Drug Classification with ML

November 2, 2023

[1]:
```
# Exploratory Data Analysis in Python for ML/Visualization
```

[2]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
import os
```

[3]:
```
drug_data = pd.read_csv("C:/Users/abhim/OneDrive/Desktop/Drug Classification ML␣
↪Models/drug200.csv")
```

[4]:
```
# See the beginning of the data
drug_data.head()
```

[4]:

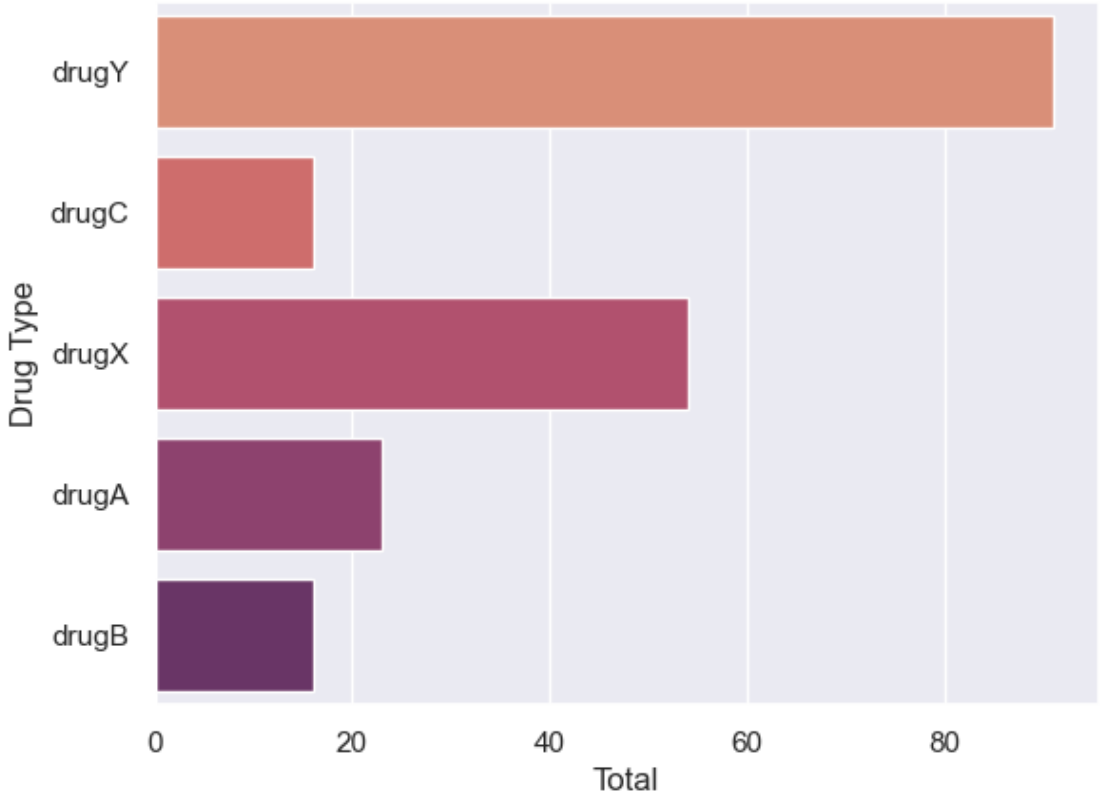
	Age	Sex	BP	Cholesterol	Na_to_K	Drug
0	23	F	HIGH	HIGH	25.355	drugY
1	47	M	LOW	HIGH	13.093	drugC
2	47	M	LOW	HIGH	10.114	drugC
3	28	F	NORMAL	HIGH	7.798	drugX
4	61	F	LOW	HIGH	18.043	drugY

[5]:
```
# Check for data types and whether there are any null data in the set
print(drug_data.info())
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 200 entries, 0 to 199
Data columns (total 6 columns):
 #   Column       Non-Null Count  Dtype
---  ------       --------------  -----
 0   Age          200 non-null    int64
 1   Sex          200 non-null    object
 2   BP           200 non-null    object
 3   Cholesterol  200 non-null    object
 4   Na_to_K      200 non-null    float64
 5   Drug         200 non-null    object
dtypes: float64(1), int64(1), object(4)
memory usage: 9.5+ KB
None
```

[6]:
```
# With python being OOP, we can access the columns of the data file as objects
print(drug_data.Drug.value_counts()) #.Drug gives access to the Drug column and␣
 ↪value_counts() returns a Series containing counts of unique values

# Drug type distribution
sns.set_theme(style="darkgrid")
sns.countplot(y="Drug", data=drug_data, palette="flare")
plt.ylabel('Drug Type')
plt.xlabel('Total')
plt.show()
```

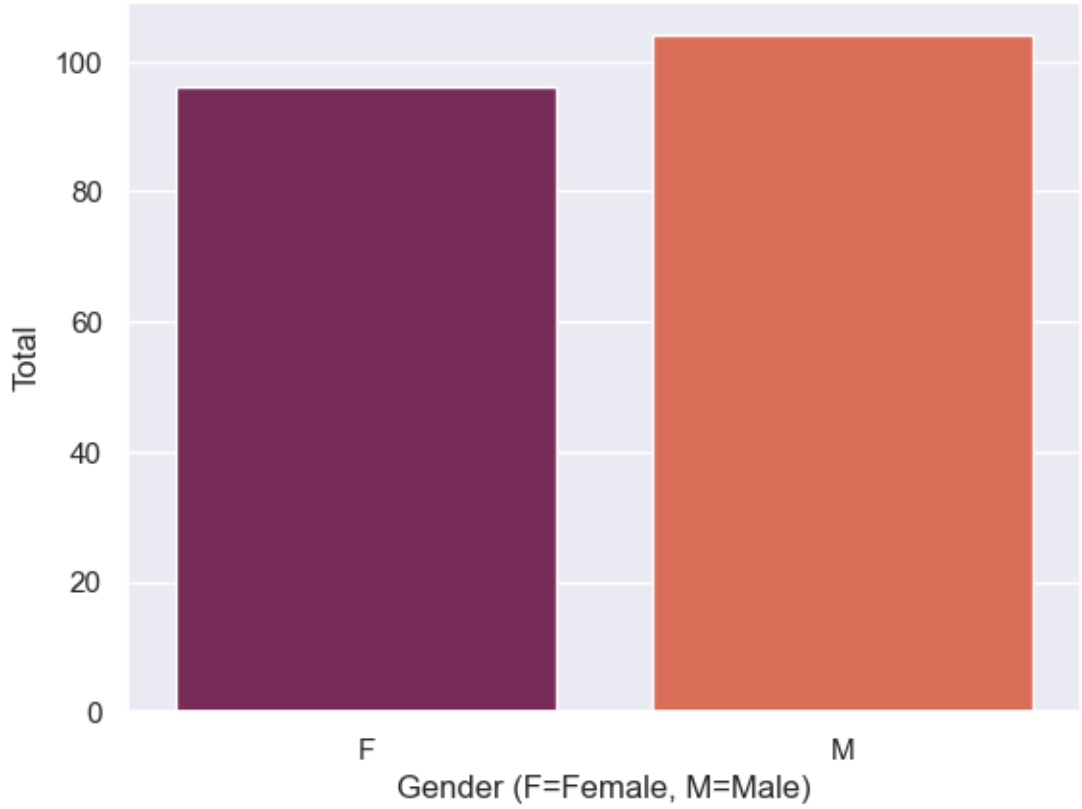
```
drugY    91
drugX    54
drugA    23
drugC    16
drugB    16
Name: Drug, dtype: int64
```



[7]:
```
# It appears patients are more on Drug Y than other drugs
```

[8]:
```
print(drug_data.Sex.value_counts())

