ID'
all_data['VAERS_ID'].duplicated().any()
```

Out[4]:
```
False
```

In [5]:
```
# check fir null/na values in Age column
print('NaN values:', all_data['AGE_YRS'].isnull().sum())
print(all_data.shape)
```

```
NaN values: 3545
(40348, 35)
```

In [6]:
```
# drop rows where age is null or na
all_data = all_data.dropna(axis=0, subset=['AGE_YRS'])
print(all_data.shape)
```

```
(36803, 35)
```

In [7]:
```
#convert the column data type to integer, age is a discrete value
# and to clean this column we'll convert it to integers
#all_data['AGE_YRS'] = df_all['AGE_YRS'].astype(int)
```

In [8]:
```
# clean Age column
all_data['AGE_YRS'].value_counts().sort_index().head(10)
```

Out[8]:
```
0.08     2
0.25     1
0.33     4
0.42     1
0.50     1
0.58     3
0.75     1
1.00     5
1.08    22
1.17     2
Name: AGE_YRS, dtype: int64
```

In [9]:
```
# Keep only patients from 16 - 99 years old

print('Shape:', all_data.shape)

filter_age = np.logical_and(all_data['AGE_YRS'] >= 16, all_data['AGE_YRS'] <100)
print('\n',filter_age.value_counts())

# drop all samples with 16<=age<100
all_data = all_data[filter_age]
print('\nShape:', all_data.shape)
```

```
Shape: (36803, 35)

 True     36674
False      129
Name: AGE_YRS, dtype: int64

Shape: (36674, 35)
```

2. symptoms_data dataset

This dataset contains all the reactions/symptoms that patients presented after obtaining the COVID-19 vaccine.

In [10]:
```
symptoms_data.head()
```

Out[10]:

	VAERS_ID	SYMPTOM1	SYMPTOMVERSION1	SYMPTOM2	SYMPTOMVERSION2	SYMPTOM3	SYMPT
0	916600	Dysphagia	23.1	Epiglottitis	23.1	NaN	
1	916601	Anxiety	23.1	Dyspnoea	23.1	NaN	
2	916602	Chest discomfort	23.1	Dysphagia	23.1	Pain in extremity	
3	916603	Dizziness	23.1	Fatigue	23.1	Mobility decreased	
4	916604	Injection site erythema	23.1	Injection site pruritus	23.1	Injection site swelling	

In [11]:
```
#Find duplicates
symptoms_data.duplicated().any()
```

Out[11]:
```
False
```

In [12]:
```
#Find duplicates of 'VAERS_ID'
print(symptoms_data['VAERS_ID'].duplicated().any())
print(symptoms_data['VAERS_ID'].duplicated().sum())

# The duplicates here means that a single patient had more than 5 symptoms
# and they were listed in different rows with the same VAERS_ID per patient.
```

```
True
16185
```

In [13]:
```
# Drop columns whose name contains a specific string from pandas DataFrame.
# Remove SYMPTOMVERSION columns
symptoms_data = symptoms_data[symptoms_data.columns.drop(list(symptoms_data.filter(rege
symptoms_data.head()
```

Out[13]:

	VAERS_ID	SYMPTOM1	SYMPTOM2	SYMPTOM3	SYMPTOM4	SYMPTOM5
0	916600	Dysphagia	Epiglottitis	NaN	NaN	NaN
1	916601	Anxiety	Dyspnoea	NaN	NaN	NaN
2	916602	Chest discomfort	Dysphagia	Pain in extremity	Visual impairment	NaN
3	916603	Dizziness	Fatigue	Mobility decreased	NaN	NaN
4	916604	Injection site erythema	Injection site pruritus	Injection site swelling	Injection site warmth	NaN

In [14]:
```
#Find duplicates of 'VAERS_ID'
print(symptoms_data['VAERS_ID'].duplicated().sum())
print(symptoms_data.shape)
```

```
16185
(56533, 6)
```

Find the most common symptoms in all the patients

In [15]:
```
#stack "SYMPTOM1", "SYMPTOM2", "SYMPTOM3" to "SYMPTOM"

symptoms_data['INDEX1'] = symptoms_data.index
symptoms_data = pd.wide_to_long(symptoms_data, stubnames='SYMPTOM', i=['INDEX1'], j='NU
symptoms_data.reset_index(drop=True, inplace=True)
symptoms_data.head()
```

Out[15]:

	VAERS_ID	SYMPTOM
0	916600	Dysphagia
1	916601	Anxiety
2	916602	Chest discomfort
3	916603	Dizziness

	VAERS_ID	SYMPTOM
4	916604	Injection site erythema

In [16]:
```
# Unique symptoms
len(symptoms_data.SYMPTOM.unique())
```

Out[16]:
```
4407
```

In [17]:
```
# remove rows with nan
symptoms_data['SYMPTOM'] = symptoms_data['SYMPTOM'].astype(str)
symptoms_data = symptoms_data[symptoms_data.SYMPTOM != 'nan']
symptoms_data.shape
```

Out[17]:
```
(190092, 2)
```

In [18]:
```
# Get the frequency of symptoms
symptoms_data['SYMPTOM'].value_counts(ascending = False).head(50)
```

Out[18]:
```
Headache                   8881
Pyrexia                    7204
Chills                     6865
Fatigue                    6418
Pain                       6034
Nausea                     5039
Dizziness                  4229
Pain in extremity          3678
Myalgia                    3416
Injection site pain        3320
Injection site erythema    2655
Arthralgia                 2505
Dyspnoea                   2407
Vomiting                   2050
Pruritus                   2044
Injection site swelling    1975
Rash                       1934
Death                      1813
Asthenia                   1799
Injection site pruritus    1619
Paraesthesia               1508
Malaise                    1495
Erythema                   1490
Diarrhoea                  1456
SARS-CoV-2 test positive   1416
Injection site warmth      1399
Urticaria                  1379
Hypoaesthesia              1280
Hyperhidrosis              1213
Lymphadenopathy            1212
COVID-19                   1190
Cough                      1141
Feeling abnormal           1101
SARS-CoV-2 test negative   1005
Heart rate increased        988
Chest discomfort            932
SARS-CoV-2 test             928
Chest pain                  882
Tremor                      865
Flushing                    836
Palpitations                833
Peripheral swelling         817
```

```
Feeling hot                 775
Injection site rash         708
Back pain                   706
Vaccination site pain       694
Tachycardia                 685
Neck pain                   684
Condition aggravated        678
Decreased appetite          669
Name: SYMPTOM, dtype: int64
```

In [19]:
```
# remove symptoms that appear less then 1,000 times
symptoms_count = symptoms_data.SYMPTOM.value_counts()
symptoms_data = symptoms_data[symptoms_data.SYMPTOM.isin(symptoms_count.index[symptoms_
symptoms_data['SYMPTOM'].value_counts(ascending = False)
```

Out[19]:
```
Headache                   8881
Pyrexia                    7204
Chills                     6865
Fatigue                    6418
Pain                       6034
Nausea                     5039
Dizziness                  4229
Pain in extremity          3678
Myalgia                    3416
Injection site pain        3320
Injection site erythema    2655
Arthralgia                 2505
Dyspnoea                   2407
Vomiting                   2050
Pruritus                   2044
Injection site swelling    1975
Rash                       1934
Death                      1813
Asthenia                   1799
Injection site pruritus    1619
Paraesthesia               1508
Malaise                    1495
Erythema                   1490
Diarrhoea                  1456
SARS-CoV-2 test positive   1416
Injection site warmth      1399
Urticaria                  1379
Hypoaesthesia              1280
Hyperhidrosis              1213
Lymphadenopathy            1212
COVID-19                   1190
Cough                      1141
Feeling abnormal           1101
SARS-CoV-2 test negative   1005
Name: SYMPTOM, dtype: int64
```

In [20]:
```
symptoms_data.shape
```

Out[20]:
```
(94170, 2)
```

In [21]:
```
#Drop all rows with "Death", as this is our dependent variable/target
symptoms_data = symptoms_data.drop(symptoms_data[symptoms_data.SYMPTOM == 'Death'].inde
symptoms_data.shape
```

Out[21]:
```
(92357, 2)
```

Hot encoding the symtoms

In [22]:
```
# Store ID column
ids = symptoms_data['VAERS_ID']

# Apply one-hot encoding
symptoms_data = symptoms_data['SYMPTOM'].str.get_dummies()

# Add the VAERS_ID column
symptoms_data.insert(loc=0, column='VAERS_ID', value=ids)

# Merging all the rows with the same ID after using dummy encoding
symptoms_data = symptoms_data.groupby(['VAERS_ID']).sum().reset_index()
symptoms_data
```

Out[22]:

	VAERS_ID	Arthralgia	Asthenia	COVID-19	Chills	Cough	Diarrhoea	Dizziness	Dyspnoea	Erythe
0	916601	0	0	0	0	0	0	0	1	
1	916602	0	0	0	0	0	0	0	0	
2	916603	0	0	0	0	0	0	1	0	
3	916604	0	0	0	0	0	0	0	0	
4	916607	0	0	0	1	0	0	0	0	
...	...	...	...	...	...	...	...	...	...	
31497	1134439	0	0	0	0	0	0	1	0	
31498	1134819	0	0	0	0	0	0	0	1	
31499	1135949	0	0	0	0	0	0	0	0	
31500	1136535	0	1	0	0	0	0	0	0	
31501	1136908	0	0	0	1	0	0	0	0	

31502 rows × 34 columns

In [23]:
```
symptoms_data.shape
```

Out[23]:
```
(31502, 34)
```

3. vax_data dataset

This dataset contains data regarding the type of vaccine that was provided to each patient.

In [24]:
```
vax_data
```

Out[24]:

	VAERS_ID	VAX_TYPE	VAX_MANU	VAX_LOT	VAX_DOSE_SERIES	VAX_ROUTE	VAX_SITE	V
0	916600	COVID19	MODERNA	037K20A	1	IM	LA	(M

	VAERS_ID	VAX_TYPE	VAX_MANU	VAX_LOT	VAX_DOSE_SERIES	VAX_ROUTE	VAX_SITE	V
1	916601	COVID19	MODERNA	025L20A	1	IM	RA	(M
2	916602	COVID19	PFIZER\BIONTECH	EL1284	1	IM	LA	B
3	916603	COVID19	MODERNA	unknown	UNK	NaN	NaN	(M
4	916604	COVID19	MODERNA	NaN	1	IM	LA	(M
...	...	...	...	...	...	...	...	
40932	1135429	COVID19	JANSSEN	NaN	UNK	IM	LA	(
40933	1135949	COVID19	JANSSEN	1805020	1	SYR	LA	(
40934	1136535	COVID19	JANSSEN	NaN	UNK	NaN	NaN	(
40935	1136622	COVID19	JANSSEN	1808609	1	IM	NaN	(
40936	1136908	COVID19	JANSSEN	NaN	1	SYR	RA	(

40937 rows × 8 columns

In [25]:
```
# unique value of 'VAX_TYPE'
vax_data.VAX_TYPE.unique()
```

Out[25]:
```
array(['COVID19', 'UNK', 'FLU4', 'DTAPHEPBIP', 'HIBV', 'RV1', 'FLUX',
       'HEP', 'MMR', 'VARZOS', 'DTAP', 'PPV', 'HPV9', 'CHOL', 'DT',
       'TTOX', 'FLU3', 'FLUC3', 'FLUC4', 'PNC13', 'FLUR4', 'MNQ', 'HPV4',
       'TDAP', 'FLUA3', 'HEPA', 'VARCEL', 'FLUA4', 'ANTH', 'IPV', 'TYP',
       'TD', 'HPVX', 'DTP', 'DTAPIPVHIB', 'RV5', 'MENB', 'RAB', 'FLUN4',
       'PNC', 'OPV', 'YF'], dtype=object)
```

Besides COVID-19 vaccines, this dataset contained other type of vaccines. Our analysis focused only in COVID-19 vaccine reactions.

In [26]:
```
#only keep rows which 'VAX_TYPE' is 'COVID19'
vax_data = vax_data[vax_data["VAX_TYPE"] == 'COVID19']
vax_data.shape
```

```
Out[26]: (40490, 8)
```

```
In [27]: #Keep only 'VAERS_ID' and 'VAX_MANU' columns in vax_data dataset
         vax_data = vax_data[['VAERS_ID','VAX_MANU']]
         print(vax_data.head())
         print(vax_data.shape)
```

```
   VAERS_ID         VAX_MANU
0    916600          MODERNA
1    916601          MODERNA
2    916602  PFIZER\BIONTECH
3    916603          MODERNA
4    916604          MODERNA
(40490, 2)
```

```
In [28]: #Find duplicates
         print(vax_data.duplicated().any())
         print(vax_data.duplicated().sum())
```

```
True
433
```

```
In [29]: #drop duplicates
         vax_data = vax_data.drop_duplicates()
         vax_data.shape
```

```
Out[29]: (40057, 2)
```

```
In [30]: #Find duplicates of 'VAERS_ID'
         print(vax_data['VAERS_ID'].duplicated().any())
         print(vax_data['VAERS_ID'].duplicated().sum())
```

```
True
13
```

There are 13 patients who took 2 different types of vax_manu (First dose with manufacture and second dose with another manufacture. Check the symptom_text for clarification.

```
In [31]: #Print all rows with duplicates "VAERS_ID"

         ids = vax_data["VAERS_ID"]
         vax_dataDuplicates = vax_data[ids.isin(ids[ids.duplicated()])]
         vax_dataDuplicates.head(26)
```

Out[31]:

	VAERS_ID	VAX_MANU
5112	922571	MODERNA
5113	922571	PFIZER\BIONTECH
5131	922592	MODERNA
5132	922592	PFIZER\BIONTECH
5258	922730	MODERNA
5259	922730	PFIZER\BIONTECH
5288	922762	MODERNA
5289	922762	PFIZER\BIONTECH

	VAERS_ID	VAX_MANU
15563	934042	MODERNA
15564	934042	PFIZER\BIONTECH
15924	934438	MODERNA
15925	934438	PFIZER\BIONTECH
18549	937422	MODERNA
18550	937422	PFIZER\BIONTECH
21914	967274	MODERNA
21915	967274	PFIZER\BIONTECH
22608	977024	MODERNA
22609	977024	PFIZER\BIONTECH
23406	988065	MODERNA
23407	988065	PFIZER\BIONTECH
28776	1046599	MODERNA
28777	1046599	PFIZER\BIONTECH
28909	1046739	MODERNA
28910	1046739	PFIZER\BIONTECH
38327	1094637	JANSSEN
38328	1094637	MODERNA

In [32]:
```
#Remove the all those 13 patients out of the study.

idx1 = set(vax_data.set_index(['VAERS_ID', 'VAX_MANU']).index)
idx2 = set(vax_dataDuplicates.set_index(['VAERS_ID', 'VAX_MANU']).index)

vax_data = pd.DataFrame(list(idx1 - idx2), columns=vax_data.columns)

vax_data.shape
```

Out[32]:
```
(40031, 2)
```

Preprocessing the data

Merging Datasets

In [33]:
```
# merge symptoms_data all_data. By default is "inner" join.
df_all = symptoms_data.merge(all_data[['VAERS_ID','AGE_YRS','SEX','DIED','L_THREAT','HO
df_all.shape
```

Out[33]:
```
(29274, 42)
```

In [34]:
```
# merge df_all with vax_data. By default is "inner" join.
```

```
df_all = df_all.merge(vax_data[['VAERS_ID','VAX_MANU']], on='VAERS_ID')
df_all
```

Out[34]:

	VAERS_ID	Arthralgia	Asthenia	COVID-19	Chills	Cough	Diarrhoea	Dizziness	Dyspnoea	Erythe
0	916601	0	0	0	0	0	0	0	1	
1	916602	0	0	0	0	0	0	0	0	
2	916603	0	0	0	0	0	0	1	0	
3	916604	0	0	0	0	0	0	0	0	
4	916607	0	0	0	1	0	0	0	0	
...	...	...	...	...	...	...	...	...	...	
29189	1134439	0	0	0	0	0	0	1	0	
29190	1134819	0	0	0	0	0	0	0	1	
29191	1135949	0	0	0	0	0	0	0	0	
29192	1136535	0	1	0	0	0	0	0	0	
29193	1136908	0	0	0	1	0	0	0	0	

29194 rows × 43 columns

After merging df_all with vax_data, the number of rows becomes less because there are some "VAERS_ID" in df_all that vax_data does not have.

In [35]:
```
df_all.shape
```

Out[35]:
```
(29194, 43)
```

In [36]:
```
# Print the value counts for categorical columns

for col in df_all.columns:
    if df_all[col].dtype == 'object':
        print('\nColumn Name:', col,)
        print(df_all[col].value_counts())
```

```
Column Name: SEX
F    22379
M     6689
U      126
Name: SEX, dtype: int64

Column Name: DIED
Y    748
Name: DIED, dtype: int64

Column Name: L_THREAT
Y    848
Name: L_THREAT, dtype: int64

Column Name: HOSPITAL
Y    2877
Name: HOSPITAL, dtype: int64

Column Name: HISTORY
None
3176
none
1452
Comments: List of non-encoded Patient Relevant History: Patient Other Relevant History
1: None                        453
Asthma
348
No
333

...
Has spinocerebellar ataxia type I
1
Medical History/Concurrent Conditions: COVID-19 (diagnosed with COVID-19:Yes); Thyroid h
ormones decreased                1
Grave's Disease, Epilepsy, Clotting Disorders
1
Medical History/Concurrent Conditions: Heart attack (Heart attack in 2011 and stent was
placed.); Stent placement        1
posterior tibialis tendinitis for about 3/4 weeks prior to vaccination
1
Name: HISTORY, Length: 10191, dtype: int64

Column Name: ALLERGIES
None                                                                                 3126
none                                                                                 1448
NKA                                                                                   540
NKDA                                                                                  492
No                                                                                    384
                                                                                     ...
NKDA & NO FOOD ALLERGIES                                                                1
Shell Fish, Cologne, Perfume, Hand sanitizer, penicillin, Zpac, coconut, peanuts        1
hives  w/ carboplatin & taxotere                                                        1
Latex, Peanuts, Percocet, Neurontin, Ferrlecit,                                         1
Zithromycin                                                                             1
Name: ALLERGIES, Length: 7697, dtype: int64