sns.set_theme(style="darkgrid")
sns.countplot(x="Sex", data=drug_data, palette="rocket")
plt.xlabel('Gender (F=Female, M=Male)')
plt.ylabel('Total')
plt.show()
```

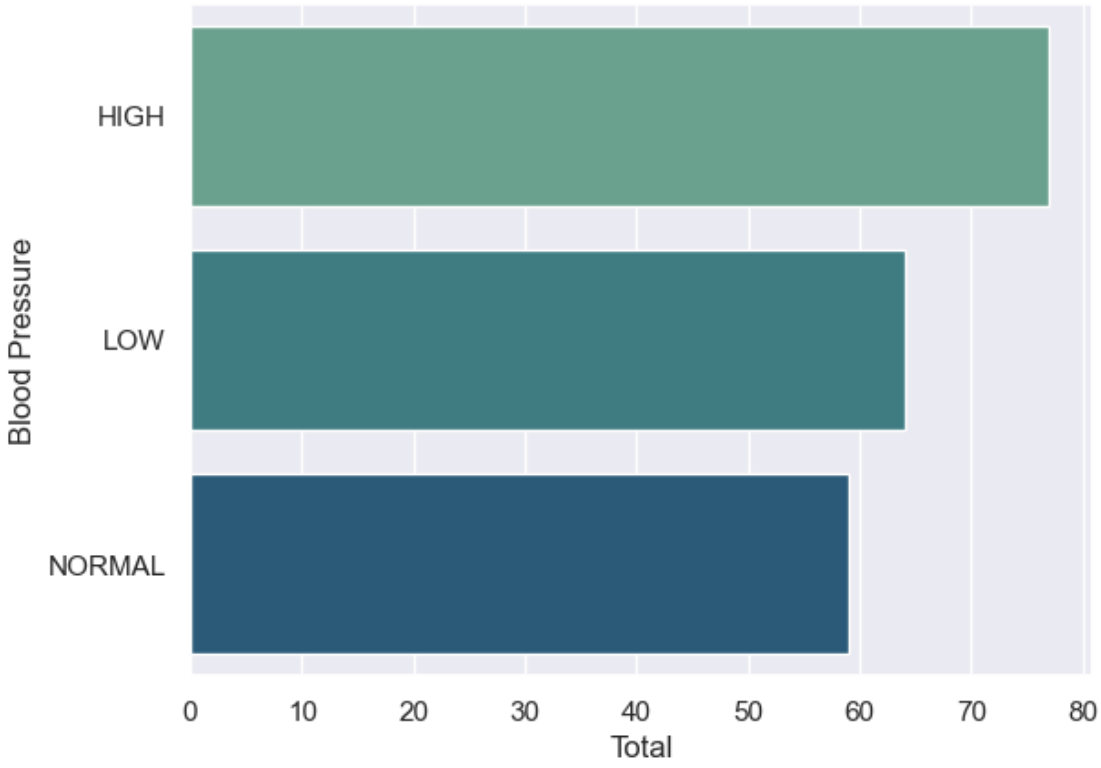
```
M    104
F     96
Name: Sex, dtype: int64
```



[9]:
```
# Sex is pretty balanced in the dataset
```

[10]:
```
print(drug_data.BP.value_counts())

sns.set_theme(style="darkgrid")
sns.countplot(y="BP", data=drug_data, palette="crest")
plt.ylabel('Blood Pressure')
plt.xlabel('Total')
plt.show()
```

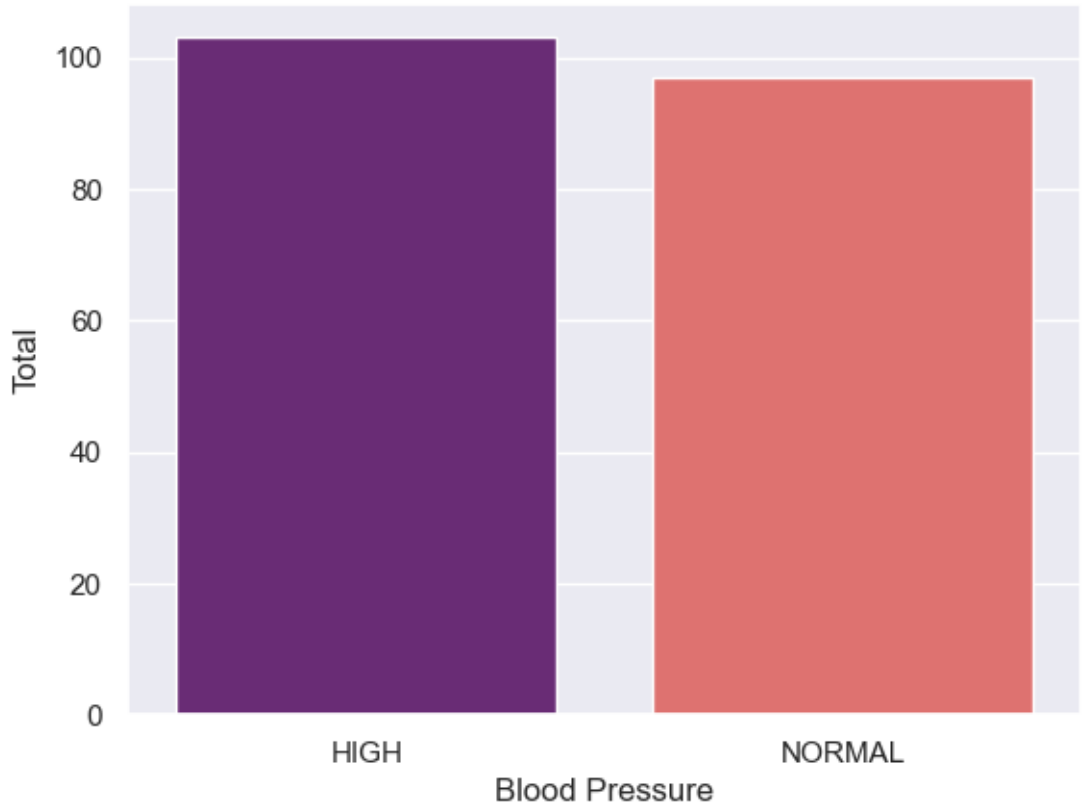
```
HIGH      77
LOW       64
NORMAL    59
Name: BP, dtype: int64
```



[11]:
```
# Looking at the BP, it appears that there is also a relative balance in the␣
 ↪number of patients who have high, low or normal BP.
# Relatively more patients though have high BP.
```

[12]:
```
print(drug_data.Cholesterol.value_counts())

sns.set_theme(style="darkgrid")
sns.countplot(x="Cholesterol", data=drug_data, palette="magma")
plt.xlabel('Blood Pressure')
plt.ylabel('Total')
plt.show()
```

```
HIGH      103
NORMAL     97
Name: Cholesterol, dtype: int64
```



[13]:
```
# Here we are given cholesterol and BP as categorical variables (just as high /␣
 ↪low/ normal).
# In the case of Cholesterol it appears the researcher is not interested in low␣
 ↪cholesterol levels rather normal and high
# Since usually those are where the problematic cases of heart disease occur
```

[14]:
```
# If we look at the data types, only age and Na/K ratio are quantitative␣
 ↪(numeric).
# The premise for this metric comes from NIH's National Heart, Lung and Blood␣
 ↪Institute (NHLBI) led research
# https://www.nih.gov/news-events/nih-research-matters/sodium/
 ↪potassium-ratio-linked-cardiovascular-disease-risk
```

[15]:
```
drug_data.describe()
```

[15]:

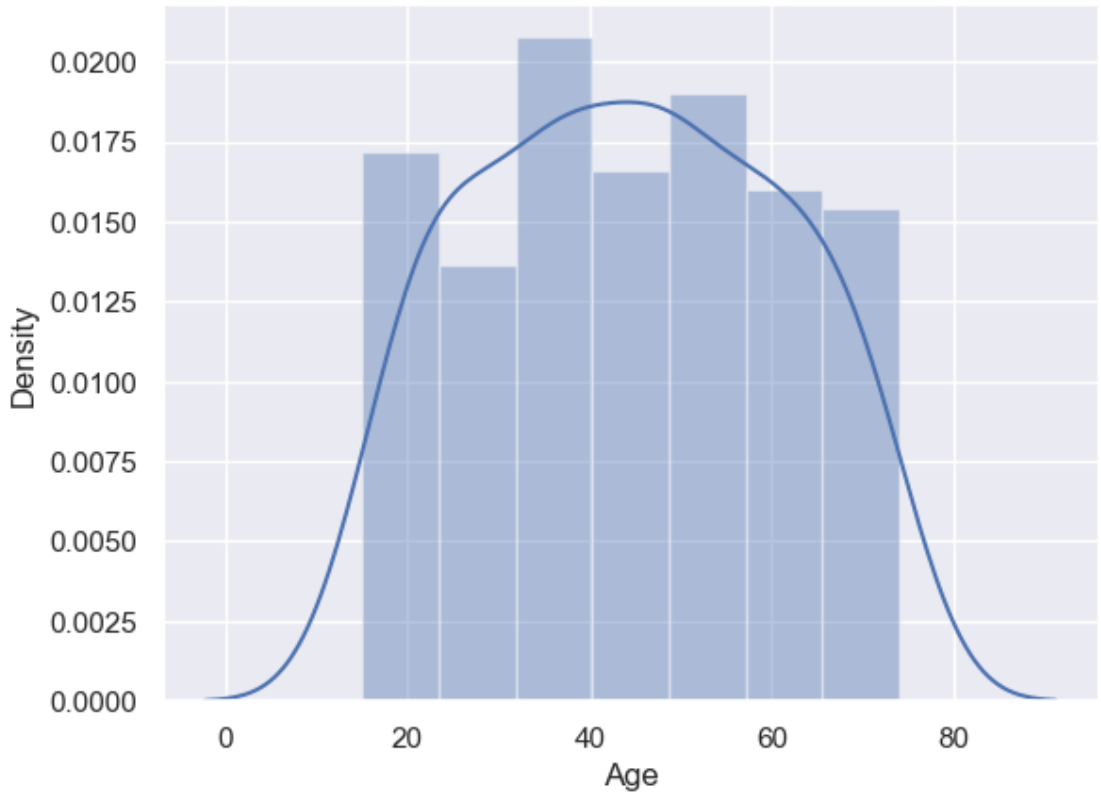
	Age	Na_to_K
count	200.000000	200.000000
mean	44.315000	16.084485
std	16.544315	7.223956
min	15.000000	6.269000

```
25%     31.000000   10.445500
50%     45.000000   13.936500
75%     58.000000   19.380000
max     74.000000   38.247000
```

[16]:
```
# Keep in mind that max age does not correlate with max Na/K ratio!
```

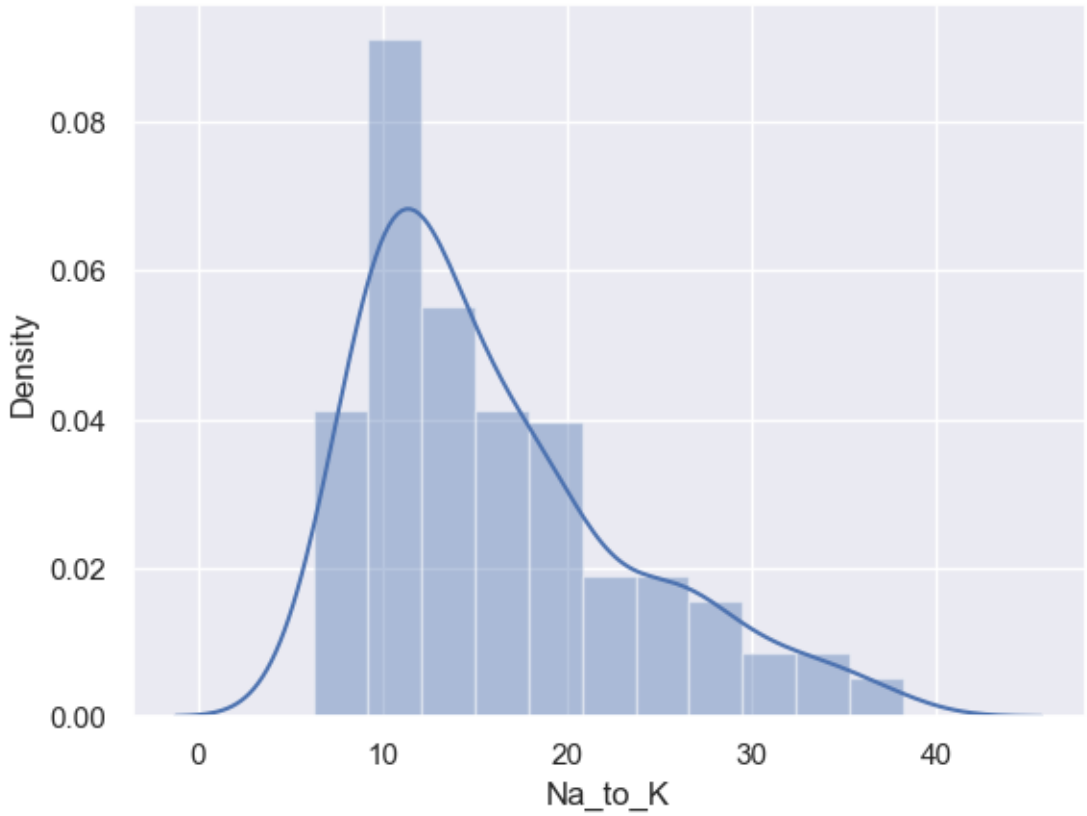
[17]:
```
# Check metric of how data are distributed
# Skewness is a metric of whether the data is symmetrically (normally)␣
 ↪distributed [or rather how assymetric the data is]
skewAge = drug_data.Age.skew(axis = 0, skipna = True)
print('Age skewness: ', skewAge)

# Plot
sns.distplot(drug_data['Age']);
```

```
Age skewness:  0.03030835703000607
C:\Users\abhim\AppData\Local\Temp\ipykernel_28348\2858418250.py:7: UserWarning:

`distplot` is a deprecated function and will be removed in seaborn v0.14.0.