Column Name: VAX_MANU
MODERNA              14068
PFIZER\BIONTECH      12688
JANSSEN               2423
```

```
UNKNOWN MANUFACTURER       15
Name: VAX_MANU, dtype: int64
```

Cleaning vaccine's manufacter column and combining related features to create our target column

In [37]:

```
import numpy as np

# Dropping rows with vaccine manufacter different than 'MODERNA','PFIZER\BIONTECH', 'JA
main_vax = ['MODERNA','PFIZER\BIONTECH', 'JANSSEN']
df_all["CLEAN_VAX"] = np.where(df_all["VAX_MANU"].isin(main_vax), df_all["VAX_MANU"], "


# create_target(row) combines related features to create the target column
def create_target(row):
    if ((row['DIED'] == 'Y') or (row['L_THREAT'] == 'Y') or (row['HOSPITAL'] == 'Y')):
        return 1
    else:
        return 0

# create target column
df_all['target'] = df_all.apply(create_target, axis = 1)

# drop columns used to create our target column and uncleaned vax_manu
df_all = df_all.drop(['DIED','L_THREAT','HOSPITAL', 'VAX_MANU'],axis=1)
df_all.head()
```

Out[37]:

	VAERS_ID	Arthralgia	Asthenia	COVID-19	Chills	Cough	Diarrhoea	Dizziness	Dyspnoea	Erythema
0	916601	0	0	0	0	0	0	0	1	0
1	916602	0	0	0	0	0	0	0	0	0
2	916603	0	0	0	0	0	0	1	0	0
3	916604	0	0	0	0	0	0	0	0	0
4	916607	0	0	0	1	0	0	0	0	0

5 rows × 41 columns

In [38]:

```
df_all.shape
```

```
Out[38]: (29194, 41)
```

Encode SEX and CLEAN_VAX columns into binary values

```
In [39]: df_all["SEX"].value_counts()
```

```
Out[39]: F    22379
         M     6689
         U      126
         Name: SEX, dtype: int64
```

```
In [40]: # drop all rows with unkown SEX
         df_all = df_all[df_all['SEX'] != 'U']
         df_all.shape
```

```
Out[40]: (29068, 41)
```

```
In [41]: df_all["CLEAN_VAX"].value_counts()
```

```
Out[41]: MODERNA            14011
         PFIZER\BIONTECH    12622
         JANSSEN             2420
         Other                 15
         Name: CLEAN_VAX, dtype: int64
```

```
In [42]: # drop all rows with Other CLEAN_VAX
         df_all = df_all[df_all['CLEAN_VAX'] != 'Other']
         df_all.shape
```

```
Out[42]: (29053, 41)
```

```
In [43]: # Transform SEX column into binary values

         # Data of SEX is converted into Binary Data
         df_gender = pd.get_dummies(df_all["SEX"])

         # Binary Data is Concatenated into Dataframe
         df_all = pd.concat((df_all, df_gender['F']), axis=1)
         df_all = df_all.drop(["SEX"], axis=1)
         df_all = df_all.rename(columns={"F": "Gender"})

         # Transform VAX column into binary values

         # Data of CLEAN_VAX is converted into Binary Data
         df_vax = pd.get_dummies(df_all["CLEAN_VAX"])

         # Binary Data is Concatenated into Dataframe
         df_all = pd.concat((df_all, df_vax['MODERNA']), axis=1)
         df_all = pd.concat((df_all, df_vax['PFIZER\BIONTECH']), axis=1)
         df_all = pd.concat((df_all, df_vax['JANSSEN']), axis=1)
         df_all = df_all.drop(["CLEAN_VAX"], axis=1)
```

```
In [44]: df_vax.value_counts()
```

```
Out[44]: JANSSEN  MODERNA  PFIZER\BIONTECH
         0        1        0                  14011
                  0        1                  12622
         1        0        0                   2420
         dtype: int64
```

In [45]:
```
df_all
```

Out[45]:

	VAERS_ID	Arthralgia	Asthenia	COVID-19	Chills	Cough	Diarrhoea	Dizziness	Dyspnoea	Erythe
0	916601	0	0	0	0	0	0	0	1	
1	916602	0	0	0	0	0	0	0	0	
2	916603	0	0	0	0	0	0	1	0	
3	916604	0	0	0	0	0	0	0	0	
4	916607	0	0	0	1	0	0	0	0	
...	...	...	...	...	...	...	...	...	...	
29189	1134439	0	0	0	0	0	0	1	0	
29190	1134819	0	0	0	0	0	0	0	1	
29191	1135949	0	0	0	0	0	0	0	0	
29192	1136535	0	1	0	0	0	0	0	0	
29193	1136908	0	0	0	1	0	0	0	0	

29053 rows × 43 columns

One-hot encoding "Allergies"

In [46]:
```
allergies_df = df_all.filter(['VAERS_ID','ALLERGIES'], axis=1)
allergies_df.head()
```

Out[46]:

	VAERS_ID	ALLERGIES
0	916601	"Dairy"
1	916602	Shellfish

	VAERS_ID	ALLERGIES
2	916603	Diclofenac, novacaine, lidocaine, pickles, tom...
3	916604	Na
4	916607	Penicillin

In [47]:
```
allergies_df['ALLERGIES'] = allergies_df['ALLERGIES'].astype(str)

# Remove punctuation
allergies_df['ALLERGIES'] = allergies_df['ALLERGIES'].str.replace('[^\w\s]','')

# Convert to lower case
allergies_df['ALLERGIES'] = allergies_df['ALLERGIES'].map(lambda x: x.lower())

# Tokenize
allergies_df['ALLERGIES'] = allergies_df['ALLERGIES'].map(lambda x: x.split())
allergies_df.head()
```

Out[47]:

	VAERS_ID	ALLERGIES
0	916601	[dairy]
1	916602	[shellfish]
2	916603	[diclofenac, novacaine, lidocaine, pickles, to...
3	916604	[na]
4	916607	[penicillin]

In [48]:
```
import nltk
nltk.download('punkt')
nltk.download('stopwords')
from nltk.corpus import stopwords
from nltk.tokenize import word_tokenize
from nltk.stem import PorterStemmer

# Stop Words
stop_words=set(stopwords.words("english"))
allergies_df['ALLERGIES'] = allergies_df['ALLERGIES'].map(lambda x: [word for word in x

# Stemming
stemmer = PorterStemmer()
allergies_df['ALLERGIES'] = allergies_df['ALLERGIES'].map(lambda x: [stemmer.stem(y) fo
allergies_df.head()
```

```
[nltk_data] Downloading package punkt to
[nltk_data]     C:\Users\andre\AppData\Roaming\nltk_data...
[nltk_data]   Package punkt is already up-to-date!
[nltk_data] Downloading package stopwords to
[nltk_data]     C:\Users\andre\AppData\Roaming\nltk_data...
[nltk_data]   Package stopwords is already up-to-date!
```

Out[48]:

	VAERS_ID	ALLERGIES
0	916601	[dairi]
1	916602	[shellfish]

	VAERS_ID	ALLERGIES
2	916603	[diclofenac, novacain, lidocain, pickl, tomato...
3	916604	[na]
4	916607	[penicillin]

In [49]:
```
allergies_df.shape
```

Out[49]:
```
(29053, 2)
```

In [50]:
```
# Unpack lists with Pandas

allergies_df = allergies_df.explode('ALLERGIES', ignore_index=True)

allergies_df.head(10)
```

Out[50]:

	VAERS_ID	ALLERGIES
0	916601	dairi
1	916602	shellfish
2	916603	diclofenac
3	916603	novacain
4	916603	lidocain
5	916603	pickl
6	916603	tomato
7	916603	milk
8	916604	na
9	916607	penicillin

In [51]:
```
#unique allergies

len(allergies_df.ALLERGIES.unique())
```

Out[51]:
```
4675
```

In [52]:
```
# Get the frequency of allergies
allergies_df['ALLERGIES'].value_counts(ascending = False)
```

Out[52]:
```
nan            10885
none            5246
sulfa           1697
penicillin      1601
allergi         1343
               ...  
hibiclen           1
buprofen           1
brewer             1
sulfamethox        1
uncod              1
Name: ALLERGIES, Length: 4674, dtype: int64
```

In [53]:
```
# Only kepp allergies that are in more than 1000 patients
allergies_count = allergies_df.ALLERGIES.value_counts()
allergies_df = allergies_df[allergies_df.ALLERGIES.isin(allergies_count.index[allergies
allergies_df['ALLERGIES'].value_counts(ascending = False)
```

Out[53]:
```
nan           10885
none           5246
sulfa          1697
penicillin     1601
allergi        1343
Name: ALLERGIES, dtype: int64
```

In [54]:
```
# Drop rows with "nan","none","allergi","food","known","unknown","reaction","na","repor

allergies_df = allergies_df.drop(allergies_df[allergies_df.ALLERGIES.isin(["nan","none"
allergies_df.shape
```

Out[54]:
```
(3298, 2)
```

In [55]:
```
# one-hot encoding

#allergies_onehot = allergies_df.set_index('VAERS_ID')['ALLERGIES'].str.get_dummies().m
#allergies_onehot.head()

# Store ID column
ids = allergies_df['VAERS_ID']

# Apply one-hot encoding
allergies_onehot = allergies_df['ALLERGIES'].str.get_dummies()

# Add the VAERS_ID column
allergies_onehot.insert(loc=0, column='VAERS_ID', value=ids)

# Merging all the rows with the same ID after using dummy encoding
allergies_onehot = allergies_onehot.groupby(['VAERS_ID']).sum().reset_index()
allergies_onehot
```

Out[55]:

	VAERS_ID	penicillin	sulfa
0	916607	1	0
1	916615	0	1
2	916619	0	1
3	916634	1	0
4	916642	1	0
...	...	...	...
3011	1126252	1	0
3012	1127237	1	0
3013	1127523	0	1
3014	1129128	0	1
3015	1130492	0	1

3016 rows × 3 columns

In [56]:
```
allergies_onehot.shape
```
Out[56]:
```
(3016, 3)
```

One hot encoding "HISTORY"

In [57]:
```
history_df = df_all.filter(['VAERS_ID','HISTORY'], axis=1)
history_df.head()
```
Out[57]:

	VAERS_ID	HISTORY
0	916601	Patient residing at nursing facility. See pati...
1	916602	None
2	916603	diverticulitis, mitral valve prolapse, osteoar...
3	916604	NaN
4	916607	High blood pressure, high cholesterol, sleep a...

In [58]:
```
history_df['HISTORY'] = history_df['HISTORY'].astype(str)

# Remove punctuation
history_df['HISTORY'] = history_df['HISTORY'].str.replace('[^\w\s]','')

# Remove digits
history_df['HISTORY'] = history_df['HISTORY'].str.replace('\d+', '')

# Convert to lower case
history_df['HISTORY'] = history_df['HISTORY'].map(lambda x: x.lower())

# Tokenize
history_df['HISTORY'] = history_df['HISTORY'].map(lambda x: x.split())
history_df.head()
```
Out[58]:

	VAERS_ID	HISTORY
0	916601	[patient, residing, at, nursing, facility, see...
1	916602	[none]
2	916603	[diverticulitis, mitral, valve, prolapse, oste...
3	916604	[nan]
4	916607	[high, blood, pressure, high, cholesterol, sle...

In [59]:
```
# Stop Words
stop_words=set(stopwords.words("english"))
history_df['HISTORY'] = history_df['HISTORY'].map(lambda x: [word for word in x if word

# Stemming
stemmer = PorterStemmer()
history_df['HISTORY'] = history_df['HISTORY'].map(lambda x: [stemmer.stem(y) for y in x
history_df.head()
```
Out[59]:

	VAERS_ID	HISTORY
0	916601	[patient, resid, nurs, facil, see, patient, ch...
1	916602	[none]
2	916603	[diverticul, mitral, valv, prolaps, osteoarthr]
3	916604	[nan]
4	916607	[high, blood, pressur, high, cholesterol, slee...

In [60]:
```
# Unpack lists with Pandas

history_df = history_df.explode('HISTORY', ignore_index=True)
history_df.head(10)
```

Out[60]:

	VAERS_ID	HISTORY
0	916601	patient
1	916601	resid
2	916601	nurs
3	916601	facil
4	916601	see
5	916601	patient
6	916601	chart
7	916602	none
8	916603	diverticul
9	916603	mitral

In [61]:
```
#unique history
len(history_df.HISTORY.unique())
```

Out[61]:
```
5668
```

In [62]:
```
history_df.shape
```

Out[62]:
```
(106269, 2)
```

In [63]:
```
# Get the frequency of symptoms
history_df['HISTORY'].value_counts(ascending = False)
```

Out[63]:
```
nan                 8780
none                5656
medic               2855
condit              2544
historyconcurr      2421
                    ...
transplantoctob        1
empir                  1
dislocatedfx           1
anklos                 1
```

```
hemositerosi          1
Name: HISTORY, Length: 5667, dtype: int64
```

In [64]:
```
# Only kepp allergies that are in more than 1000 patients
history_count = history_df.HISTORY.value_counts()
history_df = history_df[history_df.HISTORY.isin(history_count.index[history_count.gt(10
history_df['HISTORY'].value_counts(ascending = False)
```

Out[64]:
```
nan                  8780
none                 5656
medic                2855
condit               2544
historyconcurr       2421
histori              1973
asthma               1934
allergi              1869
hypertens            1686
diabet               1457
high                 1421
patient              1348
diseas               1327
relev                1212
hypothyroid          1144
blood                1116
pressur              1006
Name: HISTORY, dtype: int64
```

In [65]:
```
# Drop rows with "nan","historyconcurr","histori","patient","high",...

history_df = history_df.drop(history_df[history_df.HISTORY.isin(["nan","none","historyc
                                                                  "covid","diseas","comm
                                                                  "event","unknown","yea
                                                                  "ago"])].index)

history_df.shape
```

Out[65]:
```
(16823, 2)
```

In [66]:
```
# one-hot encoding

#history_onehot = history_df.set_index('VAERS_ID')['HISTORY'].str.get_dummies().max(lev
#history_onehot.head()

# Store ID column
ids = history_df['VAERS_ID']

# Apply one-hot encoding
history_onehot = history_df['HISTORY'].str.get_dummies()

# Add the VAERS_ID column
history_onehot.insert(loc=0, column='VAERS_ID', value=ids)

# Merging all the rows with the same ID after using dummy encoding
history_onehot = history_onehot.groupby(['VAERS_ID']).sum().reset_index()
history_onehot
```

Out[66]:

	VAERS_ID	allergi	asthma	blood	condit	diabet	hypertens	hypothyroid	medic	pressur	relev
0	916607	0	0	1	0	1	0	0	0	1	0
1	916622	0	1	0	0	0	0	0	0	0	0
2	916625	1	0	0	0	0	0	0	0	0	0

	VAERS_ID	allergi	asthma	blood	condit	diabet	hypertens	hypothyroid	medic	pressur	relev
3	916647	0	0	0	0	1	0	0	0	0	0
4	916648	0	1	0	0	0	0	0	0	0	0
...	...	...	...	...	...	...	...	...	...	...	..
8412	1130201	1	0	0	0	0	1	0	0	0	0
8413	1130492	1	1	0	0	0	0	0	0	0	0
8414	1132846	0	0	0	0	0	1	1	0	0	0
8415	1133280	0	0	0	0	1	1	0	0	0	0
8416	1134819	0	0	0	0	0	0	1	0	0	0

8417 rows × 11 columns

In [67]:
```
history_onehot.shape
```

Out[67]:
```
(8417, 11)
```

Merge allergies one hot encoding and history one hot encoding to df_all

In [68]:
```
df_merge = pd.merge(df_all, history_onehot, how="left", on='VAERS_ID')
df_merge = pd.merge(df_merge, allergies_onehot, how="left", on='VAERS_ID')