Please adapt your code to use either `displot` (a figure-level function with
similar flexibility) or `histplot` (an axes-level function for histograms).

For a guide to updating your code to use the new functions, please see
https://gist.github.com/mwaskom/de44147ed2974457ad6372750bbe5751

  sns.distplot(drug_data['Age']);
```



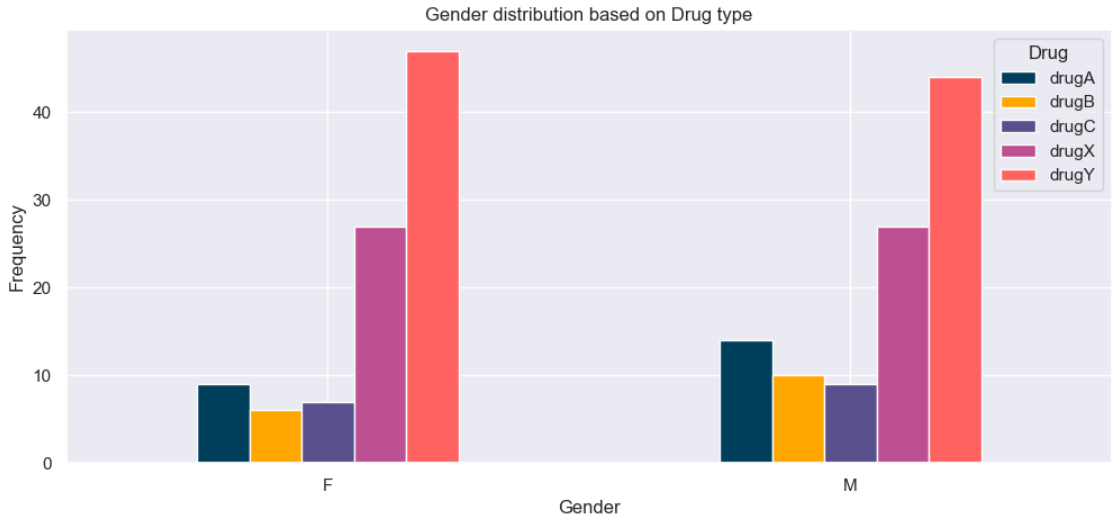
[18]:
```
skewNatoK = drug_data.Na_to_K.skew(axis = 0, skipna = True)
print('Na to K skewness: ', skewNatoK)

sns.distplot(drug_data['Na_to_K']);
```

```
Na to K skewness:  1.039341186028881

C:\Users\abhim\AppData\Local\Temp\ipykernel_28348\485059803.py:4: UserWarning:

`distplot` is a deprecated function and will be removed in seaborn v0.14.0.

Please adapt your code to use either `displot` (a figure-level function with
similar flexibility) or `histplot` (an axes-level function for histograms).

For a guide to updating your code to use the new functions, please see
https://gist.github.com/mwaskom/de44147ed2974457ad6372750bbe5751

  sns.distplot(drug_data['Na_to_K']);
```

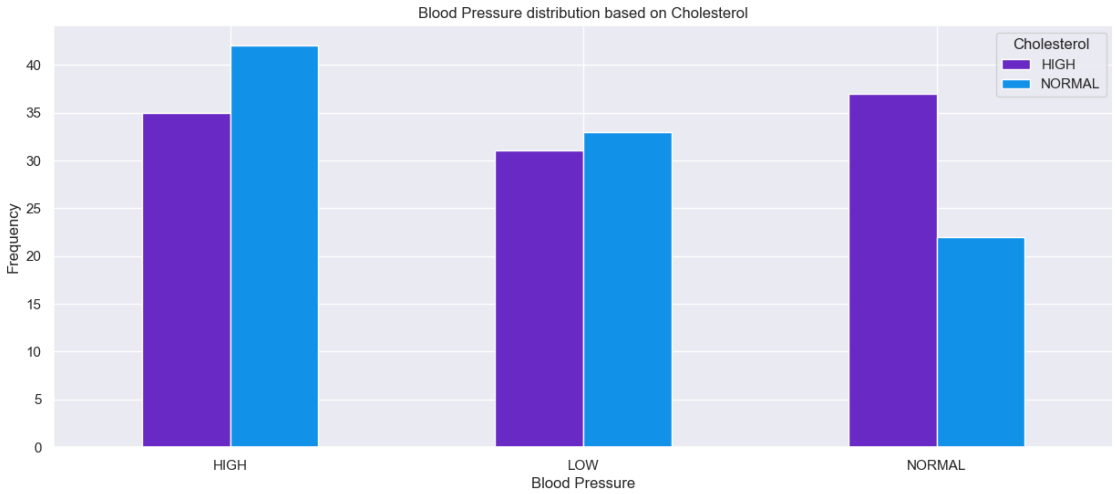


[19]:
```
# We see that the Na/K ratio is skewed right, indicating that patients have␣
↪higher values of Na/K and that the data is not symmetrically distributed
```

[20]:
```
pd.crosstab(drug_data.Sex,drug_data.Drug).
↪plot(kind="bar",figsize=(12,5),color=['#003f5c','#ffa600','#58508d','#bc5090','#ff6361'])
plt.title('Gender distribution based on Drug type')
plt.xlabel('Gender')
plt.xticks(rotation=0)
plt.ylabel('Frequency')
plt.show()
```

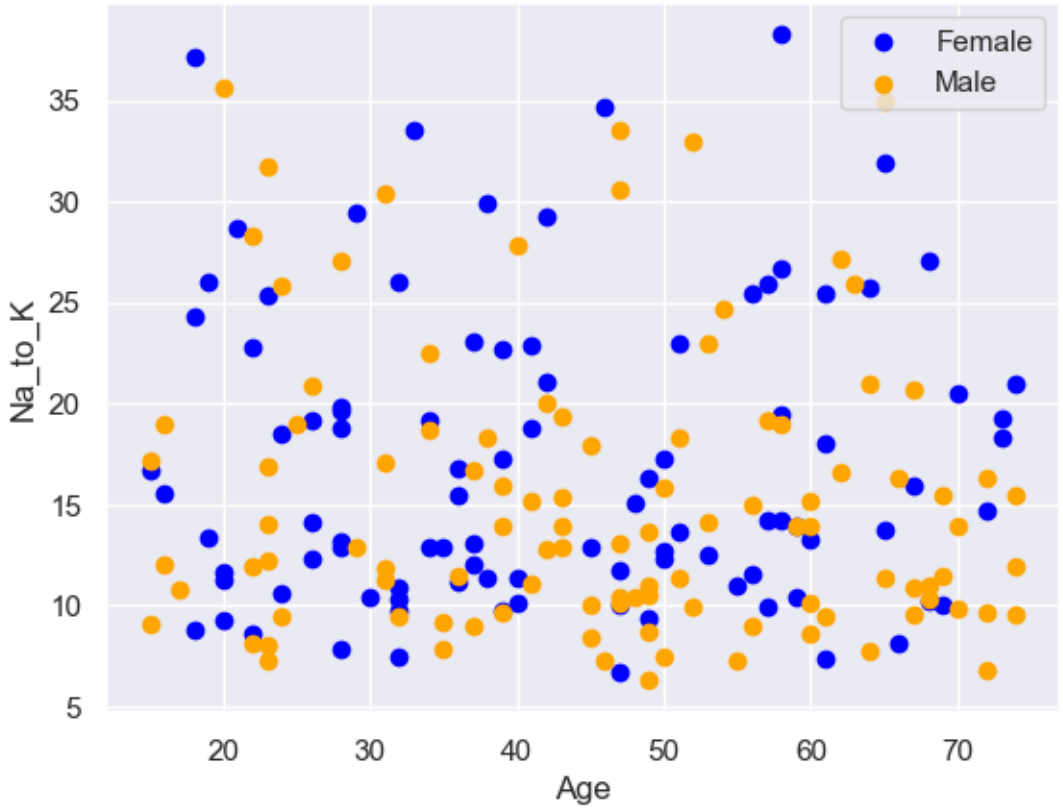


[21]:
```
pd.crosstab(drug_data.BP,drug_data.Cholesterol).
  ↪plot(kind="bar",figsize=(15,6),color=['#6929c4','#1192e8'])
plt.title('Blood Pressure distribution based on Cholesterol')
plt.xlabel('Blood Pressure')
plt.xticks(rotation=0)
plt.ylabel('Frequency')
plt.show()
```



[22]:
```
# Scatter Plot for Na/K vs age sorted by gender

plt.scatter(x=drug_data.Age[drug_data.Sex=='F'], y=drug_data.Na_to_K[(drug_data.
  ↪Sex=='F')], c="Blue") # take all age and Na/K values by Female
```

```
plt.scatter(x=drug_data.Age[drug_data.Sex=='M'], y=drug_data.Na_to_K[(drug_data.
  ↪Sex=='M')], c="Orange")
plt.legend(["Female", "Male"])
plt.xlabel("Age")
plt.ylabel("Na_to_K")
plt.show()
```



[23]:
```
# Now let's prepare the data for ML analysis
```

[24]:
```
# The age will be divided into 7 age categories:

# Below 20 y.o. <20s
# 20 - 29 y.o.  20s
# 30 - 39 y.o.  30s
# 40 - 49 y.o.  40s
# 50 - 59 y.o.  50s
# 60 - 69 y.o.  60s
# Above 70.    >70
```

[25]:
```
bin_age = [0, 19, 29, 39, 49, 59, 69, 80]
category_age = ['<20s', '20s', '30s', '40s', '50s', '60s', '>60s']
drug_data['Age_binned'] = pd.cut(drug_data['Age'], bins=bin_age,␣
 ↪labels=category_age)
drug_data = drug_data.drop(['Age'], axis = 1)
```

[26]:
```
# We drop the age column from the data since we bin it

drug_data
```

[26]:

	Sex	BP	Cholesterol	Na_to_K	Drug	Age_binned
0	F	HIGH	HIGH	25.355	drugY	20s
1	M	LOW	HIGH	13.093	drugC	40s
2	M	LOW	HIGH	10.114	drugC	40s
3	F	NORMAL	HIGH	7.798	drugX	20s
4	F	LOW	HIGH	18.043	drugY	60s
..	..	…	…	…	…	…
195	F	LOW	HIGH	11.567	drugC	50s
196	M	LOW	HIGH	12.006	drugC	<20s
197	M	NORMAL	HIGH	9.894	drugX	50s
198	M	NORMAL	NORMAL	14.020	drugX	20s
199	F	LOW	NORMAL	11.349	drugX	40s

[200 rows x 6 columns]

[27]:
```
#  The chemical ratio will be divided into 4 categories:

# Below 10.
# 10 - 20.
# 20 - 30.
# Above 30.
```

[28]:
```
bin_NatoK = [0, 9, 19, 29, 50]
category_NatoK = ['<10', '10-20', '20-30', '>30']
drug_data['Na_to_K_binned'] = pd.cut(drug_data['Na_to_K'], bins=bin_NatoK,␣
 ↪labels=category_NatoK)
drug_data = drug_data.drop(['Na_to_K'], axis = 1)
```

[29]:
```
drug_data
```

[29]:

	Sex	BP	Cholesterol	Drug	Age_binned	Na_to_K_binned
0	F	HIGH	HIGH	drugY	20s	20-30
1	M	LOW	HIGH	drugC	40s	10-20
2	M	LOW	HIGH	drugC	40s	10-20
3	F	NORMAL	HIGH	drugX	20s	<10
4	F	LOW	HIGH	drugY	60s	10-20
..	..	…	…	…	…	…

```
195   F     LOW        HIGH  drugC        50s          10-20
196   M     LOW        HIGH  drugC       <20s          10-20
197   M  NORMAL        HIGH  drugX        50s          10-20
198   M  NORMAL      NORMAL  drugX        20s          10-20
199   F     LOW      NORMAL  drugX        40s          10-20

[200 rows x 6 columns]
```

[30]:
```
# Now we have binned data for age groups and ranges of Na/K ratio.
# We do this since the clinical research data is presented by groups of age and␣
 ↪also the physiological parameter range
```

[31]:
```
# Begin Machine Learning - We will do a 70/30 split on training/testing
```

[32]:
```
from sklearn.metrics import confusion_matrix
from sklearn.metrics import classification_report
```

[33]:
```
# OK since the goal is to predict which drug to give the patient, we want to␣
 ↪drop the drug column from the data set since that will be what we use as a␣
 ↪label and also predict
X = drug_data.drop(["Drug"], axis=1) # axis = 1, drop the column. axis = 0,␣
 ↪drop the row
y = drug_data["Drug"]

from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.3,␣
 ↪random_state = 0)
# we also randomize the rows of the data by a seed so that it takes away any␣
 ↪bias that order may confer (you'll see that in the table below)
```

[34]:
```
# Feature Engineering - The FE method that used is one-hot encoding, which is␣
 ↪transforming categorical variables into a form that could be provided to ML␣
 ↪algorithms to do a better prediction.
X_train = pd.get_dummies(X_train)
X_test = pd.get_dummies(X_test)
# Each variable is converted in as many 0/1 variables as there are different␣
 ↪values. Columns in the output are each named after a value; if the input is␣
 ↪a DataFrame, the name of the original variable is prepended to the value.
```

[35]:
```
# To better understand what one-hot encoding has done via get_dummies lets look␣
 ↪at part of the dataset:
X_train.head()
```

[35]:
```
     Sex_F  Sex_M  BP_HIGH  BP_LOW  BP_NORMAL  Cholesterol_HIGH  \
131      0      1        0       1          0                 0
96       1      0        0       1          0                 1
181      1      0        0       0          1                 1
```

```
19       1      0        1       0          0                0
153      1      0        0       1          0                0