# store patient's ID
patients_VAERS_ID = df_merge['VAERS_ID']

#df_merge = df_merge.drop(['VAERS_ID', "HISTORY", "ALLERGIES", "CLEAN_VAX"],axis=1)
df_merge = df_merge.drop(['VAERS_ID', "HISTORY", "ALLERGIES"],axis=1)
df_merge.head()
```

Out[68]:

	Arthralgia	Asthenia	COVID-19	Chills	Cough	Diarrhoea	Dizziness	Dyspnoea	Erythema	Fatigue	...
0	0	0	0	0	0	0	0	1	0	0	...
1	0	0	0	0	0	0	0	0	0	0	...
2	0	0	0	0	0	0	1	0	0	1	...
3	0	0	0	0	0	0	0	0	0	0	...
4	0	0	0	1	0	0	0	0	0	0	...

5 rows × 52 columns

In [69]:
```
df_merge.shape
```

Out[69]:
```
(29053, 52)
```

In [70]:
```
#Fill NaN with 0. NaN occurs because we merge "left"
df_merge = df_merge.fillna(0)
df_merge.head()
```

Out[70]:

	Arthralgia	Asthenia	COVID-19	Chills	Cough	Diarrhoea	Dizziness	Dyspnoea	Erythema	Fatigue	...
0	0	0	0	0	0	0	0	1	0	0	...
1	0	0	0	0	0	0	0	0	0	0	...
2	0	0	0	0	0	0	1	0	0	1	...
3	0	0	0	0	0	0	0	0	0	0	...
4	0	0	0	1	0	0	0	0	0	0	...

5 rows × 52 columns

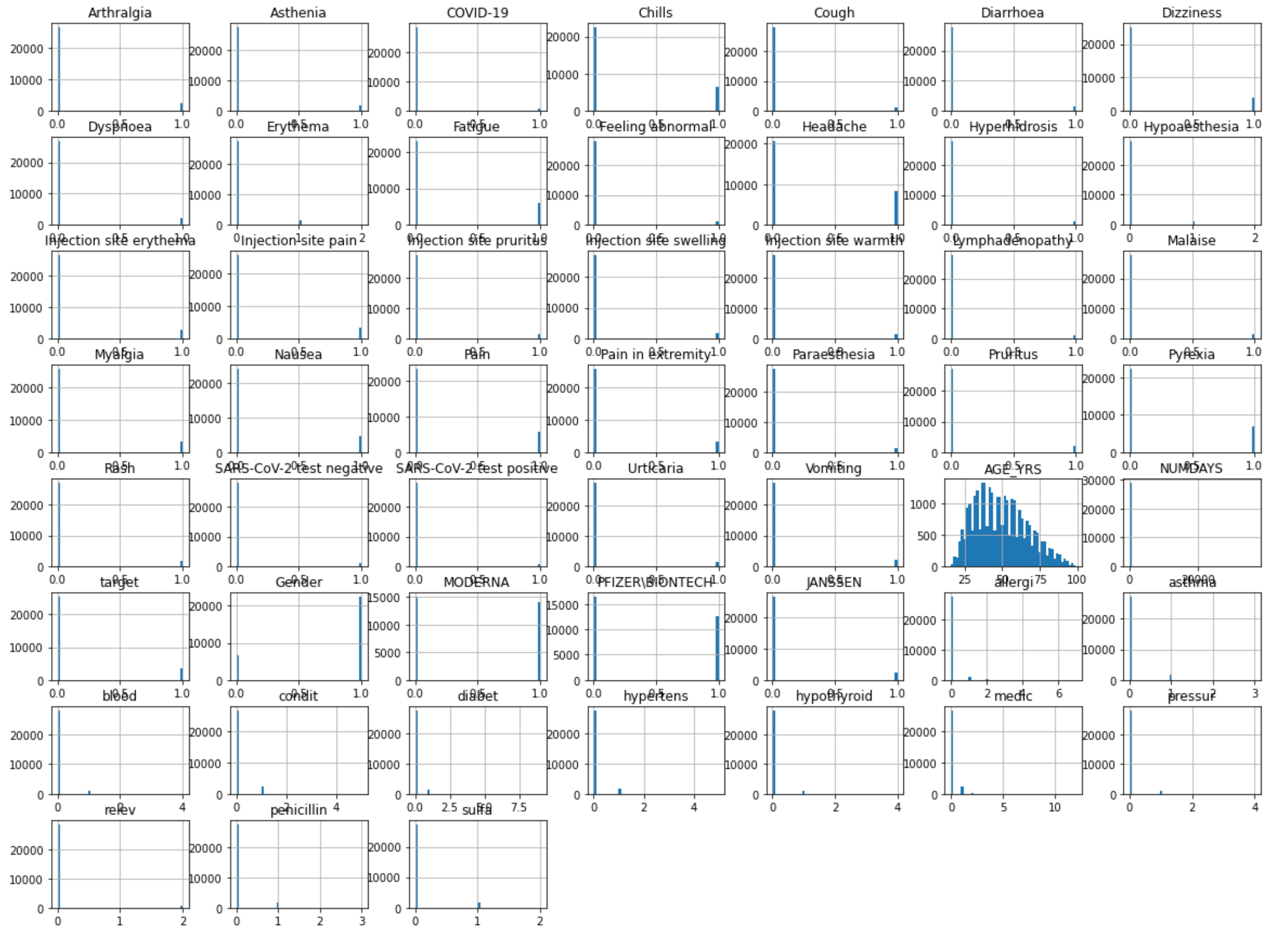
In [71]:
```
# Keep only features that don't have feature vector = 0.

df_merge = df_merge[df_merge.drop(['AGE_YRS', 'NUMDAYS', 'target'], axis=1).sum(axis=1)

df_merge.shape
```

Out[71]:
```
(29053, 52)
```

In [72]:
```
df_merge.to_csv('cleaned_data.csv', encoding='utf-8')
```

Exploratory Data Analysis (With Clean Dataset)

In [73]:
```
# Import Matplotlib for plotting
import matplotlib.pyplot as plt
%matplotlib inline

df_merge.hist(bins=50, figsize=(20,15));
```

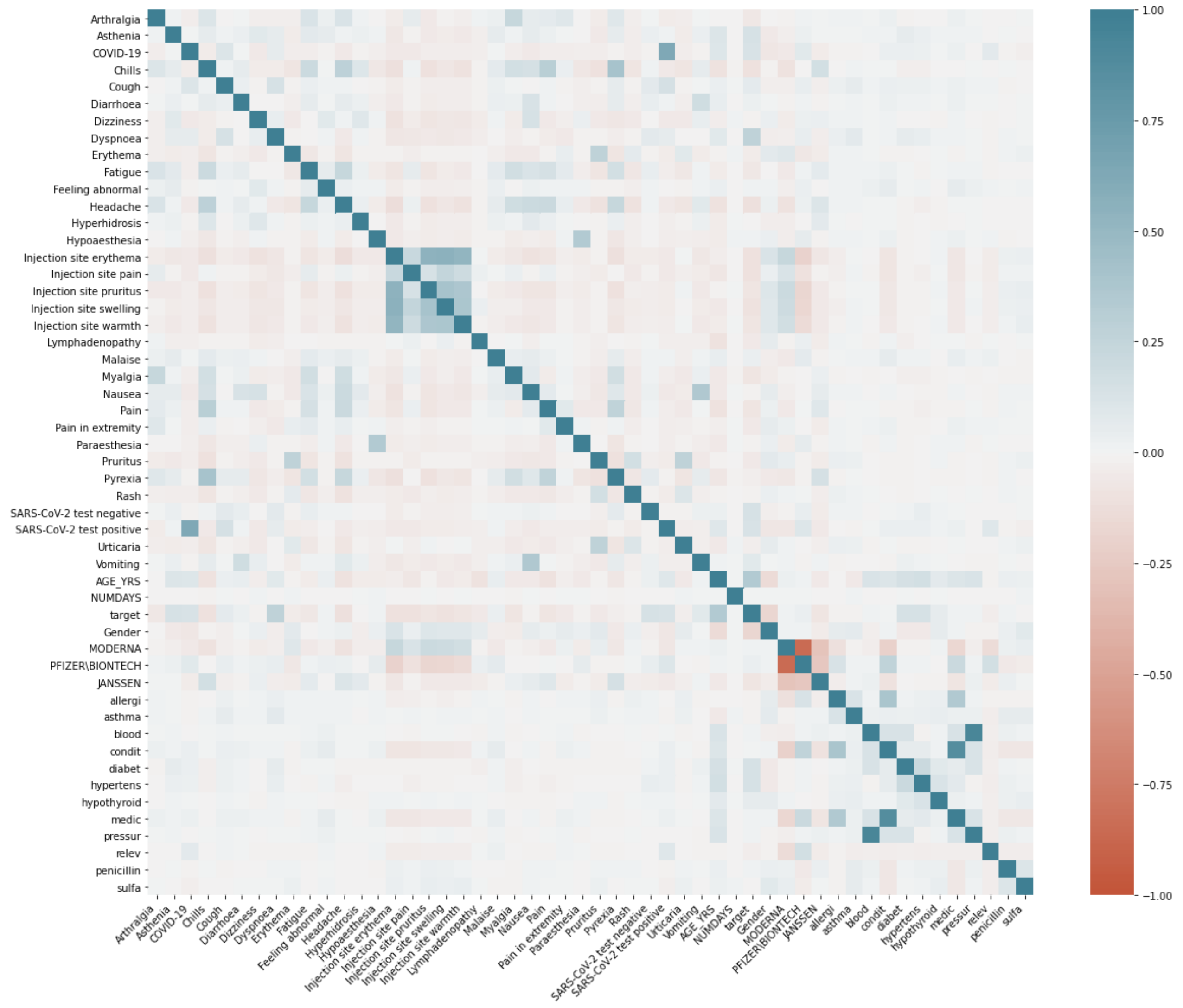


```
In [74]: # Variable Correlations with target
         df_merge.corr()['target'].sort_values(ascending=False)
```

```
Out[74]: target                      1.000000
         AGE_YRS                     0.338083
         Dyspnoea                    0.269475
         Asthenia                    0.147948
         hypertens                   0.147573
         SARS-CoV-2 test negative    0.146734
         diabet                      0.142609
         SARS-CoV-2 test positive    0.139795
         COVID-19                    0.139074
         Vomiting                    0.082831
         Cough                       0.067850
         hypothyroid                 0.053677
         PFIZER\BIONTECH             0.037456
         Malaise                     0.036731
         Diarrhoea                   0.025644
         Hypoaesthesia               0.018954
         pressur                     0.017443
         blood                       0.016703
         penicillin                  0.016396
         medic                       0.015218
         Feeling abnormal            0.010334
         MODERNA                     0.008076
         condit                      0.001240
         NUMDAYS                     0.000823
         sulfa                      -0.003435
         Hyperhidrosis              -0.003970
         Paraesthesia               -0.007940
         asthma                     -0.008577
         Dizziness                  -0.010958
```

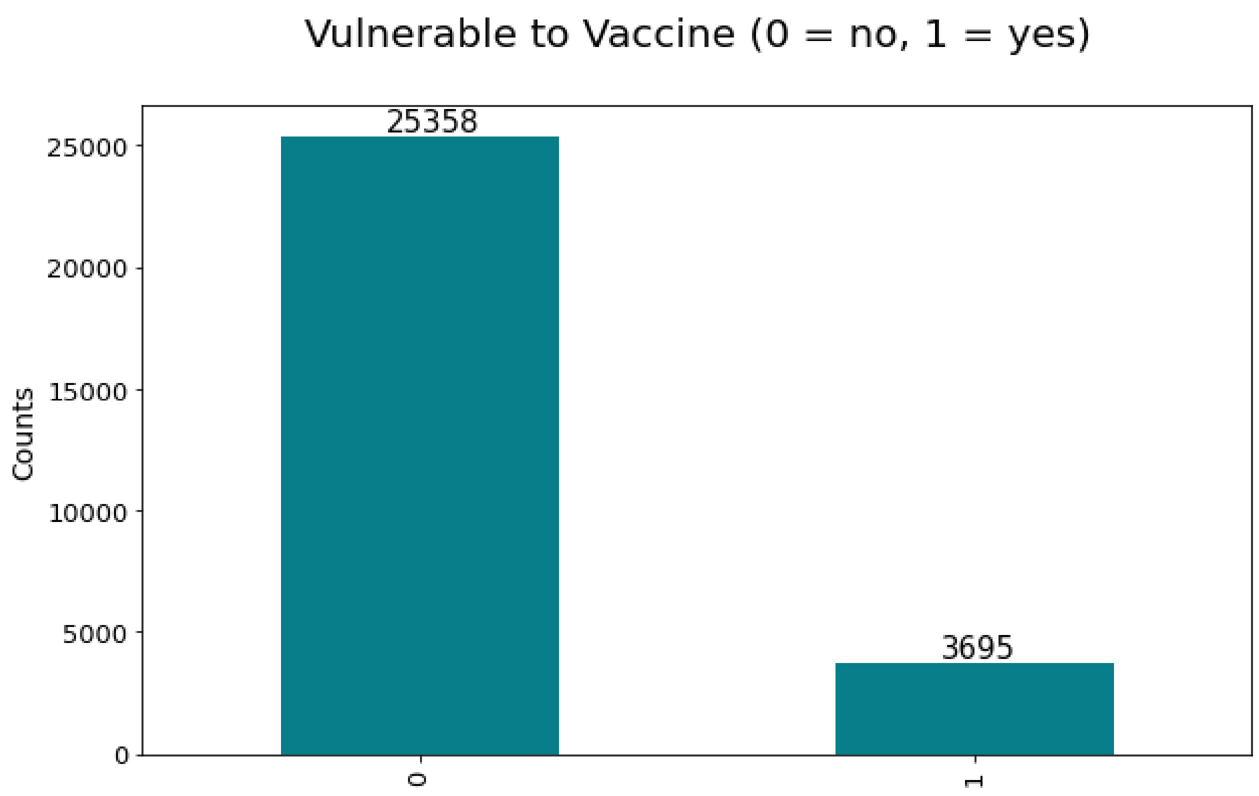
```
Nausea                       -0.020873
Rash                         -0.021250
allergi                      -0.022125
Pyrexia                      -0.023654
Urticaria                    -0.026058
relev                        -0.037674
Erythema                     -0.046453
Lymphadenopathy              -0.053753
Pruritus                     -0.054346
Pain in extremity            -0.059325
Arthralgia                   -0.065501
Fatigue                      -0.068493
Injection site warmth        -0.080216
Pain                         -0.081597
JANSSEN                      -0.081793
Myalgia                      -0.083460
Injection site pruritus      -0.085394
Injection site swelling      -0.088326
Injection site pain          -0.104425
Chills                       -0.106652
Injection site erythema      -0.109196
Headache                     -0.115307
Gender                       -0.172210
Name: target, dtype: float64
```

In [75]:
```python
from seaborn import heatmap, diverging_palette

fig, ax = plt.subplots(figsize=(20, 16))

corr = df_merge.corr()
ax = heatmap(corr, vmin=-1, vmax=1, center=0,
    cmap=diverging_palette(20, 220, n=200), square=True, annot=False)

ax.set_xticklabels( ax.get_xticklabels(),
    rotation=45, horizontalalignment='right');
```



Classification Models

```
In [77]: import matplotlib.pyplot as plt

         # showing how are dataset is unbalanced
         ax = df_merge['target'].value_counts().plot(kind='bar', figsize=(10, 6), fontsize=13, c
         ax.set_title('Vulnerable to Vaccine (0 = no, 1 = yes)', size=20, pad=30)
         ax.set_ylabel('Counts', fontsize=14)

         for i in ax.patches:
             ax.text(i.get_x() + 0.19, i.get_height() + 250, str(round(i.get_height(), 2)), font
```



Classification with Unbalanced Dataset

In [78]:
```
from sklearn.preprocessing import StandardScaler, PolynomialFeatures
from sklearn.pipeline import Pipeline
from sklearn.pipeline import make_pipeline
from sklearn.model_selection import GridSearchCV

from sklearn.metrics import confusion_matrix, precision_score, recall_score, f1_score,
from sklearn.model_selection import train_test_split
from sklearn.metrics import plot_confusion_matrix, roc_auc_score, accuracy_score
```

Split Dataset into training and test set

In [79]:
```
allData = df_merge
y = df_merge['target'] # 1D targer vector
X = df_merge.drop(labels='target', axis=1)

# Split data into train and test set
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.20, random_state

# Scale the data
scaler = StandardScaler()
scaler.fit(X_train)

X_train = scaler.transform(X_train)
X_test = scaler.transform(X_test)
```

Handling Imbalanced data with Synthetic Minority Oversampling TEchnique - SMOTE

In [80]:
```
!pip install imbalanced-learn

from imblearn.over_sampling import SMOTE
```

```
smt = SMOTE(random_state=42)
X_train_SMOTE, y_train_SMOTE = smt.fit_resample(X_train, y_train)

print(f'''\nShape of X before SMOTE: {X_train.shape}
Shape of X after SMOTE: {X_train_SMOTE.shape}''')

print('\nBalance of positive and negative classes (%):')
y_train_SMOTE.value_counts(normalize=True) * 100
```

```
Requirement already satisfied: imbalanced-learn in c:\users\andre\anaconda3\lib\site-pac
kages (0.8.0)
Requirement already satisfied: scikit-learn>=0.24 in c:\users\andre\anaconda3\lib\site-p
ackages (from imbalanced-learn) (0.24.2)
Requirement already satisfied: joblib>=0.11 in c:\users\andre\anaconda3\lib\site-package
s (from imbalanced-learn) (0.17.0)
Requirement already satisfied: numpy>=1.13.3 in c:\users\andre\anaconda3\lib\site-packag
es (from imbalanced-learn) (1.19.2)
Requirement already satisfied: scipy>=0.19.1 in c:\users\andre\anaconda3\lib\site-packag
es (from imbalanced-learn) (1.5.2)
Requirement already satisfied: threadpoolctl>=2.0.0 in c:\users\andre\anaconda3\lib\site
-packages (from scikit-learn>=0.24->imbalanced-learn) (2.1.0)

Shape of X before SMOTE: (23242, 51)
Shape of X after SMOTE: (40552, 51)

Balance of positive and negative classes (%):
```

Out[80]:
```
1    50.0
0    50.0
Name: target, dtype: float64
```

Fucntion to print any classifier report

In [81]:
```
from sklearn.metrics import plot_confusion_matrix, roc_auc_score, accuracy_score
from sklearn.metrics import average_precision_score, balanced_accuracy_score, plot_prec

def print_report_classifiers(model, y_train_pred, y_test_pred, X_test=X_test, Y_test=y_
                             auc=True, conf_train=True):

    print("\nTraining Accuracy: {0:0.4f}".format(accuracy_score(Y_train, y_train_pred))
    print("Test Accuracy: {0:0.4f}".format(accuracy_score(Y_test, y_test_pred)))

    print("\nTest Confusion Matrix:")
    print(confusion_matrix(Y_test, y_test_pred))

    print(classification_report(Y_test, y_test_pred))

    if auc:
        if model in ["svm_rbf_clf"]:
            #print("ROC-AUC Score:",roc_auc_score(Y_test, model.decision_function(X_tes
            average_precision = average_precision_score(y_test, model.decision_function
        else:
            #print("ROC-AUC Score:",roc_auc_score(Y_test, model.predict_proba(X_test)[:
            average_precision = average_precision_score(y_test, model.predict_proba(X_t

        if conf_train:
            disp = plot_precision_recall_curve(model, X_test, y_test)
            disp.ax_.set_title('2-class Precision-Recall curve: '
                    'AP={0:0.2f}'.format(average_precision))
        print("Precision-Recall AUC: {:0.2f}".format(average_precision))

    print("Balanced accuaracy: {:0.2f}".format(balanced_accuracy_score(Y_test, y_test_p
    #plot_roc_curve(model, Xtest, ytest)
    #plt.show()
```

- Model: KNN

In [82]:
```
from sklearn.neighbors import KNeighborsClassifier

knnclf = KNeighborsClassifier()
knnclf.fit(X_train, y_train)

y_train_predicted = knnclf.predict(X_train)
y_test_predicted = knnclf.predict(X_test)

print_report_classifiers(knnclf, y_train_predicted, y_test_predicted, conf_train=False)
```

```
Training Accuracy: 0.9154
Test Accuracy: 0.8957

Test Confusion Matrix:
[[4914  168]
 [ 438  291]]
              precision    recall  f1-score   support

           0       0.92      0.97      0.94      5082
           1       0.63      0.40      0.49       729

    accuracy                           0.90      5811
   macro avg       0.78      0.68      0.72      5811
weighted avg       0.88      0.90      0.89      5811