     Cholesterol_NORMAL  Age_binned_<20s  Age_binned_20s  Age_binned_30s  \
131                   1                0               0               0
96                    0                0               0               0
181                   0                0               0               0
19                    1                0               0               1
153                   1                0               0               0

     Age_binned_40s  Age_binned_50s  Age_binned_60s  Age_binned_>60s  \
131               0               1               0                0
96                0               1               0                0
181               0               1               0                0
19                0               0               0                0
153               0               0               0                1

     Na_to_K_binned_<10  Na_to_K_binned_10-20  Na_to_K_binned_20-30  \
131                   0                     0                     0
96                    0                     0                     0
181                   0                     1                     0
19                    0                     0                     1
153                   0                     1                     0

     Na_to_K_binned_>30
131                   1
96                    1
181                   0
19                    0
153                   0
```

[36]:
```
# We see that here we have put a "1" wherever the variable has a value and 0␣
 ↪where it does not have a value!
# so the first row is a male patient with low BP, normal cholesterol, in the␣
 ↪50s with an Na/K > 30
```

[37]:
```
y_train.head()
```

[37]:
```
131    drugY
96     drugY
181    drugX
19     drugY
153    drugX
Name: Drug, dtype: object
```

[38]:
```
# It appears that patient 131 (as we will call him) is getting drug Y!
```

```
# And from visual, it appears the drug may be dependent on the Na/K ratio -␣
 ↪being > 20 since patients 131, 96 and 19 are all getting Drug Y!
```

[39]:
```
X_test.head()
```

[39]:

	Sex_F	Sex_M	BP_HIGH	BP_LOW	BP_NORMAL	Cholesterol_HIGH
18	0	1	0	1	0	1
170	1	0	0	0	1	1
107	0	1	0	1	0	1
98	0	1	1	0	0	0
177	0	1	0	0	1	1

	Cholesterol_NORMAL	Age_binned_<20s	Age_binned_20s	Age_binned_30s
18	0	0	1	0
170	0	0	1	0
107	0	0	0	0
98	1	0	1	0
177	0	0	1	0

	Age_binned_40s	Age_binned_50s	Age_binned_60s	Age_binned_>60s
18	0	0	0	0
170	0	0	0	0
107	1	0	0	0
98	0	0	0	0
177	0	0	0	0

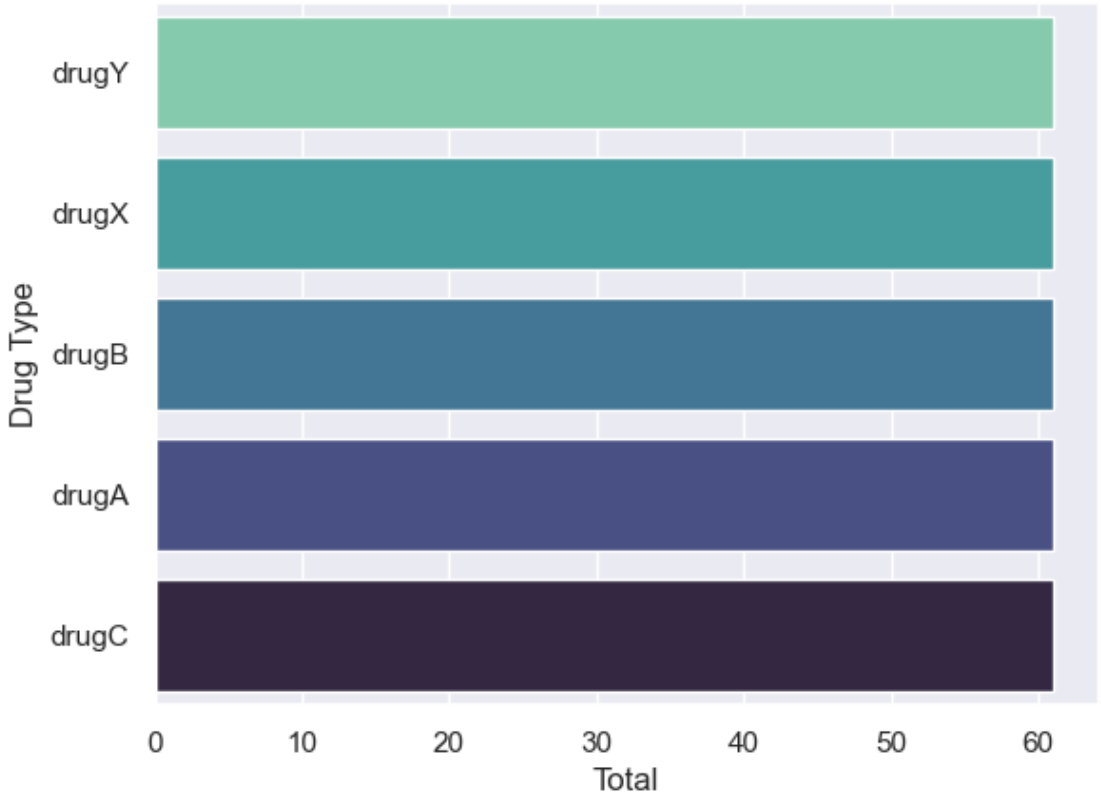
	Na_to_K_binned_<10	Na_to_K_binned_10-20	Na_to_K_binned_20-30
18	1	0	0
170	0	1	0
107	0	0	1
98	0	0	0
177	0	0	1

	Na_to_K_binned_>30
18	0
170	0
107	0
98	1
177	0

[40]:
```
# Since we know that Drug Y is more prominent in the dataset, to balance the␣
 ↪classification problem, we would need to use oversampling to overcome␣
 ↪overfitting
from imblearn.over_sampling import SMOTE
X_train, y_train = SMOTE().fit_resample(X_train, y_train)
```

[41]:
```
# SMOTE stands for Synthetic Minority Oversampling Technique
# A general downside of the approach is that synthetic examples are created␣
 ↪without considering the majority class, possibly resulting in ambiguous␣
 ↪examples if there is a strong overlap for the classes.
```

[42]:
```
sns.set_theme(style="darkgrid")
sns.countplot(y=y_train, data=drug_data, palette="mako_r")
plt.ylabel('Drug Type')
plt.xlabel('Total')
plt.show()
```



[43]:
```
# By resampling the minority data, we create a scenario in which the amounts of␣
 ↪drug is more uniform to avoid any bias and overfitting in the system
# By the same token, we also resample the patient data as well! But in randomly␣
 ↪doing so based on which patients get which drug in the training set
```

[44]:
```
# Logistic Regression:
from sklearn.linear_model import LogisticRegression
LRclassifier = LogisticRegression(solver='liblinear', max_iter=5000) #liblinear␣
 ↪is a linear classifier for data supporting log reg and SVM: https://www.csie.
 ↪ntu.edu.tw/~cjlin/papers/liblinear.pdf
```

```
LRclassifier.fit(X_train, y_train)

y_pred = LRclassifier.predict(X_test) # we will predict which drug a patient␣
 ↪will get based on the fit we got from training and compare it to the test␣
 ↪labels to determine accuracy

print(classification_report(y_test, y_pred)) # how did the model perform?
print(confusion_matrix(y_test, y_pred))

from sklearn.metrics import accuracy_score
LRAcc = accuracy_score(y_pred,y_test) # In multilabel classification, this␣
 ↪function computes subset accuracy: the set of labels predicted for a sample␣
 ↪must exactly match the corresponding set of labels in y_true. Here y_true =␣
 ↪y_test
print('Logistic Regression accuracy is: {:.2f}%'.format(LRAcc*100))
```

```
              precision    recall  f1-score   support

       drugA       0.71      1.00      0.83         5
       drugB       0.75      1.00      0.86         3
       drugC       0.67      1.00      0.80         4
       drugX       0.81      0.94      0.87        18
       drugY       0.95      0.70      0.81        30

    accuracy                           0.83        60
   macro avg       0.78      0.93      0.83        60
weighted avg       0.86      0.83      0.83        60

[[ 5  0  0  0  0]
 [ 0  3  0  0  0]
 [ 0  0  4  0  0]
 [ 0  0  0 17  1]
 [ 2  1  2  4 21]]
Logistic Regression accuracy is: 83.33%
```

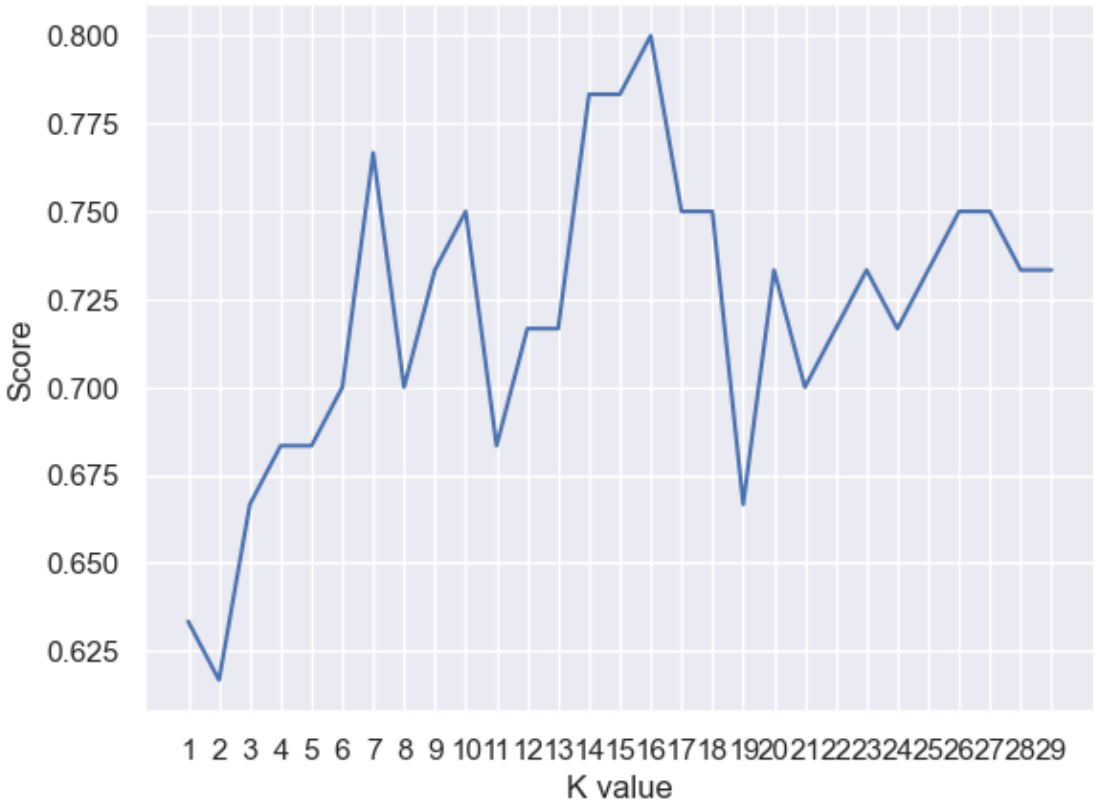
[45]:
```
# from LR confusion matrix, we learn that drug Y had the most␣
 ↪misclassifications!
```

[46]:
```
# K Neighbors Classification - based on euclidian distance of where points are␣
 ↪relative to each other, so if we have the other parameters summarized for␣
 ↪the x variable and our drug as y, a distance is computed, and may also be␣
 ↪computed for each class of data
# https://www.ibm.com/topics/knn

from sklearn.neighbors import KNeighborsClassifier
KNclassifier = KNeighborsClassifier(n_neighbors=20) # how many neighbors do we␣
 ↪want to account for to classify a point?
```

```
KNclassifier.fit(X_train, y_train)

y_pred = KNclassifier.predict(X_test)

print(classification_report(y_test, y_pred))
print(confusion_matrix(y_test, y_pred))

from sklearn.metrics import accuracy_score
KNAcc = accuracy_score(y_pred,y_test)
print('K Neighbours accuracy is: {:.2f}%'.format(KNAcc*100))
```

```
              precision    recall  f1-score   support

       drugA       0.40      0.80      0.53         5
       drugB       0.50      0.33      0.40         3
       drugC       0.50      0.50      0.50         4
       drugX       0.82      1.00      0.90        18
       drugY       0.86      0.63      0.73        30

    accuracy                           0.73        60
   macro avg       0.62      0.65      0.61        60
weighted avg       0.77      0.73      0.73        60

[[ 4  1  0  0  0]
 [ 1  1  0  0  1]
 [ 0  0  2  0  2]
 [ 0  0  0 18  0]
 [ 5  0  2  4 19]]
K Neighbours accuracy is: 73.33%
```

[47]:
```
# If we are to iterate through number of neighbors to consider, what is max␣
 ↪accuracy we can achieve with KNN?
scoreListknn = []
for i in range(1,30):
    KNclassifier = KNeighborsClassifier(n_neighbors = i)
    KNclassifier.fit(X_train, y_train)
    scoreListknn.append(KNclassifier.score(X_test, y_test))

plt.plot(range(1,30), scoreListknn)
plt.xticks(np.arange(1,30,1))
plt.xlabel("K value")
plt.ylabel("Score")
plt.show()
KNAccMax = max(scoreListknn)
print("KNN Acc Max {:.2f}%".format(KNAccMax*100))
```




```
KNN Acc Max 80.00%
```

[48]:
```
# It appears this output may be GPU dependent
```

[50]:
```
# SVM -  a supervised machine learning problem where we try to find a␣
 ↪hyperplane that best separates the two classes.
# This is different from LR in that LR is probabilistic, while SVM has more␣
 ↪mathematical/statistical founding:
# https://www.analyticsvidhya.com/blog/2021/10/
 ↪support-vector-machinessvm-a-complete-guide-for-beginners/

from sklearn.svm import SVC
SVCclassifier = SVC(kernel='linear', max_iter=251)
SVCclassifier.fit(X_train, y_train)

y_pred = SVCclassifier.predict(X_test)

print(classification_report(y_test, y_pred))
print(confusion_matrix(y_test, y_pred))

from sklearn.metrics import accuracy_score
```

```
SVCAcc = accuracy_score(y_pred,y_test)
print('SVC accuracy is: {:.2f}%'.format(SVCAcc*100))
```