Precision-Recall AUC: 0.45
Balanced accuaracy: 0.68
```

KNN Hyperparameter Tuning

In [ ]:
```
%%time

#List Hyperparameters
leaf_size = [1,10,20,30,40,50]
n_neighbors = list(range(3,15,2))
metric = ['euclidean','manhattan']
p=[1,2]

#Convert to dictionary
hyperparameters = dict(n_neighbors=n_neighbors, p=p, metric = metric)

#Create new KNN object
knnclf2 = KNeighborsClassifier()

#Use GridSearch
clf = GridSearchCV(knnclf2, hyperparameters, cv=5, scoring='f1')

#Fit the model
best_model = clf.fit(X_train_SMOTE, y_train_SMOTE)

#Print The value of best Hyperparameters
print('Best p:', best_model.best_estimator_.get_params()['p'])
print('Best n_neighbors:', best_model.best_estimator_.get_params()['n_neighbors'])
print('Best Metric:', best_model.best_estimator_.get_params()['metric'])
print('Best leaf_size:', best_model.best_estimator_.get_params()['leaf_size'])
```

For hyperparameter tunning we will leave the cells with the code used to find the optimal parameters in the form of a raw cells (for the models where Hyperparameter tunning took more than a few minutes) and report the results.

Optimal Parameters for KNN:

- p: 1
- n_neighbors: 5
- Metric: manhattan
- leaf_size: 30

In [83]:
```
%%time
# knn optimal parameters with SMOTE
knnclffinal = KNeighborsClassifier(leaf_size=30, n_neighbors=5,
                                   p=1, metric='manhattan')

knnclffinal.fit(X_train_SMOTE, y_train_SMOTE)

y_train_predicted = knnclffinal.predict(X_train_SMOTE)
y_test_predicted = knnclffinal.predict(X_test)

print_report_classifiers(knnclffinal, y_train_predicted, y_test_predicted,
                         Y_train=y_train_SMOTE, conf_train=False)
```

```
Training Accuracy: 0.9346
Test Accuracy: 0.8246

Test Confusion Matrix:
[[4345  737]
 [ 282  447]]
              precision    recall  f1-score   support

           0       0.94      0.85      0.90      5082
           1       0.38      0.61      0.47       729

    accuracy                           0.82      5811
   macro avg       0.66      0.73      0.68      5811
weighted avg       0.87      0.82      0.84      5811

Precision-Recall AUC: 0.38
Balanced accuaracy: 0.73
Wall time: 2min 36s
```

In [84]:
```
%%time
# knn optimal parameters
knnclffinal = KNeighborsClassifier(leaf_size=30, n_neighbors=5,
                                   p=1, metric='manhattan')

knnclffinal.fit(X_train, y_train)

y_train_predicted = knnclffinal.predict(X_train)
y_test_predicted = knnclffinal.predict(X_test)

print_report_classifiers(knnclffinal, y_train_predicted,
                         y_test_predicted, conf_train=False)
```

```
Training Accuracy: 0.9190
Test Accuracy: 0.8997

Test Confusion Matrix:
```

```
[[4939  143]
 [ 440  289]]
              precision    recall  f1-score   support

           0       0.92      0.97      0.94      5082
           1       0.67      0.40      0.50       729

    accuracy                           0.90      5811
   macro avg       0.79      0.68      0.72      5811
weighted avg       0.89      0.90      0.89      5811

Precision-Recall AUC: 0.46
Balanced accuaracy: 0.68
Wall time: 1min 2s
```

- Model: Naive Bayes

Gaussian NB Hyperparameter Tuning with unbalance dataset

In [85]:
```
%%time
from sklearn.naive_bayes import GaussianNB

param_grid = {'var_smoothing': [1.0, 2.0, 3.0, 4.0]}

gnb = GaussianNB()

gnb = GridSearchCV(gnb, param_grid, scoring='recall', cv=10, verbose=1, n_jobs=-1)
gnb.fit(X_train, y_train)

params_optimal = gnb.best_params_

print("Best Score (accuracy): %f" % gnb.best_score_)
print("Optimal Hyperparameter Values: ", params_optimal)
```

```
Fitting 10 folds for each of 4 candidates, totalling 40 fits
Best Score (accuracy): 0.603839
Optimal Hyperparameter Values:  {'var_smoothing': 1.0}
Wall time: 4.58 s
```

Gaussian NB optimal parameters

In [86]:
```
# Train the Optimal Guassian NB Model
gaussianNB_clf = GaussianNB(var_smoothing=1.0)

gaussianNB_clf.fit(X_train, y_train)
y_train_predicted = gaussianNB_clf.predict(X_train)
y_test_predicted = gaussianNB_clf.predict(X_test)

print_report_classifiers(gaussianNB_clf, y_train_predicted, y_test_predicted,
                         auc=True, conf_train=False)
```

```
Training Accuracy: 0.8365
Test Accuracy: 0.8339

Test Confusion Matrix:
[[4372  710]
 [ 255  474]]
              precision    recall  f1-score   support

           0       0.94      0.86      0.90      5082
           1       0.40      0.65      0.50       729
```

```
    accuracy                           0.83      5811
   macro avg       0.67      0.76      0.70      5811
weighted avg       0.88      0.83      0.85      5811

Precision-Recall AUC: 0.45
Balanced accuaracy: 0.76
```

Bernoulli NB with unblanced dataset

In [87]:
```python
%%time
from sklearn.naive_bayes import BernoulliNB

param_grid = {'alpha': [1, 2, 3, 4, 5, 6]}

bnb = BernoulliNB()

bnb = GridSearchCV(bnb, param_grid, scoring='recall', cv=10, verbose=1, n_jobs=-1)
bnb.fit(X_train, y_train)

params_optimal = bnb.best_params_

print("Best Score (accuracy): %f" % bnb.best_score_)
print("Optimal Hyperparameter Values: ", params_optimal)
```

```
Fitting 10 folds for each of 6 candidates, totalling 60 fits
Best Score (accuracy): 0.480786
Optimal Hyperparameter Values:  {'alpha': 1}
Wall time: 908 ms
```

In [88]:
```python
# Train the Optimal Bernoulli NB Model
bernoulliNB_clf = BernoulliNB(alpha=2)
bernoulliNB_clf.fit(X_train, y_train)

y_train_predicted = bernoulliNB_clf.predict(X_train)
y_test_predicted = bernoulliNB_clf.predict(X_test)

print_report_classifiers(bernoulliNB_clf, y_train_predicted, y_test_predicted,
                         auc=True, conf_train=False)
```

```
Training Accuracy: 0.8865
Test Accuracy: 0.8881

Test Confusion Matrix:
[[4784  298]
 [ 352  377]]
              precision    recall  f1-score   support

           0       0.93      0.94      0.94      5082
           1       0.56      0.52      0.54       729

    accuracy                           0.89      5811
   macro avg       0.74      0.73      0.74      5811
weighted avg       0.88      0.89      0.89      5811

Precision-Recall AUC: 0.54
Balanced accuaracy: 0.73
```

Gaussian NB with SMOTE

In [89]:
```python
%%time
from sklearn.naive_bayes import GaussianNB

param_grid = {'var_smoothing': [10,100,1000,1001]}
```

```
gnb = GaussianNB()

gnb = GridSearchCV(gnb, param_grid, scoring='f1', cv=10, verbose=1, n_jobs=-1)
gnb.fit(X_train_SMOTE, y_train_SMOTE)

params_optimal = gnb.best_params_

print("Best Score (accuracy): %f" % gnb.best_score_)
print("Optimal Hyperparameter Values: ", params_optimal)
```

```
Fitting 10 folds for each of 4 candidates, totalling 40 fits
Best Score (accuracy): 0.792028
Optimal Hyperparameter Values:  {'var_smoothing': 10}
Wall time: 1.28 s
```

In [90]:

```
# Train the Optimal Guassian NB Model
gaussianNB_clf = GaussianNB(var_smoothing=100)
gaussianNB_clf.fit(X_train_SMOTE, y_train_SMOTE)

y_train_predicted = gaussianNB_clf.predict(X_train_SMOTE)
y_test_predicted = gaussianNB_clf.predict(X_test)

print_report_classifiers(gaussianNB_clf, y_train_predicted, y_test_predicted,
                        Y_train=y_train_SMOTE, auc=True, conf_train=False)
```

```
Training Accuracy: 0.7777
Test Accuracy: 0.7064

Test Confusion Matrix:
[[3503 1579]
 [ 127  602]]
              precision    recall  f1-score   support

           0       0.97      0.69      0.80      5082
           1       0.28      0.83      0.41       729

    accuracy                           0.71      5811
   macro avg       0.62      0.76      0.61      5811
weighted avg       0.88      0.71      0.76      5811

Precision-Recall AUC: 0.55
Balanced accuaracy: 0.76
```

Bernoulli NB with SMOTE

In [91]:

```
%%time
from sklearn.naive_bayes import BernoulliNB

param_grid = {'alpha': [15,16,17]}

bnb = BernoulliNB()

bnb = GridSearchCV(bnb, param_grid, scoring='f1', cv=10, verbose=1, n_jobs=-1)
bnb.fit(X_train_SMOTE, y_train_SMOTE)

params_optimal = bnb.best_params_

print("Best Score (accuracy): %f" % bnb.best_score_)
print("Optimal Hyperparameter Values: ", params_optimal)
```

```
Fitting 10 folds for each of 3 candidates, totalling 30 fits
Best Score (accuracy): 0.778535
```

```
Optimal Hyperparameter Values:  {'alpha': 16}
Wall time: 915 ms
```

In [92]:
```python
# Train the Optimal Bernoulli NB Model
bernoulliNB_clf = BernoulliNB(alpha=16)
bernoulliNB_clf.fit(X_train_SMOTE, y_train_SMOTE)

y_train_predicted = bernoulliNB_clf.predict(X_train_SMOTE)
y_test_predicted = bernoulliNB_clf.predict(X_test)

print_report_classifiers(bernoulliNB_clf, y_train_predicted, y_test_predicted,
                        Y_train=y_train_SMOTE, auc=True, conf_train=False)
```

```
Training Accuracy: 0.7790
Test Accuracy: 0.7710

Test Confusion Matrix:
[[3926 1156]
 [ 175  554]]
              precision    recall  f1-score   support

           0       0.96      0.77      0.86      5082
           1       0.32      0.76      0.45       729

    accuracy                           0.77      5811
   macro avg       0.64      0.77      0.65      5811
weighted avg       0.88      0.77      0.80      5811

Precision-Recall AUC: 0.54
Balanced accuaracy: 0.77
```

Model: Logistic Regression

LR Hyperparameter runing

In [93]:
```python
%%time
from sklearn.linear_model import LogisticRegression

param_grid = {'solver': ['liblinear', 'newton-cg', 'lbfgs', 'sag', 'saga'],
              'tol': [1e-3, 1e-4], 'max_iter':[150, 200],
              'C': [0.1, 1, 5, 10], 'class_weight':[None, 'balanced']}

lg_reg = LogisticRegression(random_state=42)

lg_reg_cv = GridSearchCV(lg_reg, param_grid, scoring='recall', cv=5)
lg_reg_cv.fit(X_train, y_train)

params_optimal = lg_reg_cv.best_params_

print("Best Score (accuracy): %f" % lg_reg_cv.best_score_)
print("Optimal Hyperparameter Values: ", params_optimal)
```

```
C:\Users\andre\anaconda3\lib\site-packages\sklearn\linear_model\_sag.py:328: Convergence
Warning: The max_iter was reached which means the coef_ did not converge
  warnings.warn("The max_iter was reached which means "
C:\Users\andre\anaconda3\lib\site-packages\sklearn\linear_model\_sag.py:328: Convergence
Warning: The max_iter was reached which means the coef_ did not converge
  warnings.warn("The max_iter was reached which means "
C:\Users\andre\anaconda3\lib\site-packages\sklearn\linear_model\_sag.py:328: Convergence
Warning: The max_iter was reached which means the coef_ did not converge
  warnings.warn("The max_iter was reached which means "
Best Score (accuracy): 0.771408
```

```
Optimal Hyperparameter Values:  {'C': 0.1, 'class_weight': 'balanced', 'max_iter': 150,
'solver': 'liblinear', 'tol': 0.001}
Wall time: 5min 19s
```

Optimal Parameters for LR:

- C: 0.1
- max_iter: 150
- solver: liblinear
- tol: 0.001
- class_weight: Balanced

In [94]:
```
%%time
from sklearn.linear_model import LogisticRegression
# Train the Optimal LR Model
lg_reg_clf = LogisticRegression(solver='liblinear', tol=0.001,
                                max_iter= 150, C=0.1, class_weight='balanced')
lg_reg_clf.fit(X_train, y_train)

y_train_predicted = lg_reg_clf.predict(X_train)
y_test_predicted = lg_reg_clf.predict(X_test)

print_report_classifiers(lg_reg_clf, y_train_predicted, y_test_predicted,
                        auc=True, conf_train=False)
```

```
Training Accuracy: 0.8023
Test Accuracy: 0.7992

Test Confusion Matrix:
[[4075 1007]
 [ 160  569]]
              precision    recall  f1-score   support

           0       0.96      0.80      0.87      5082
           1       0.36      0.78      0.49       729

    accuracy                           0.80      5811
   macro avg       0.66      0.79      0.68      5811
weighted avg       0.89      0.80      0.83      5811

Precision-Recall AUC: 0.60
Balanced accuaracy: 0.79
Wall time: 242 ms
```

LR hyperparameter tuning with SMOTE

In [95]:
```
%%time
from sklearn.linear_model import LogisticRegression

param_grid = {'solver': ['liblinear', 'newton-cg', 'lbfgs', 'sag', 'saga'],
              'tol': [1e-3, 1e-4], 'max_iter':[110,150],'C': [1,5,6]}

lg_reg = LogisticRegression(random_state=42)

lg_reg_cv = GridSearchCV(lg_reg, param_grid, scoring='recall', cv=5)
lg_reg_cv.fit(X_train_SMOTE, y_train_SMOTE)

params_optimal = lg_reg_cv.best_params_

print("Best Score (accuracy): %f" % lg_reg_cv.best_score_)
print("Optimal Hyperparameter Values: ", params_optimal)
```

```
Best Score (accuracy): 0.798037
Optimal Hyperparameter Values:  {'C': 1, 'max_iter': 110, 'solver': 'liblinear', 'tol': 
0.001}
Wall time: 2min 52s
```

Optimal Parameters for LS SMOTE:

- C: 1
- max_iter: 110
- solver: liblinear
- tol: 0.001

In [96]:
```
# Train the Optimal LR Model

lg_reg_clf = LogisticRegression(solver='liblinear', tol=0.001,
                                max_iter= 110, C=1)
lg_reg_clf.fit(X_train_SMOTE, y_train_SMOTE)

y_train_predicted = lg_reg_clf.predict(X_train_SMOTE)
y_test_predicted = lg_reg_clf.predict(X_test)

print_report_classifiers(lg_reg_clf, y_train_predicted, y_test_predicted,
                        Y_train=y_train_SMOTE, auc=True, conf_train=False)
```

```
Training Accuracy: 0.8052
Test Accuracy: 0.8002

Test Confusion Matrix:
[[4087  995]
 [ 166  563]]
              precision    recall  f1-score   support

           0       0.96      0.80      0.88      5082
           1       0.36      0.77      0.49       729

    accuracy                           0.80      5811
   macro avg       0.66      0.79      0.68      5811
weighted avg       0.89      0.80      0.83      5811

Precision-Recall AUC: 0.61
Balanced accuaracy: 0.79
```

- Model: Support Vector Machine

Implement LinearSVC with default values

In [97]:
```
from sklearn.svm import LinearSVC, SVC

# Implement Linear SVC with default paramenters with CLASS WEIGHT
linear_svc_clf = LinearSVC(random_state=42)
linear_svc_clf.fit(X_train, y_train)

# Prediction of training set
y_train_predicted = linear_svc_clf.predict(X_train)
# Prediction of test set
y_test_predicted = linear_svc_clf.predict(X_test)

print_report_classifiers(linear_svc_clf, y_train_predicted, y_test_predicted,
                         auc=False, conf_train=False)
```

```
Training Accuracy: 0.9035
Test Accuracy: 0.9071

Test Confusion Matrix:
[[4998   84]
 [ 456  273]]
              precision    recall  f1-score   support

           0       0.92      0.98      0.95      5082
           1       0.76      0.37      0.50       729

    accuracy                           0.91      5811
   macro avg       0.84      0.68      0.73      5811
weighted avg       0.90      0.91      0.89      5811

Balanced accuaracy: 0.68
```

```
C:\Users\andre\anaconda3\lib\site-packages\sklearn\svm\_base.py:985: ConvergenceWarning:
Liblinear failed to converge, increase the number of iterations.
  warnings.warn("Liblinear failed to converge, increase "
```

Hyperparameter tunning for LinearSVC

In [ ]:
```
%%time
# Hyperparameter tunning for the LinearSVC
param_grid = {'C': [1, 10, 100],
              'max_iter':[1000, 2000, 3000],
              'tol': [0.001, 0.0001],
              'penalty': ['l1', 'l2'],
              'class_weight': [None, 'balanced']
              }

clf_svc = LinearSVC(loss="squared_hinge", random_state=42, dual=False)
clf_svc_cv = GridSearchCV(clf_svc, param_grid, scoring='recall', cv=5, verbose=1, n_job
clf_svc_cv.fit(X_train, y_train.ravel())

params_optimal_svc = clf_svc_cv.best_params_
print("Best Score (accuracy): %f" % clf_svc_cv.best_score_)
print("Optimal Hyperparameter Values: ", params_optimal_svc)
print("\n")
```

Optimal Parameters for LinearSVC:

- C: 1
- max_iter: 1000
- tol: 0.001
- class_weight: balanced
- penalty: l1
- dual: False

LinearSVC with optimal values - imbalanced data

In [98]:
```
%%time

linear_svc_clf = LinearSVC(C=1, max_iter=1000, tol=0.001,
                           loss="squared_hinge", random_state=42,
                           dual=False, class_weight='balanced', penalty='l1')

# train LienarSVC model
linear_svc_clf.fit(X_train, y_train)
```

```
y_train_predicted = linear_svc_clf.predict(X_train)
y_test_predicted = linear_svc_clf.predict(X_test)

print_report_classifiers(linear_svc_clf, y_train_predicted,
                         y_test_predicted, auc=False, conf_train=False)
```

```
Training Accuracy: 0.8063
Test Accuracy: 0.8030

Test Confusion Matrix:
[[4102  980]
 [ 165  564]]
              precision    recall  f1-score   support

           0       0.96      0.81      0.88      5082
           1       0.37      0.77      0.50       729

    accuracy                           0.80      5811
   macro avg       0.66      0.79      0.69      5811
weighted avg       0.89      0.80      0.83      5811

Balanced accuaracy: 0.79
Wall time: 320 ms
```

LinearSVC optimal values - SMOTE

In [99]:
```
# Implement Linear SVC optimal parameters with SMOTE
linear_svc_clf = LinearSVC(C=1, max_iter=1000, tol=0.001,
                           loss="squared_hinge", random_state=42,
                           dual=False, penalty='l1')

# train LienarSVC model
linear_svc_clf.fit(X_train_SMOTE, y_train_SMOTE)

y_train_predicted = linear_svc_clf.predict(X_train_SMOTE)
y_test_predicted = linear_svc_clf.predict(X_test)

print_report_classifiers(linear_svc_clf, y_train_predicted,
                         y_test_predicted, Y_train=y_train_SMOTE,
                         auc=False, conf_train=False)
```

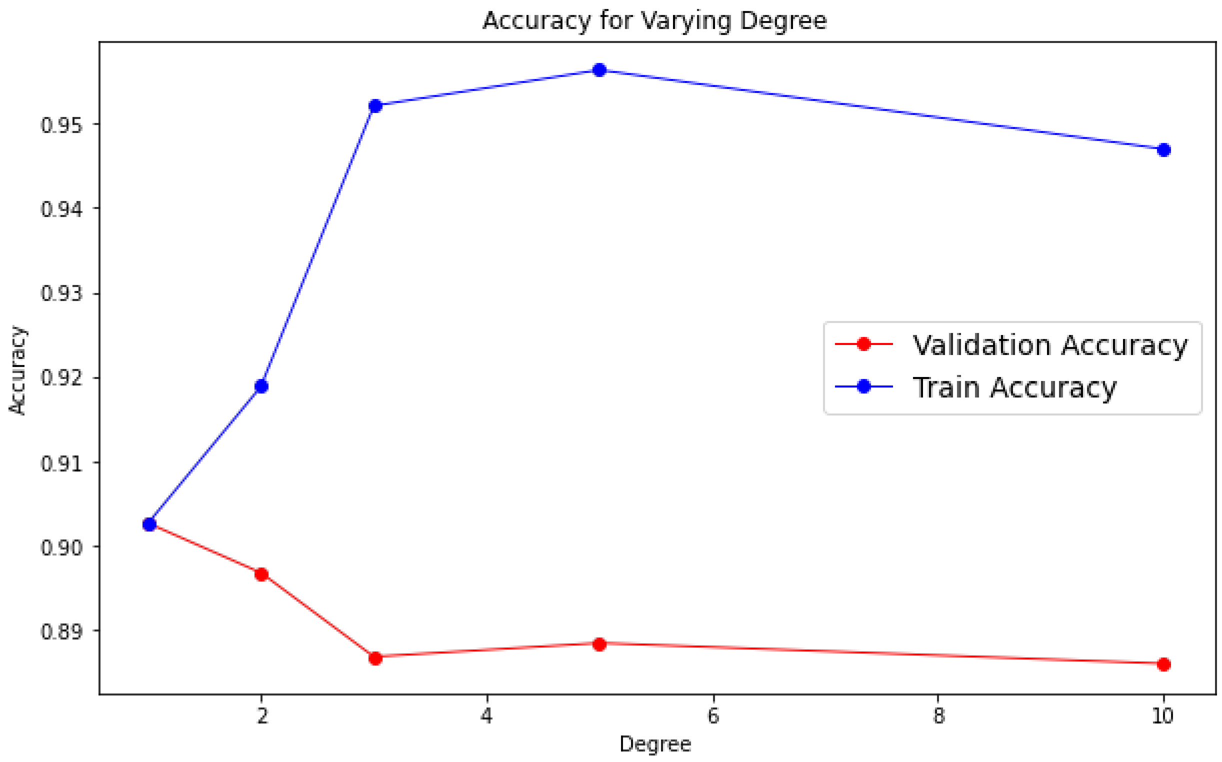
```
Training Accuracy: 0.8053
Test Accuracy: 0.8021

Test Confusion Matrix:
[[4101  981]
 [ 169  560]]
              precision    recall  f1-score   support

           0       0.96      0.81      0.88      5082
           1       0.36      0.77      0.49       729

    accuracy                           0.80      5811
   macro avg       0.66      0.79      0.69      5811
weighted avg       0.89      0.80      0.83      5811

Balanced accuaracy: 0.79
```

LinearSVC seems to be fitting the data set. There is barely no difference in the performance in the train set and test set. However the results show that the model does a better job classifying class 0 (patients who didn't or enconuter high risk reactions from the vaccine) due to the dataset being unbalanced.

Let's see how the dataset performs when we use **polynomial kernels with SVM**:

Hyperparameter tunning for polynomial SVM - Finding Optimal degree

In [ ]:
```
%%time

# Split data set into train and test set
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.20, random_state

# Split Training data into Traing and Validation Fold
X_train_fold, X_val_fold, y_train_fold, y_val_fold = train_test_split(X_train, y_train,

# Scale the train and test set
scaler = StandardScaler()
scaler.fit(X_train)

X_train = scaler.transform(X_train)

degreeList = [1, 2, 3, 5]

accuracy_train, accuracy_val = [], []

for degree in degreeList:

    model = SVC(C=10, kernel='poly', degree=degree, gamma='auto')

    model.fit(X_train_fold, y_train_fold)

    # Make prediction
    y_train_predicted = model.predict(X_train_fold)
    y_val_predicted = model.predict(X_val_fold)

    accuracy_train.append(model.score(X_train_fold, y_train_fold))
    accuracy_val.append(model.score(X_val_fold, y_val_fold))


plt.figure(figsize=(10, 6))
plt.plot(degreeList, accuracy_val, "ro-", alpha=1.0, linewidth=1.0, label="Validation A
plt.plot(degreeList, accuracy_train, "bo-", alpha=1.0, linewidth=1.0, label="Train Accu

plt.legend(loc="best", fontsize=14)
plt.xlabel("Degree")
plt.ylabel("Accuracy")
plt.title("Accuracy for Varying Degree")
plt.show()


# Find the value of degree that gives max validation accuracy
j = 0
max_val_accuracy = accuracy_val[j]
optimal_degree = 1

for i in degreeList:
    if(accuracy_val[j] > max_val_accuracy):
        max_val_accuracy = accuracy_val[j]
        optimal_degree = i
    j +=1

print("Optimal Degree: ", optimal_degree)
print("\n")
```



Optimal Degree: 1

- Model: Multilayer Perceptron

Hyperparameter tuning MLP

In [ ]:
```
%%time

from sklearn.neural_network import MLPClassifier

param_grid = {'hidden_layer_sizes': [(5,), (10,), (50,), (100,), (150,)],
              'activation':['logistic', 'relu', 'tanh'],
              'alpha': (0.1, 0.01, 0.001),
              'tol': (0.001, 0.0001),
              'learning_rate_init':[0.1, 0.01, 0.001],
              'learning_rate': ['adaptive', 'constant']}

clf_mlp = MLPClassifier(solver='adam', early_stopping=False)

clf_mlp_cv = GridSearchCV(clf_mlp, param_grid, scoring='f1', cv=5, verbose=1, n_jobs=-1
clf_mlp_cv.fit(X_train, y_train)


params_optimal_mlp = clf_mlp_cv.best_params_

print("Best Score (accuracy): %f" % clf_mlp_cv.best_score_)

print("Optimal Hyperparameter Values: ", params_optimal_mlp)
```

Wall time: 1h 28min 50s

For MLP we decided to use solver='adam' due to recommendations by sklearn documentation regarding the size of the dataset. Early_stopping = True was also used to aovid overtraining and overfitting on the training set.

Optimal Parameters for LinearSVC:

- hidden_layer_sizes: 50
- activation: logistic
- alpha: 0.1
- tol: 0.0001
- learning_rate_init: 0.01
- learning_rate: adaptive

MLP with optimal parameters

In [100…
```
%%time

from sklearn.neural_network import MLPClassifier


mlp_clf = MLPClassifier(random_state=42, hidden_layer_sizes=(50,), alpha=0.1, solver='a
                      learning_rate='adaptive', activation='logistic', verbose=False,
                      learning_rate_init=0.01, tol=0.0001, early_stopping=True)

mlp_clf.fit(X_train, y_train)


print("No. of Iterations:", mlp_clf.n_iter_ )

y_train_predicted = mlp_clf.predict(X_train)
y_test_predicted = mlp_clf.predict(X_test)

print_report_classifiers(mlp_clf, y_train_predicted, y_test_predicted,
                        auc=True, conf_train=False)
```

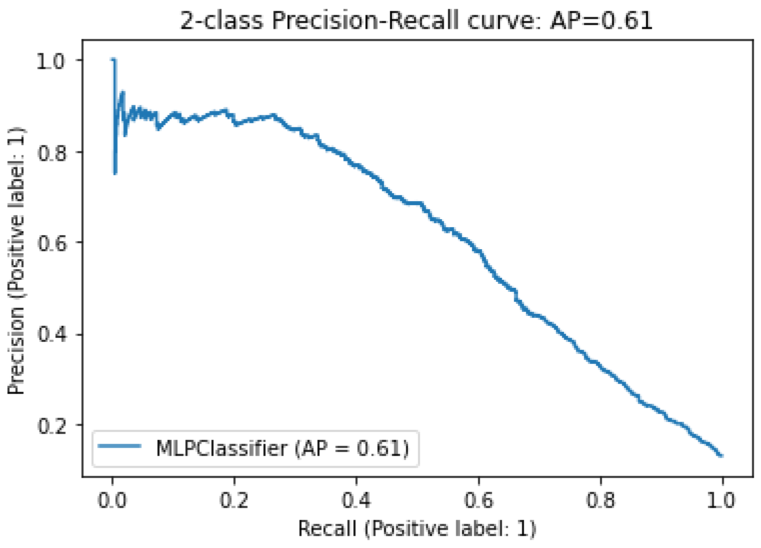
```
No. of Iterations: 24

Training Accuracy: 0.9074
Test Accuracy: 0.9145

Test Confusion Matrix:
[[5004   78]
 [ 419  310]]
              precision    recall  f1-score   support

           0       0.92      0.98      0.95      5082
           1       0.80      0.43      0.56       729

    accuracy                           0.91      5811
   macro avg       0.86      0.70      0.75      5811
weighted avg       0.91      0.91      0.90      5811

Precision-Recall AUC: 0.64
Balanced accuaracy: 0.70
Wall time: 2.64 s
```

MLP optimal parameters with SMOTE

In [101…
```
from sklearn.metrics import precision_recall_curve, auc

mlp_clf_SMOTE = MLPClassifier(random_state=42, hidden_layer_sizes=(50,), alpha=0.1, sol
                      learning_rate='adaptive', activation='logistic', verbose=False,
                      learning_rate_init=0.01, tol=0.0001, early_stopping=True)
```

```
mlp_clf_SMOTE.fit(X_train_SMOTE, y_train_SMOTE);

print("No. of Iterations:", mlp_clf_SMOTE.n_iter_ )

# perdiction on training set
y_train_predicted = mlp_clf_SMOTE.predict(X_train_SMOTE)
# predictions on test set
y_test_predicted = mlp_clf_SMOTE.predict(X_test)

print_report_classifiers(mlp_clf_SMOTE, y_train_predicted, y_test_predicted,
                         Y_train =y_train_SMOTE, auc=True, conf_train=True)
```

```
No. of Iterations: 54

Training Accuracy: 0.8470
Test Accuracy: 0.8143

Test Confusion Matrix:
[[4180  902]
 [ 177  552]]
              precision    recall  f1-score   support

           0       0.96      0.82      0.89      5082
           1       0.38      0.76      0.51       729

    accuracy                           0.81      5811
   macro avg       0.67      0.79      0.70      5811
weighted avg       0.89      0.81      0.84      5811

Precision-Recall AUC: 0.61
Balanced accuaracy: 0.79
```

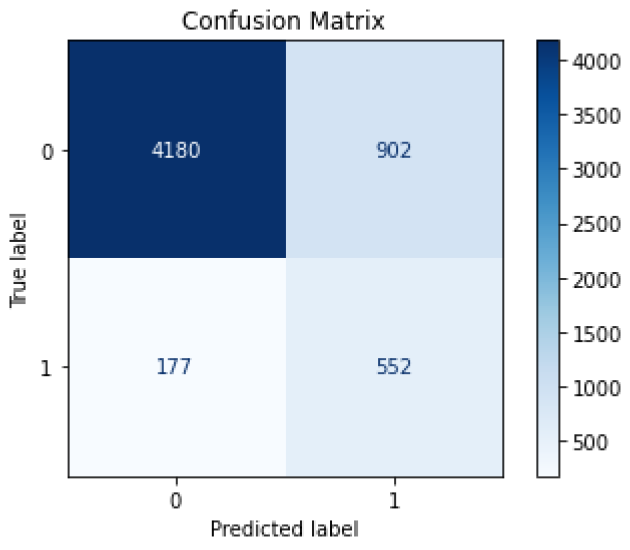


In [102…
```
from sklearn.model_selection import cross_val_score

# validating our model with train set without SMOTE using cross-val
# to make sure the model is not overfitting the dataset. We use f1 score
#
from imblearn.pipeline import make_pipeline

def evaluate_model(X_train, y_train, model):

    model.fit(X_train, y_train)
    test_pred = model.predict(X_test)
    scores = cross_val_score(model, X_train, y_train, cv=3, scoring="f1")
    scores_ba = cross_val_score(model, X_train, y_train, cv=3, scoring="balanced_accura
    diff = scores.mean() - f1_score(y_test, test_pred)


    print(f"Training Accuracy:{model.score(X_train, y_train)}")
    print(f"Testing Accuracy: {model.score(X_test, y_test)}")

    print(f"\nTest F1-score: {f1_score(y_test, test_pred)}")
    print(f"Cross-Val F1-score: {scores.mean()} +/- {scores.std()}")
    print(f"\nTest Balance accuracy: {balanced_accuracy_score(y_test, test_pred)}")
    print(f"Cross-Val Balance accuracy: {scores_ba.mean()} +/- {scores_ba.std()}")

pipeline = make_pipeline(smt, mlp_clf_SMOTE)
evaluate_model(X_train, y_train, pipeline)
```

```
Training Accuracy:0.8345667326391877
Testing Accuracy: 0.814317673378076

Test F1-score: 0.5057260650480989
Cross-Val F1-score: 0.505379471856166 +/- 0.01201256964873245

Test Balance accuracy: 0.7898562343006788
Cross-Val Balance accuracy: 0.7665827330320774 +/- 0.011037901793746304
```

In [103…

```
disp = plot_confusion_matrix(mlp_clf_SMOTE, X_test, y_test, cmap=plt.cm.Blues)
disp.ax_.set_title('Confusion Matrix')
plt.show()
```



- Model: Random Forest

In [104…

```
%%time
from sklearn.ensemble import RandomForestClassifier

rfclf = RandomForestClassifier(random_state=42)
rfclf.fit(X_train_SMOTE, y_train_SMOTE)

y_train_predicted = rfclf.predict(X_train_SMOTE)
y_test_predicted = rfclf.predict(X_test)

print_report_classifiers(rfclf, y_train_predicted, y_test_predicted,
                         Y_train=y_train_SMOTE, auc=True, conf_train=False)
```

```
Training Accuracy: 0.9984
```

```
Test Accuracy: 0.8935

Test Confusion Matrix:
[[4819  263]
 [ 356  373]]
              precision    recall  f1-score   support

           0       0.93      0.95      0.94      5082
           1       0.59      0.51      0.55       729

    accuracy                           0.89      5811
   macro avg       0.76      0.73      0.74      5811
weighted avg       0.89      0.89      0.89      5811

Precision-Recall AUC: 0.58
Balanced accuaracy: 0.73
Wall time: 7.98 s
```

Random Forest Hyperparameter Tuning

```
In [ ]: #List Hyperparameters
        bootstrap = [True, False]
        max_depth = [20, 50, 100, None]
        max_features = ['auto', 'sqrt']
        min_samples_leaf = [1, 4]
        min_samples_split = [2, 10]
        n_estimators = [1000, 2000]

        `r
        #Convert to dictionary
        hyperparameters = dict(bootstrap=bootstrap,
                               max_depth=max_depth, max_features = max_features,
                              min_samples_leaf = min_samples_leaf, min_samples_split = min_samp
                              n_estimators = n_estimators)

        #Create new RF object
        rfclf2 = RandomForestClassifier(random_state=42)

        #Use GridSearch
        clf = GridSearchCV(rfclf2, hyperparameters, cv=10)

        #Fit the model
        best_model = clf.fit(X_train_SMOTE, y_train_SMOTE)

        #Print The value of best Hyperparameters
        print('Best bootstrap:', best_model.best_estimator_.get_params()['bootstrap'])
        print('Best max_depth:', best_model.best_estimator_.get_params()['max_depth'])
        print('Best max_features:', best_model.best_estimator_.get_params()['max_features'])
        print('Best min_samples_leaf:', best_model.best_estimator_.get_params()['min_samples_le
        print('Best min_samples_split:', best_model.best_estimator_.get_params()['min_samples_s
        print('n_estimators:', best_model.best_estimator_.get_params()['n_estimators'])
```

Optimal Parameters for Random Forest (SMOTE):

- bootstrap: False
- max_depth: 50
- max_features: auto
- min_samples_leaf: 1
- min_samples_split: 10
- n_estimators: 2000

RF optimal parameter with SMOTE

```
In [105…
%%time

rfclffinal = RandomForestClassifier(random_state=42, bootstrap=False, max_depth = 50,
                                    max_features = 'auto', min_samples_leaf = 1,
                                    min_samples_split = 10, n_estimators = 2000)

rfclffinal.fit(X_train_SMOTE, y_train_SMOTE)

y_train_predicted = rfclffinal.predict(X_train_SMOTE)
y_test_predicted = rfclffinal.predict(X_test)

print_report_classifiers(rfclffinal, y_train_predicted, y_test_predicted,
                         Y_train=y_train_SMOTE, auc=True, conf_train=False)
```

```
Training Accuracy: 0.9873
Test Accuracy: 0.8993

Test Confusion Matrix:
[[4841  241]
 [ 344  385]]
              precision    recall  f1-score   support

           0       0.93      0.95      0.94      5082
           1       0.62      0.53      0.57       729

    accuracy                           0.90      5811
   macro avg       0.77      0.74      0.76      5811
weighted avg       0.89      0.90      0.90      5811

Precision-Recall AUC: 0.60
Balanced accuaracy: 0.74
Wall time: 3min 39s
```

RF optimal parameter imbalaced data

```
In [106…
%%time
rfclffinal = RandomForestClassifier(random_state=42, bootstrap=False,max_depth = 50,
                                    max_features = 'auto', min_samples_leaf = 1,
                                    min_samples_split = 10, n_estimators = 2000,
                                   class_weight='balanced')

rfclffinal.fit(X_train, y_train)

y_train_predicted = rfclffinal.predict(X_train)
y_test_predicted = rfclffinal.predict(X_test)

print_report_classifiers(rfclffinal, y_train_predicted,
                         y_test_predicted, auc=True, conf_train=False)
```

```
Training Accuracy: 0.9724
Test Accuracy: 0.8887

Test Confusion Matrix:
[[4706  376]
 [ 271  458]]
              precision    recall  f1-score   support

           0       0.95      0.93      0.94      5082
           1       0.55      0.63      0.59       729

    accuracy                           0.89      5811
```

```
   macro avg       0.75      0.78      0.76      5811
weighted avg       0.90      0.89      0.89      5811

Precision-Recall AUC: 0.62
Balanced accuaracy: 0.78
Wall time: 1min 38s
```

RF optimal parameters with boostrap = True

We decided to use boostrap to help with the imbalanced distribution of classes of our dataset.

In [107…

```
rfclffinal = RandomForestClassifier(random_state=42, bootstrap=True, max_depth = 50,
                                    max_features = 'auto', min_samples_leaf = 1,
                                    min_samples_split = 10, n_estimators = 2000)

rfclffinal.fit(X_train_SMOTE, y_train_SMOTE)

y_train_predicted = rfclffinal.predict(X_train_SMOTE)
y_test_predicted = rfclffinal.predict(X_test)

print_report_classifiers(rfclffinal, y_train_predicted, y_test_predicted,
                         Y_train=y_train_SMOTE, auc=True, conf_train=False)
```

```
Training Accuracy: 0.9739
Test Accuracy: 0.8981

Test Confusion Matrix:
[[4814  268]
 [ 324  405]]
              precision    recall  f1-score   support

           0       0.94      0.95      0.94      5082
           1       0.60      0.56      0.58       729

    accuracy                           0.90      5811
   macro avg       0.77      0.75      0.76      5811
weighted avg       0.89      0.90      0.90      5811

Precision-Recall AUC: 0.62
Balanced accuaracy: 0.75
```

In [108…

```
%%time
rfclffinal = RandomForestClassifier(random_state=42, bootstrap=True, max_depth = 50,
                                    max_features = 'auto', min_samples_leaf = 1,
                                    min_samples_split = 10, n_estimators = 2000,
                                   class_weight='balanced')

rfclffinal.fit(X_train, y_train)

y_train_predicted = rfclffinal.predict(X_train)
y_test_predicted = rfclffinal.predict(X_test)

print_report_classifiers(rfclffinal, y_train_predicted,
                         y_test_predicted, auc=True, conf_train=False)
```

```
Training Accuracy: 0.9639
Test Accuracy: 0.9007

Test Confusion Matrix:
[[4790  292]
 [ 285  444]]
              precision    recall  f1-score   support
```

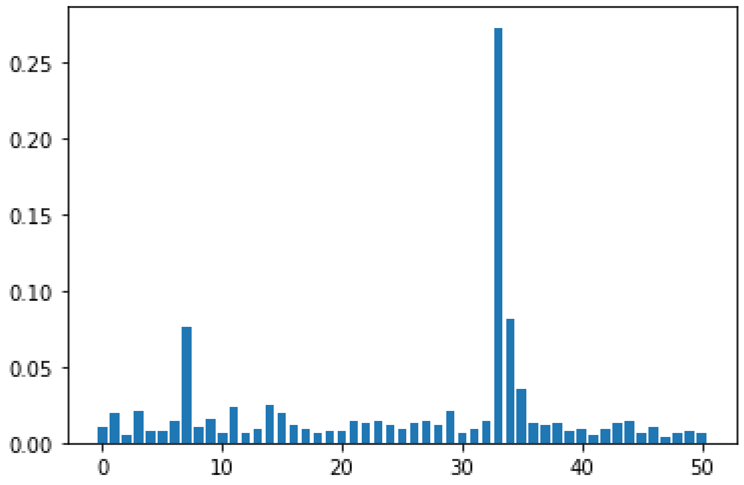
```
           0       0.94      0.94      0.94      5082
           1       0.60      0.61      0.61       729

    accuracy                           0.90      5811
   macro avg       0.77      0.78      0.77      5811
weighted avg       0.90      0.90      0.90      5811

Precision-Recall AUC: 0.64
Balanced accuaracy: 0.78
Wall time: 1min 8s
```

In [109…

```
%%time
from matplotlib import pyplot

# get feature importance from RF
importance = rfclffinal.feature_importances_

# summarize feature importance
for i,v in enumerate(importance):
        print('Feature: %0d, Score: %.5f' % (i,v))

# plot feature importance
pyplot.bar([x for x in range(len(importance))], importance)
pyplot.show()
```

```
Feature: 0, Score: 0.01072
Feature: 1, Score: 0.01932
Feature: 2, Score: 0.00520
Feature: 3, Score: 0.02128
Feature: 4, Score: 0.00782
Feature: 5, Score: 0.00759
Feature: 6, Score: 0.01451
Feature: 7, Score: 0.07585
Feature: 8, Score: 0.01054
Feature: 9, Score: 0.01570
Feature: 10, Score: 0.00662
Feature: 11, Score: 0.02366
Feature: 12, Score: 0.00666
Feature: 13, Score: 0.00947
Feature: 14, Score: 0.02455
Feature: 15, Score: 0.02008
Feature: 16, Score: 0.01218
Feature: 17, Score: 0.00849
Feature: 18, Score: 0.00593
Feature: 19, Score: 0.00732
Feature: 20, Score: 0.00818
Feature: 21, Score: 0.01483
Feature: 22, Score: 0.01281
Feature: 23, Score: 0.01410
Feature: 24, Score: 0.01220
Feature: 25, Score: 0.00897
Feature: 26, Score: 0.01283
Feature: 27, Score: 0.01408
Feature: 28, Score: 0.01224
Feature: 29, Score: 0.02054
Feature: 30, Score: 0.00690
Feature: 31, Score: 0.00896
Feature: 32, Score: 0.01416
Feature: 33, Score: 0.27300
Feature: 34, Score: 0.08124
Feature: 35, Score: 0.03576
Feature: 36, Score: 0.01257
Feature: 37, Score: 0.01191
Feature: 38, Score: 0.01320
```

```
Feature: 39, Score: 0.00706
Feature: 40, Score: 0.00841
Feature: 41, Score: 0.00485
Feature: 42, Score: 0.00847
Feature: 43, Score: 0.01282
Feature: 44, Score: 0.01428
Feature: 45, Score: 0.00612
Feature: 46, Score: 0.01055
Feature: 47, Score: 0.00416
Feature: 48, Score: 0.00658
Feature: 49, Score: 0.00786
Feature: 50, Score: 0.00690
```



```
Wall time: 731 ms
```

Feature 7, 33 and Feature 34 are most important, these are age and numdays in hospital. However some symptoms are still important.

```
In [110…  df_merge.columns
```

```
Out[110…  Index(['Arthralgia', 'Asthenia', 'COVID-19', 'Chills', 'Cough', 'Diarrhoea',
                 'Dizziness', 'Dyspnoea', 'Erythema', 'Fatigue', 'Feeling abnormal',
                 'Headache', 'Hyperhidrosis', 'Hypoaesthesia', 'Injection site erythema',
                 'Injection site pain', 'Injection site pruritus',
                 'Injection site swelling', 'Injection site warmth', 'Lymphadenopathy',
                 'Malaise', 'Myalgia', 'Nausea', 'Pain', 'Pain in extremity',
                 'Paraesthesia', 'Pruritus', 'Pyrexia', 'Rash',
                 'SARS-CoV-2 test negative', 'SARS-CoV-2 test positive', 'Urticaria',
                 'Vomiting', 'AGE_YRS', 'NUMDAYS', 'target', 'Gender', 'MODERNA',
                 'PFIZER\BIONTECH', 'JANSSEN', 'allergi', 'asthma', 'blood', 'condit',
                 'diabet', 'hypertens', 'hypothyroid', 'medic', 'pressur', 'relev',
                 'penicillin', 'sulfa'],
                dtype='object')
```

Model: Gradient Boosting

GB with unbalanced dataset

%%time from sklearn.ensemble import GradientBoostingClassifier param_grid = {#'learning_rate': [0.05,0.1,0.2], #'n_estimators': [100, 300, 500, 1000], #'max_depth': list(range(1,11)), #'min_samples_split':list(range(2,15)), #'min_samples_leaf': [5,10,20,30] } grad_boost = GradientBoostingClassifier(random_state=42, n_estimators=100, learning_rate=0.1, max_depth=8, min_samples_leaf=30, min_samples_split=2) grad_boost_cv = GridSearchCV(grad_boost, param_grid, scoring='f1', cv=5, n_jobs=-1, verbose=3) grad_boost_cv.fit(X_train, y_train) params_optimal = grad_boost_cv.best_params_ print("Best Score (accuracy): %f" % grad_boost_cv.best_score_) print("Optimal Hyperparameter Values: ", params_optimal)

Optimal Parameters for GB with unbalanced dataset f1:

- learning_rate: 0.1
- max_depth: 8
- min_samples_leaf: 30
- min_samples_split: 2
- n_estimators: 300

In [111…

```
%%time
from sklearn.ensemble import GradientBoostingClassifier

# Train the Optimal GB Model
grad_boost_clf = GradientBoostingClassifier(random_state=42, n_estimators=300,
                                             learning_rate=0.1, max_depth=8,
                                            min_samples_leaf=30, min_samples_split=2)

grad_boost_clf.fit(X_train, y_train)

y_train_predicted = grad_boost_clf.predict(X_train)
y_test_predicted = grad_boost_clf.predict(X_test)

print_report_classifiers(grad_boost_clf, y_train_predicted, y_test_predicted,
                         auc=True, conf_train=False)
```

```
Training Accuracy: 0.9449
Test Accuracy: 0.9081

Test Confusion Matrix:
[[4919  163]
 [ 371  358]]
              precision    recall  f1-score   support

           0       0.93      0.97      0.95      5082
           1       0.69      0.49      0.57       729

    accuracy                           0.91      5811
   macro avg       0.81      0.73      0.76      5811
weighted avg       0.90      0.91      0.90      5811

Precision-Recall AUC: 0.63
Balanced accuaracy: 0.73
Wall time: 26.6 s
```

GB with SMOTE

In [112…

```
grad_boost_clf = GradientBoostingClassifier(random_state=42, n_estimators=100,
                                             learning_rate=0.1, max_depth=8,
                                            min_samples_leaf=30, min_samples_split=2)

grad_boost_clf.fit(X_train_SMOTE, y_train_SMOTE)

y_train_predicted = grad_boost_clf.predict(X_train_SMOTE)
y_test_predicted = grad_boost_clf.predict(X_test)

print_report_classifiers(grad_boost_clf, y_train_predicted, y_test_predicted,
                         Y_train=y_train_SMOTE, auc=True, conf_train=False)
```

```
Training Accuracy: 0.9442
Test Accuracy: 0.9026

Test Confusion Matrix:
[[4831  251]
 [ 315  414]]
```

```
              precision    recall  f1-score   support

           0       0.94      0.95      0.94      5082
           1       0.62      0.57      0.59       729

    accuracy                           0.90      5811
   macro avg       0.78      0.76      0.77      5811
weighted avg       0.90      0.90      0.90      5811

Precision-Recall AUC: 0.64
Balanced accuaracy: 0.76
```

- Model: Easy ensemble

Default Values

In [113…

```
%%time
from imblearn.ensemble import EasyEnsembleClassifier

# define model
easy_ensem = EasyEnsembleClassifier(n_estimators=100)

easy_ensem.fit(X_train, y_train)

y_train_predicted = easy_ensem.predict(X_train)
y_test_predicted = easy_ensem.predict(X_test)

print_report_classifiers(easy_ensem, y_train_predicted,
                         y_test_predicted, auc=True, conf_train=False)
```

```
Training Accuracy: 0.8193
Test Accuracy: 0.8126

Test Confusion Matrix:
[[4162  920]
 [ 169  560]]
              precision    recall  f1-score   support

           0       0.96      0.82      0.88      5082
           1       0.38      0.77      0.51       729

    accuracy                           0.81      5811
   macro avg       0.67      0.79      0.70      5811
weighted avg       0.89      0.81      0.84      5811

Precision-Recall AUC: 0.62
Balanced accuaracy: 0.79
Wall time: 1min 39s
```

- Model: AdaBoost

AdaBoost Imbalanced data

In [114…

```
from sklearn.ensemble import AdaBoostClassifier

adaboost_clf = AdaBoostClassifier(n_estimators=100, random_state=42)
adaboost_clf.fit(X_train, y_train)

y_train_predicted = adaboost_clf.predict(X_train)
y_test_predicted = adaboost_clf.predict(X_test)
```

```
print_report_classifiers(adaboost_clf, y_train_predicted,
                         y_test_predicted, auc=True, conf_train=False)
```

```
Training Accuracy: 0.9078
Test Accuracy: 0.9093

Test Confusion Matrix:
[[4964  118]
 [ 409  320]]
              precision    recall  f1-score   support

           0       0.92      0.98      0.95      5082
           1       0.73      0.44      0.55       729

    accuracy                           0.91      5811
   macro avg       0.83      0.71      0.75      5811
weighted avg       0.90      0.91      0.90      5811

Precision-Recall AUC: 0.62
Balanced accuaracy: 0.71
```

AdaBoost SMOTE

In [115…

```
from sklearn.ensemble import AdaBoostClassifier

adaboost_clf = AdaBoostClassifier(n_estimators=100, random_state=42)

adaboost_clf.fit(X_train_SMOTE, y_train_SMOTE)

y_train_predicted = adaboost_clf.predict(X_train_SMOTE)
y_test_predicted = adaboost_clf.predict(X_test)

print_report_classifiers(adaboost_clf, y_train_predicted, y_test_predicted,
                         Y_train=y_train_SMOTE, auc=True, conf_train=False)
```

```
Training Accuracy: 0.9027
Test Accuracy: 0.8720

Test Confusion Matrix:
[[4598  484]
 [ 260  469]]
              precision    recall  f1-score   support

           0       0.95      0.90      0.93      5082
           1       0.49      0.64      0.56       729

    accuracy                           0.87      5811
   macro avg       0.72      0.77      0.74      5811
weighted avg       0.89      0.87      0.88      5811

Precision-Recall AUC: 0.61
Balanced accuaracy: 0.77
```

Clustering

In [116…

```
# let's see data again

# include only patients from the final clean data set
cluster_data_withID = symptoms_data[symptoms_data['VAERS_ID'].isin(list(patients_VAERS_

# Drop "VAERS_ID" to perform clustering
```

```
cluster_data = cluster_data_withID.drop('VAERS_ID', 1)
cluster_data
```

Out[116…

	Arthralgia	Asthenia	COVID-19	Chills	Cough	Diarrhoea	Dizziness	Dyspnoea	Erythema	Fatigu
0	0	0	0	0	0	0	0	1	0	
1	0	0	0	0	0	0	0	0	0	
2	0	0	0	0	0	0	1	0	0	
3	0	0	0	0	0	0	0	0	0	
4	0	0	0	1	0	0	0	0	0	
...	...	...	...	...	...	...	...	...	...	
31497	0	0	0	0	0	0	1	0	0	
31498	0	0	0	0	0	0	0	1	0	
31499	0	0	0	0	0	0	0	0	0	
31500	0	1	0	0	0	0	0	0	0	
31501	0	0	0	1	0	0	0	0	0	

29053 rows × 33 columns

In [117…

```
import numpy as np
import pandas as pd
import seaborn as sns
from matplotlib import pyplot as plt
from sklearn.cluster import KMeans
from sklearn.metrics import silhouette_score
from sklearn.metrics import davies_bouldin_score
```

In [118…

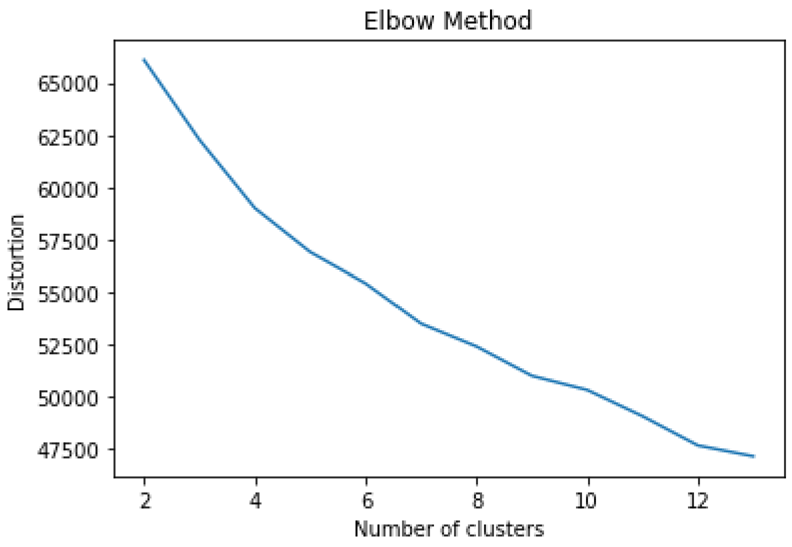
```
def print_interpret_clusters(predicted_labels, df):

    # Number of patients in each cluster
    unique_elements, counts_elements = np.unique(predicted_labels, return_counts = True
    print(np.asarray((unique_elements, counts_elements)))

    # interpret clusters
    interpret_data = df.copy()
    interpret_data['cluster_labels'] = predicted_labels

    # compute the mean of each symptom for each cluster
    df_mean = (interpret_data.groupby('cluster_labels').mean())

    results = pd.DataFrame(columns=['Variable', 'Var'])
    for column in df_mean.columns[1:]:
        results.loc[len(results), :] = [column, np.var(df_mean[column])]

    # select the 10 most recurrent symptoms across all clusters
    selected_columns = list(results.sort_values('Var', ascending=False,).head(10).Varia
    # plot the mean of the 10 most recurrent symtpoms
    tidy = interpret_data[selected_columns].melt(id_vars='cluster_labels')
    sns.barplot(x='cluster_labels', y='value', hue='variable', data=tidy)
```

- Model: K-Means++ Clustering

In [119…

```
# elbow method to determine number of clusters
wcss = []
for i in range(2, 14):
    kmeans = KMeans(n_clusters=i, init='k-means++', max_iter=300, n_init=10, random_sta
    pred_cl = kmeans.fit_predict(cluster_data)
    print('k={} DB Score: {:.02f}'.format(i, davies_bouldin_score(cluster_data, pred_cl
    wcss.append(kmeans.inertia_)

plt.plot(range(2, 14), wcss)
plt.title('Elbow Method')
plt.xlabel('Number of clusters')
plt.ylabel('Distortion')
plt.show()
```

```
k=2 DB Score: 2.61
k=3 DB Score: 2.40
k=4 DB Score: 2.44
k=5 DB Score: 2.36
k=6 DB Score: 2.41
k=7 DB Score: 2.36
k=8 DB Score: 2.43
k=9 DB Score: 2.42
k=10 DB Score: 2.39
k=11 DB Score: 2.29
k=12 DB Score: 2.25
k=13 DB Score: 2.19
```



In [120…

```
from sklearn.metrics import davies_bouldin_score

# categorize data using optimum number of clusters: 5
kmeans = KMeans(n_clusters=5, init='k-means++', max_iter=300, n_init=10, random_state=4
pred_y_kmeans = kmeans.fit_predict(cluster_data)

# Silhouette Score
print('Silhoutte Score: {}\n'.format(silhouette_score(cluster_data, pred_y_kmeans)))
print('DB Score: {}\n'.format(davies_bouldin_score(cluster_data, pred_y_kmeans)))
```

```
unique_elements, counts_elements = np.unique(pred_y_kmeans, return_counts = True)
print(np.asarray((unique_elements, counts_elements)))
```

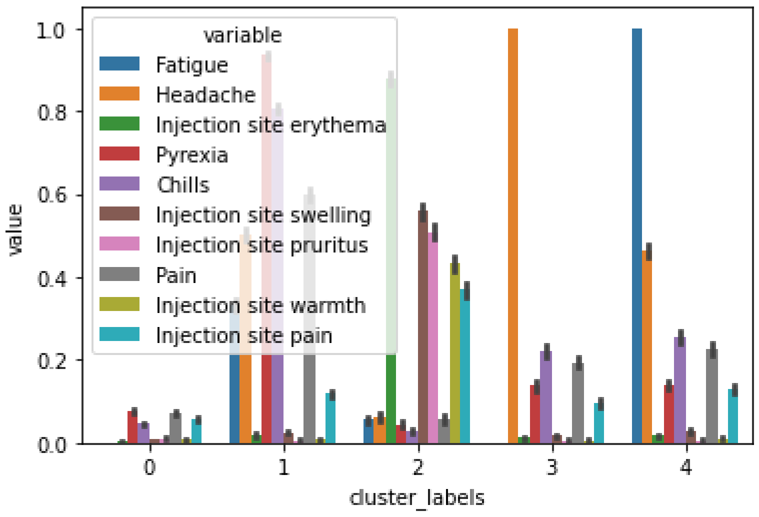
```
Silhoutte Score: 0.12274732447685241

DB Score: 2.355321742778679

[[    0     1     2     3     4]
 [13332  4893  2691  3813  4324]]
```

Interpret Clusters for KMeans++ k = 5

In [127...

```
print_interpret_clusters(pred_y_kmeans, cluster_data)
```

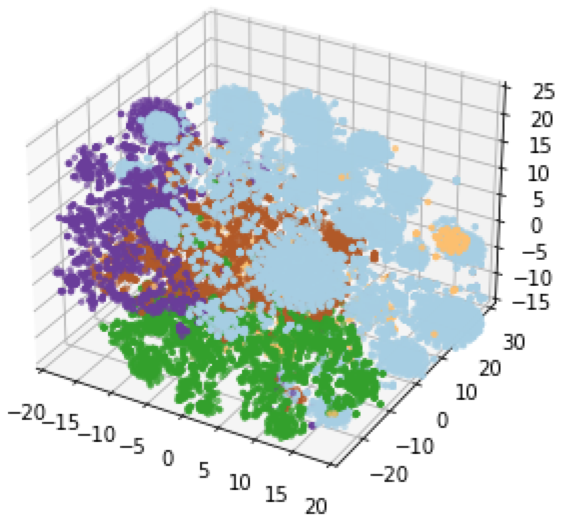
```
[[    0     1     2     3     4]
 [13332  4893  2691  3813  4324]]
```



Visualizing Clusters

In [ ]:

```
%%time
# visualizing clusters with T-SNE: used for high-dimensional data like ours
# visualizing clusters with T-SNE: used for high-dimensional data like ours

from sklearn.manifold import TSNE
from matplotlib.animation import FuncAnimation

def prepare_tsne(n_components, data, kmeans_labels):
    names = ['x', 'y', 'z']
    matrix = TSNE(n_components=n_components).fit_transform(data)
    df_matrix = pd.DataFrame(matrix)
    df_matrix.rename({i:names[i] for i in range(n_components)}, axis=1, inplace=True)
    df_matrix['labels'] = kmeans_labels
    return df_matrix

def plot_animation(df, label_column, name):
    def update(num):
        ax.view_init(200, num)

    N=360
    fig = plt.figure()
    ax = fig.add_subplot(111, projection='3d')
    ax.scatter(tsne_3d_df['x'], tsne_3d_df['y'], tsne_3d_df['z'], c=tsne_3d_df[label_co
               s=6, depthshade=True, cmap='Paired')
    ax.set_zlim(-15, 25)
    ax.set_xlim(-20, 20)
    plt.tight_layout()
    ani = animation.FuncAnimation(fig, update, N, blit=False, interval=50)
    ani.save('{}.gif'.format(name), writer='imagemagick')
    plt.show()

tsne_3d_df = prepare_tsne(3, cluster_data, pred_y_kmeans)
plot_animation(tsne_3d_df, 'labels', 'Kmeans')
# tfne_3d_df
```



In [128…

```
# interpret clusters
interpret_data = cluster_data.copy()
interpret_data['cluster_labels'] = pred_y_kmeans

# How common is each cluster, and which one yields to more deaths?

# Counts of each cluster
interpret_data['cluster_labels'].value_counts(ascending = False)
```

Out[128…

```
0    13332
1     4893
4     4324
3     3813
2     2691
Name: cluster_labels, dtype: int64
```

In [129…

```
# Which one represents more deaths/life threaths/hospital visits?
symptoms_data2 = cluster_data_withID.copy()
symptoms_data2['cluster_labels'] = pred_y_kmeans
cluster_target_data = symptoms_data2.merge(df_all[['VAERS_ID','target', 'AGE_YRS']], on

summary = cluster_target_data.groupby(['cluster_labels'])['target'].sum().rename("targe
# percentage of each cluster at high-risk
pcts = (summary / interpret_data['cluster_labels'].value_counts().sort_index())*100
pcts
```

Out[129…

```
cluster_labels
0    19.074407
1     6.683017
2     1.077666
3     9.834776
4     9.736355
dtype: float64
```

In [130…

```
# In what cluster are the high-risk patients located?
# percentage of all hih-risk patients per cluster
pcts = (summary / summary.sum())*100
pcts
```

Out[130…

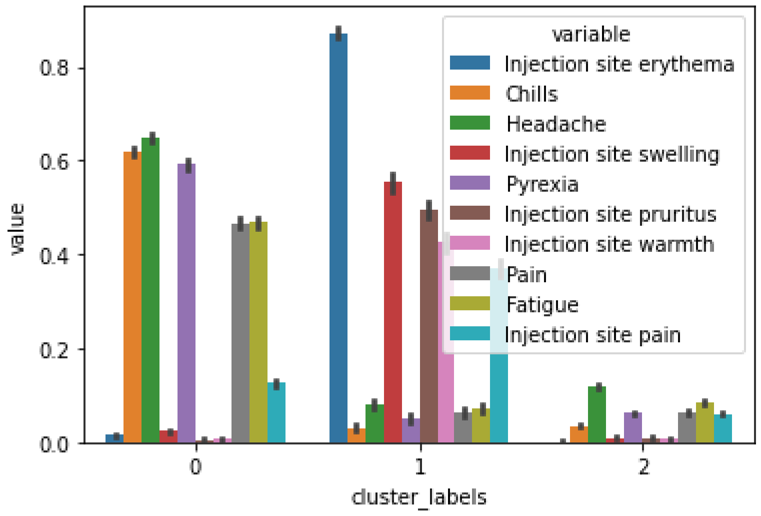
```
cluster_labels
0    68.822733
1     8.849797
2     0.784844
3    10.148850
4    11.393775
Name: target_count, dtype: float64
```

Interpret Clusters for KMeans++ k = 3

In [131…

```
# categorize data using KMeans++ k = 3
kmeans = KMeans(n_clusters=3, init='k-means++', max_iter=300, n_init=10, random_state=4
pred_y_kmeans3 = kmeans.fit_predict(cluster_data)

# Silhouette Score
print('Silhoutte Score: {:.3f}'.format(silhouette_score(cluster_data, pred_y_kmeans3)))
print('DB Score: {:.3f}\n'.format(davies_bouldin_score(cluster_data, pred_y_kmeans3)))

print_interpret_clusters(pred_y_kmeans3, cluster_data)
```

```
Silhoutte Score: 0.129
DB Score: 2.396

[[    0     1     2]
 [ 9589  2797 16667]]
```



- [9589] Cluster 0: chills, headache, fever, chills, pain and fatigue
- [2797] Cluster 1: only injection site reactions
- [16667] Cluster 2: no main symptoms

Further analysis of the K-Means++ clusters was done in R with the dataset and the labels from 3 and 5 clusters. The results are shown in the project report

- Model: BIRCH Clustering

In [121…

```
from sklearn.cluster import Birch
```

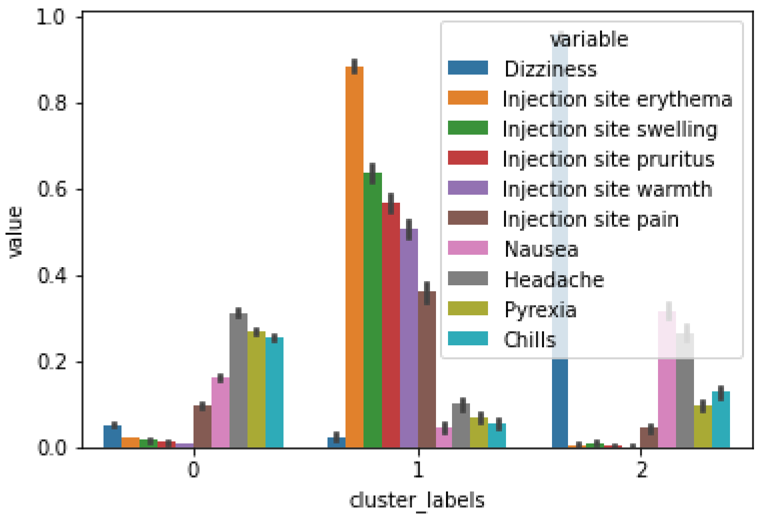
```
brc = Birch(branching_factor=50, n_clusters=3, threshold=1.5)
pred_y_birch = brc.fit_predict(cluster_data)

# Silhouette Score
print('Silhoutte Score: {}'.format(silhouette_score(cluster_data, pred_y_birch)))
print('DB Score: {}\n'.format(davies_bouldin_score(cluster_data, pred_y_birch)))

unique_elements, counts_elements = np.unique(pred_y_birch, return_counts = True)
print(np.asarray((unique_elements, counts_elements)))
```

```
Silhoutte Score: 0.06631019344838797
DB Score: 2.5255455678893637

[[    0     1     2]
 [23830  2338  2885]]
```

In [122…

```
print_interpret_clusters(pred_y_birch, cluster_data)
```

```
[[    0     1     2]
 [23830  2338  2885]]
```

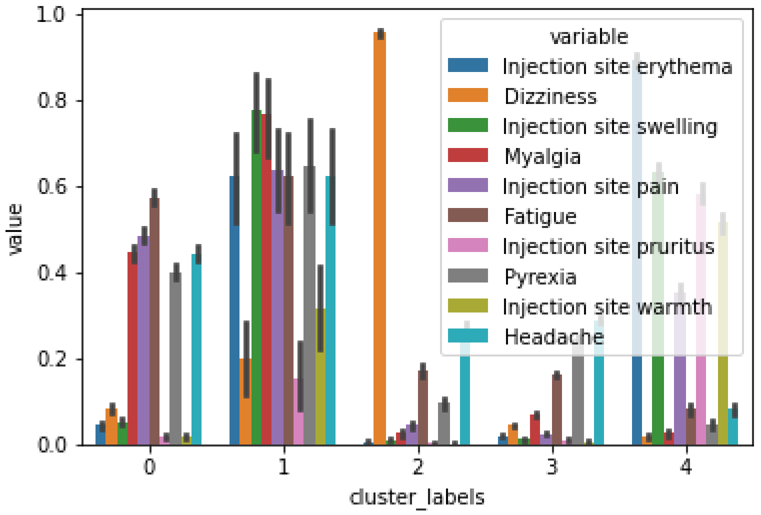


- [13332] Cluster 0, no main symptoms
- [4893] Cluster 1, fever, chills, pain, headache and fatigue
- [2691] Cluster 2, only injection site reactions
- [3813] Cluster 3, mainly headache, ~20% chills, fever and pain
- [4324] Cluster 4, Fatigue, headache, ~20% chills, fever and pain

In [123…

```
brc = Birch(branching_factor=50, n_clusters=5, threshold=1.5)
pred_y_birch5 = brc.fit_predict(cluster_data)

# Silhouette Score
print('Silhoutte Score: {}'.format(silhouette_score(cluster_data, pred_y_birch5)))
print('DB Score: {}\n'.format(davies_bouldin_score(cluster_data, pred_y_birch5)))

print_interpret_clusters(pred_y_birch5, cluster_data)
```

```
Silhoutte Score: 0.07018289456937489
DB Score: 3.069578031196215

[[    0     1     2     3     4]
 [ 3712    85  2885 20118  2253]]
```



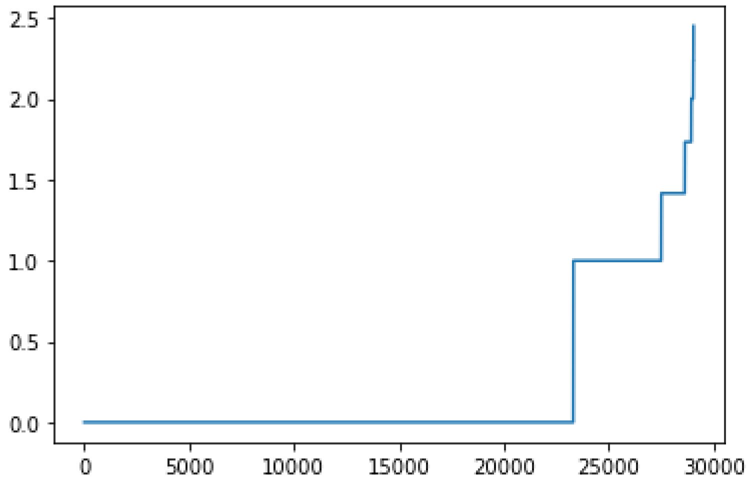
- Model: DBSCAN Clustering

In [124…

```
# first find optimal value of epsilon, which is the point of max curvature
from sklearn.neighbors import NearestNeighbors

neigh = NearestNeighbors(n_neighbors=2)
nbrs = neigh.fit(cluster_data)
distances, indices = nbrs.kneighbors(cluster_data)
distances = np.sort(distances, axis=0)
distances = distances[:,1]
plt.plot(distances)
```

Out[124…

```
[<matplotlib.lines.Line2D at 0x1a0094b2b20>]
```



In [125…

```
from sklearn.cluster import DBSCAN

min_samples = cluster_data.shape[1]+1 #  Rule of thumb; number of dimensions D in the d
dbscan = DBSCAN(eps=1, min_samples=min_samples)
pred_y_dbscan = dbscan.fit_predict(cluster_data)

# Silhouette Score
print('Silhoutte Score: {}'.format(silhouette_score(cluster_data, pred_y_dbscan)))
print('DB Score : {}\n'.format(davies_bouldin_score(cluster_data, pred_y_birch)))

unique_elements, counts_elements = np.unique(pred_y_dbscan, return_counts = True)
print(np.asarray((unique_elements, counts_elements)))
```

```
Silhoutte Score: 0.21293894606573366
DB Score : 2.5255455678893637

[[   -1     0]
 [ 2685 26368]]
```

In [126…

```
#DBSCAN Creates only few clusters... not useful for this purpose
```

Spectral Clustering

In [132…

```
from sklearn.cluster import SpectralClustering
from sklearn.metrics import silhouette_score
```

In [133…

```
%%time

all_predictions=[]

num_cluster = [3, 4, 5]

for n in num_cluster:
    spectral_cl = SpectralClustering(n_clusters=n,
                            assign_labels='discretize', random_state=42)

    pred_clusters = spectral_cl.fit_predict(cluster_data)
    all_predictions.append(pred_clusters)

    # Silhouette Score
    print('Silhouette Score Spectral: {:.3f}'.format(silhouette_score(cluster_data, pre
    print('DB Score : {:.3f}'.format(davies_bouldin_score(cluster_data, pred_clusters))

    # Number of patients in each cluster
    unique_elements, counts_elements = np.unique(pred_clusters, return_counts = True)
    print(np.asarray((unique_elements, counts_elements)))
    print()
```

```
Silhouette Score Spectral: 0.137
DB Score : 2.322
[[    0     1     2]
 [18242  8427  2384]]

Silhouette Score Spectral: 0.136
DB Score : 1.992
[[    0     1     2     3]
 [18242  8425  2382     4]]

Silhouette Score Spectral: 0.104
DB Score : 2.339
[[    0     1     2     3     4]
 [12681  6969  2297  7102     4]]

Wall time: 33min 8s
```

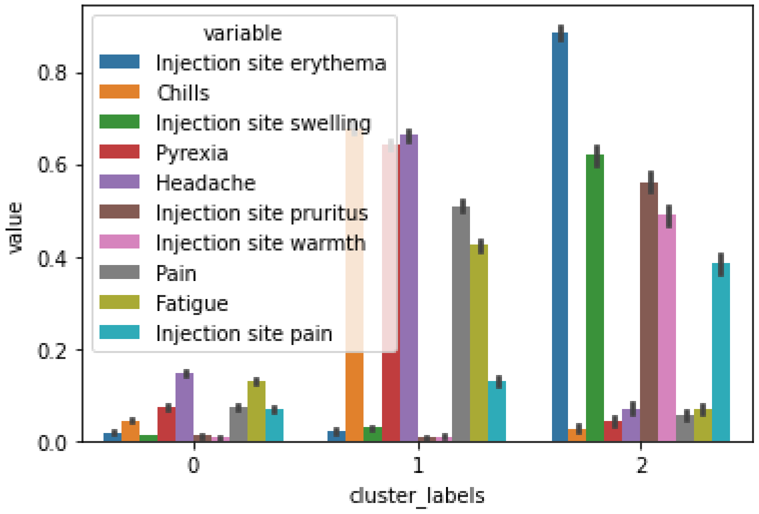
The highest score is for cluster = 3

In [134…

```
%%time
spectral_cl = SpectralClustering(n_clusters=3,
                            assign_labels='discretize', random_state=42)

pred_sp = spectral_cl.fit_predict(cluster_data)

# Silhouette Score
```

```
print('Silhouette Score Spectral: {:.3f}'.format(silhouette_score(cluster_data, pred_sp
print('DB Score: {:.3f}\n'.format(davies_bouldin_score(cluster_data, pred_sp)))

print_interpret_clusters(pred_sp, cluster_data)
print()
```

```
Silhouette Score Spectral: 0.137
DB Score: 2.322

[[    0     1     2]
 [18242  8427  2384]]

Wall time: 10min 22s
```



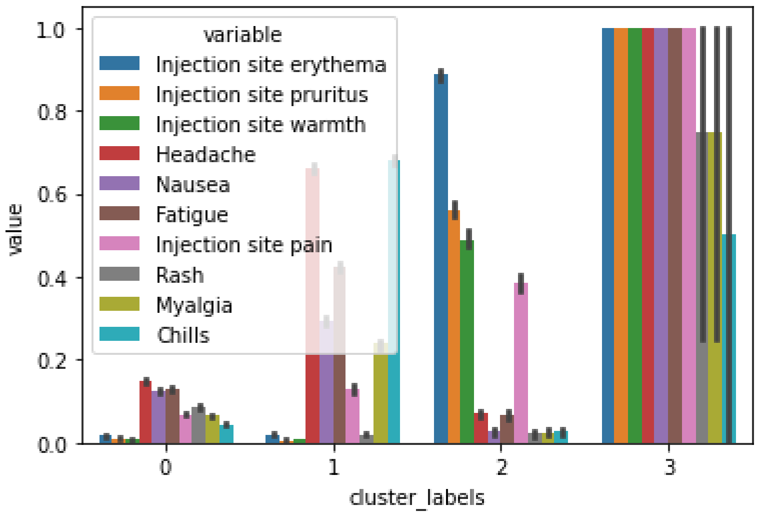
- [18242] cluster 0 : almost no symptoms, some headaches and fatigue
- [8427] cluster 1 : chills, fever, headache, pain, fatigue
- [2384] cluster 2 : injection site symptoms (itch, redness, swelling, warmt, pain)

Spectral cluster n=4

In [135…

```
%%time
spectral_cl = SpectralClustering(n_clusters=4,
                                 assign_labels='discretize', random_state=42)

pred_sp4 = spectral_cl.fit_predict(cluster_data)

# Silhouette Score
print('Silhouette Score Spectral: {:.3f}'.format(silhouette_score(cluster_data, pred_sp
print('DB Score: {:.3f}\n'.format(davies_bouldin_score(cluster_data, pred_sp4)))

print_interpret_clusters(pred_sp4, cluster_data)
print()
```

```
Silhouette Score Spectral: 0.136
DB Score: 1.992

[[    0     1     2     3]
 [18242  8425  2382     4]]

Wall time: 9min 32s
```



We can see how the last cluster of spectral clustering has only 4 samples and could be reduced to 3 clusters with the same characteristics from the results with 3 clusters. Spectral clustering with 5 clusters is expected to have very similar behavior as with 4 clusters.

Gaussian Mixture

In [136…

```
%%time

from sklearn.mixture import GaussianMixture

all_predictions=[]

num_cluster = [3, 4, 5]

for n in num_cluster:

    gm_cluster = GaussianMixture(n_components=n, covariance_type='full', random_state=4

    pred_clusters = gm_cluster.fit_predict(cluster_data)
    all_predictions.append(pred_clusters)

    # Silhouette Score
    print('Silhouette Score: {:.3f}'.format(silhouette_score(cluster_data, pred_cluster
    print('DB Score: {:.3f}'.format(davies_bouldin_score(cluster_data, pred_clusters)))

    # Number of patients in each cluster
    unique_elements, counts_elements = np.unique(pred_clusters, return_counts = True)
    print(np.asarray((unique_elements, counts_elements)))
    print()
```

```
Silhouette Score: 0.058
DB Score: 3.723
[[    0     1     2]
 [18349  9656  1048]]

Silhouette Score: 0.053
DB Score: 3.481
[[    0     1     2     3]
 [18395  8921   904   833]]

Silhouette Score: 0.078
DB Score: 3.577
[[    0     1     2     3     4]
```

```
 [ 4958 13265  1889  4314  4627]]
```

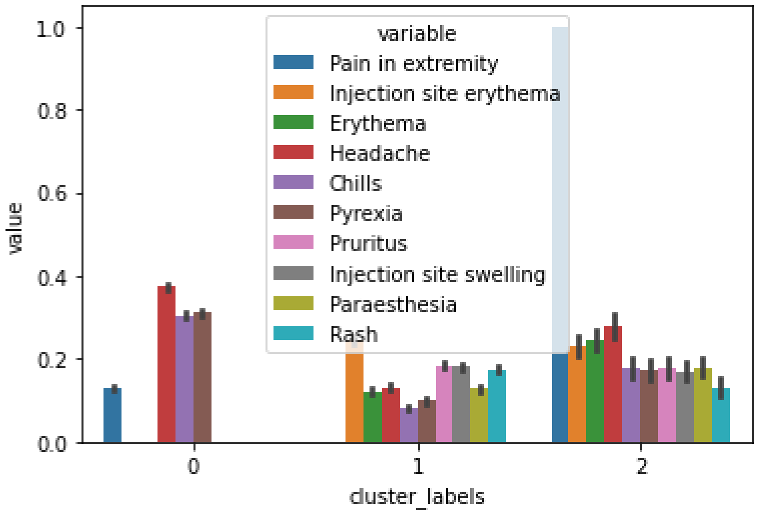
```
Wall time: 39.2 s
```

Gaussian Mixtures with 3 clusters

In [137...

```python
gm_cluster = GaussianMixture(n_components=3, covariance_type='full', random_state=42)

pred_gauss3 = gm_cluster.fit_predict(cluster_data)

# Silhouette Score
print('Silhouette Score: {:.3f}'.format(silhouette_score(cluster_data, pred_gauss3)))
print('DB Score: {:.3f}'.format(davies_bouldin_score(cluster_data, pred_gauss3)))


print_interpret_clusters(pred_gauss3, cluster_data)
```

```
Silhouette Score: 0.058
DB Score: 3.723
[[    0     1     2]
 [18349  9656  1048]]
```



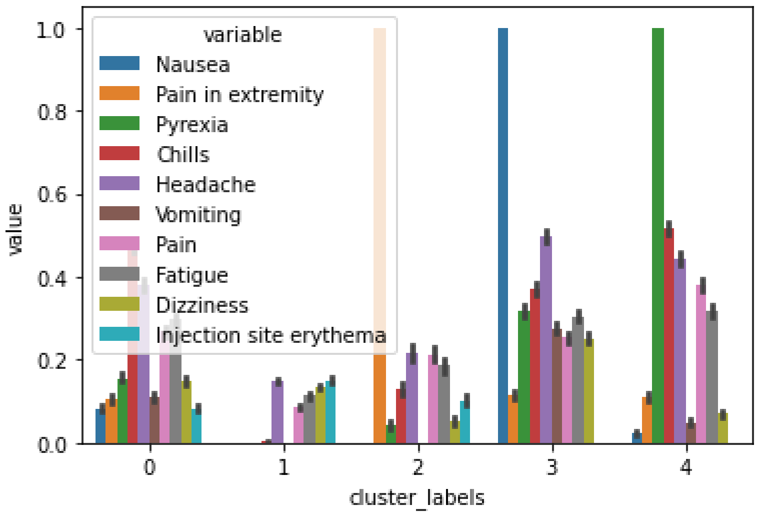
These clusters seem to have overlaping symptoms with close values. We will disregard these results

Gaussian Mixtures with 5 clusters

In [138...

```python
gm_cluster = GaussianMixture(n_components=5, covariance_type='full', random_state=42)

pred_gauss5 = gm_cluster.fit_predict(cluster_data)

print_interpret_clusters(pred_gauss5, cluster_data)
```

```
[[    0     1     2     3     4]
 [ 4958 13265  1889  4314  4627]]
```



Using 5 clusters in Gaussian Mixtures we can see how the clusters overlap in features like headache (purple), chills (red), fatigue(gray) and pain (pink). The clusters are not clearly separated.

We will disregard the results from the Gaussian mixture algorithm

- Model: Agglomerative

In [139...
```
from sklearn.cluster import AgglomerativeClustering
```

In [140...
```
%%time
from sklearn.cluster import AgglomerativeClustering

agglomerative = AgglomerativeClustering(n_clusters=2)
pred_y_agglomerative = agglomerative.fit_predict(cluster_data)

# Silhouette Score
print('Affinity Propagation: {}'.format(silhouette_score(cluster_data, pred_y_agglomera
```

```
Affinity Propagation: 0.10291866817555377
Wall time: 1min 11s
```

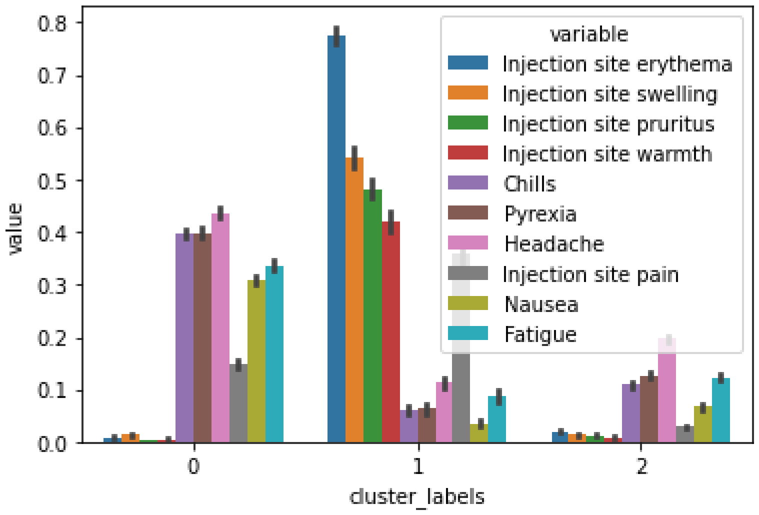
In [141...
```
%%time
from matplotlib import pyplot
from numpy import unique
from numpy import where
from sklearn.cluster import AgglomerativeClustering

range_n_clusters = range(3,6)
#sil_score = []

for k in range_n_clusters:
    agglomerative = AgglomerativeClustering(n_clusters=k)
    pred_y_agglomerative = agglomerative.fit_predict(cluster_data)
    score = silhouette_score(cluster_data, pred_y_agglomerative)
    print("For n_clusters =", k,
          "The average silhouette_score is :", score)
    #sil_score.append(score)
```

```
For n_clusters = 3 The average silhouette_score is : 0.06912384728059194
For n_clusters = 4 The average silhouette_score is : 0.07069402081486571
For n_clusters = 5 The average silhouette_score is : 0.04527529600672926
Wall time: 3min 29s
```

Agglomerative clusters = 3

```
In [142…
agglomerative = AgglomerativeClustering(n_clusters=3)
pred_y_agglomerative3 = agglomerative.fit_predict(cluster_data)

print_interpret_clusters(pred_y_agglomerative3, cluster_data)
```

```
[[    0     1     2]
 [12383  2880 13790]]
```

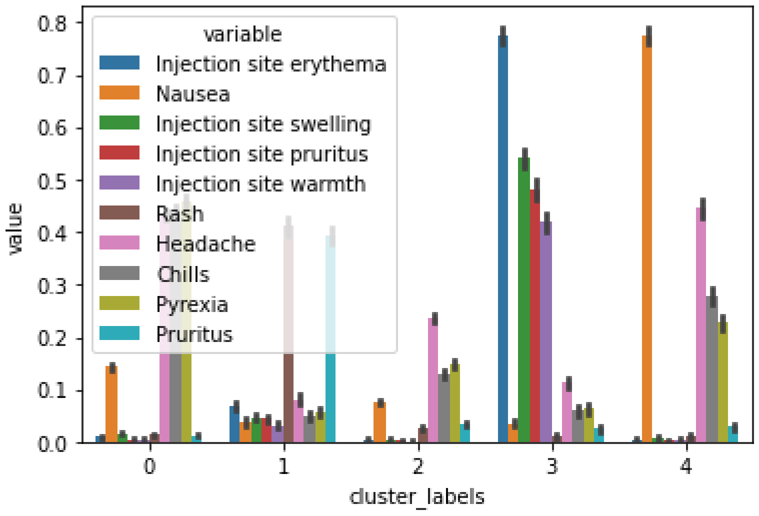


- [12383] cluster 0: chills, fever, headache, fatigue, nausea
- [2880] cluster 1: injection site symptoms (itch, redness, swelling, warmth, pain)
- [13790] cluster 2: almost no symptoms, some headache and fatigue

Agglomerative clusters = 5

```
In [143…
from sklearn.cluster import AgglomerativeClustering

agglomerative = AgglomerativeClustering(n_clusters=5)
pred_y_agglomerative5 = agglomerative.fit_predict(cluster_data)

print_interpret_clusters(pred_y_agglomerative5, cluster_data)
```

```
[[    0     1     2     3     4]
 [ 9132  3370 10420  2880  3251]]
```



- [9132] cluster 0: headache, chills, fever, some nausea
- [3370] cluster 1: rash and itching
- [10420] cluster 2: almost no symptoms, ~20% had headache ~10% chills, fever
- [2880] cluster 3: injection site symptoms
- [3251] cluster 4: Nausea, headache, ~20% chills, fever

In [ ]:
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%%time
# visualizing clusters with T-SNE: used for high-dimensional data like ours

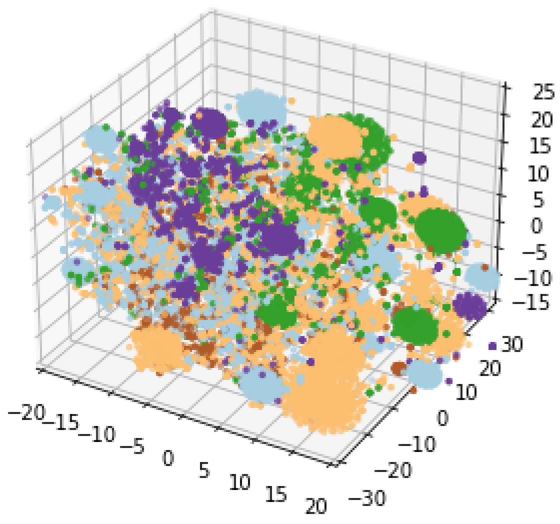
from sklearn.manifold import TSNE

def prepare_tsne(n_components, data, kmeans_labels):
    names = ['x', 'y', 'z']
    matrix = TSNE(n_components=n_components).fit_transform(data)
    df_matrix = pd.DataFrame(matrix)
    df_matrix.rename({i:names[i] for i in range(n_components)}, axis=1, inplace=True)
    df_matrix['labels'] = kmeans_labels
    return df_matrix

def plot_animation(df, label_column, name):
    def update(num):
        ax.view_init(200, num)

    N=360
    fig = plt.figure()
    ax = fig.add_subplot(111, projection='3d')
    ax.scatter(tsne_3d_df['x'], tsne_3d_df['y'], tsne_3d_df['z'], c=tsne_3d_df[label_co
               s=6, depthshade=True, cmap='Paired')
    ax.set_zlim(-15, 25)
    ax.set_xlim(-20, 20)
    plt.tight_layout()
    ani = animation.FuncAnimation(fig, update, N, blit=False, interval=50)
    ani.save('{}.gif'.format(name), writer='imagemagick')
    plt.show()

tsne_3d_df = prepare_tsne(3, cluster_data, pred_y_agglomerative5)
plot_animation(tsne_3d_df, 'labels', 'Agglomerative')
# tfne_3d_df
```



In [ ]:

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In [144…

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# Store the clean dataset with the kmeans cluster labels
# to be used for further analysis in R
df_clusters = df_merge.copy()
df_clusters['kmeans_5'] = pred_y_kmeans
df_clusters['kmeans_3'] = pred_y_kmeans3

df_clusters.to_csv('cleaned_data_clusters.csv', encoding='utf-8')
```