```
              precision    recall  f1-score   support

       drugA       0.67      0.80      0.73         5
       drugB       0.75      1.00      0.86         3
       drugC       0.67      1.00      0.80         4
       drugX       0.82      1.00      0.90        18
       drugY       0.95      0.70      0.81        30

    accuracy                           0.83        60
   macro avg       0.77      0.90      0.82        60
weighted avg       0.86      0.83      0.83        60

[[ 4  0  0  0  1]
 [ 0  3  0  0  0]
 [ 0  0  4  0  0]
 [ 0  0  0 18  0]
 [ 2  1  2  4 21]]
SVC accuracy is: 83.33%
```

```
C:\Users\abhim\anaconda3\Lib\site-packages\sklearn\svm\_base.py:299:
ConvergenceWarning: Solver terminated early (max_iter=251).  Consider pre-
processing your data with StandardScaler or MinMaxScaler.
  warnings.warn(
```

[51]:
```
# Naive Bayes - Uses the liklihood ratios of an event occuring to calculate the␣
 ↪probability of a posterior event occuring
# e.g., if it is sunny outside, then we go play - P(Play|Sunny) =␣
 ↪P(Sunny|Play)P(Play)/P(Sunny) Class probability goes in numerator
# https://www.analyticsvidhya.com/blog/2017/09/naive-bayes-explained/

# Categorical NB - Categorical Naive Bayes is useful if the features are␣
 ↪categorically distributed. We have to encode the categorical variable in the␣
 ↪numeric format using the ordinal encoder for using this algorithm.
from sklearn.naive_bayes import CategoricalNB
NBclassifier1 = CategoricalNB()
NBclassifier1.fit(X_train, y_train)

y_pred = NBclassifier1.predict(X_test)

print(classification_report(y_test, y_pred))
print(confusion_matrix(y_test, y_pred))

from sklearn.metrics import accuracy_score
NBAcc1 = accuracy_score(y_pred,y_test)
print('Naive Bayes accuracy is: {:.2f}%'.format(NBAcc1*100))
```

```
              precision    recall  f1-score   support

       drugA       0.71      1.00      0.83         5
       drugB       0.75      1.00      0.86         3
       drugC       0.50      0.50      0.50         4
       drugX       0.75      1.00      0.86        18
       drugY       1.00      0.70      0.82        30

    accuracy                           0.82        60
   macro avg       0.74      0.84      0.77        60
weighted avg       0.86      0.82      0.81        60

[[ 5  0  0  0  0]
 [ 0  3  0  0  0]
 [ 0  0  2  2  0]
 [ 0  0  0 18  0]
 [ 2  1  2  4 21]]
Naive Bayes accuracy is: 81.67%
```

[52]:
```
# Gaussian NB - gaussiannb is used in classification tasks and it assumes that␣
 ↪feature values follow a gaussian distribution.

from sklearn.naive_bayes import GaussianNB
NBclassifier2 = GaussianNB()
NBclassifier2.fit(X_train, y_train)

y_pred = NBclassifier2.predict(X_test)

print(classification_report(y_test, y_pred))
print(confusion_matrix(y_test, y_pred))

from sklearn.metrics import accuracy_score
NBAcc2 = accuracy_score(y_pred,y_test)
print('Gaussian Naive Bayes accuracy is: {:.2f}%'.format(NBAcc2*100))
```

```
              precision    recall  f1-score   support

       drugA       1.00      0.20      0.33         5
       drugB       0.75      1.00      0.86         3
       drugC       1.00      0.50      0.67         4
       drugX       1.00      0.39      0.56        18
       drugY       0.63      0.97      0.76        30

    accuracy                           0.70        60
   macro avg       0.88      0.61      0.64        60
weighted avg       0.80      0.70      0.66        60

[[ 1  0  0  0  4]
```

```
 [ 0  3  0  0  0]
 [ 0  0  2  0  2]
 [ 0  0  0  7 11]
 [ 0  1  0  0 29]]
Gaussian Naive Bayes accuracy is: 70.00%
```

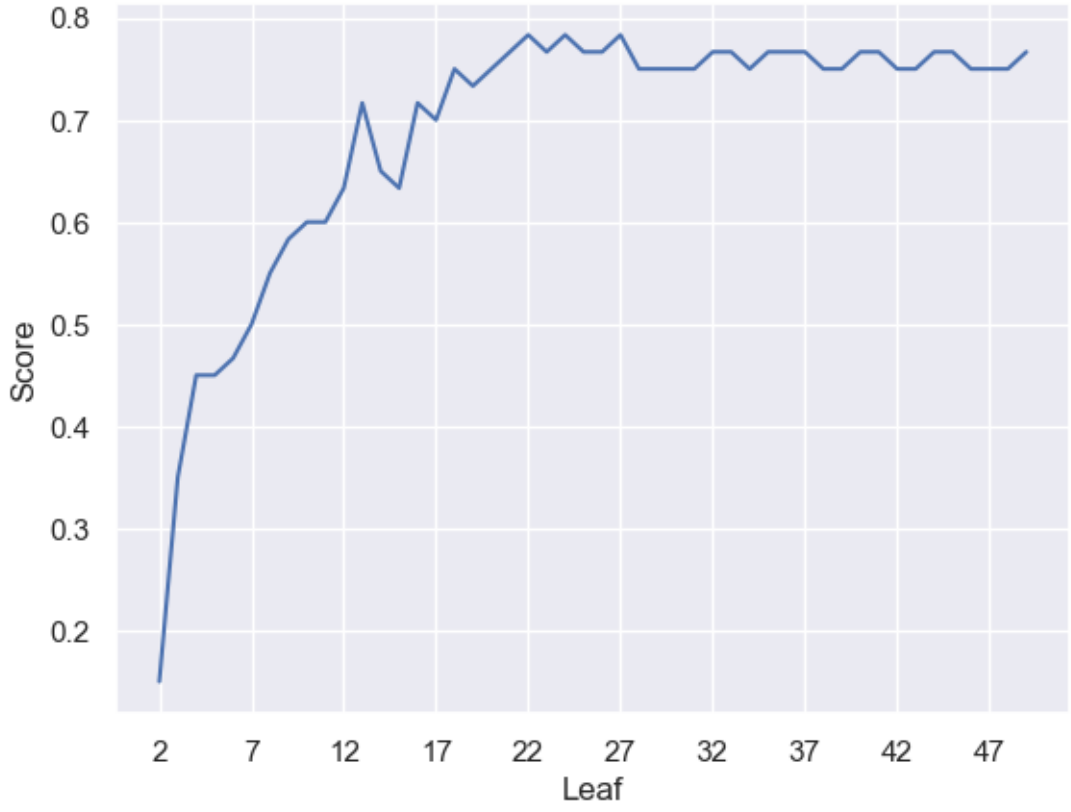
[53]:
```
# If we hadn't balanced the data, we may have been able to use Complement NB - which is used on imbalanced datasets.
# However, the trend we are observing is that with most of the ML algorithms, drug Y is most misclassified
```

[54]:
```
# Decision Trees - They are classification systems which use nodes and rely on entropy and the weight of a decision to determine how to traverse a final classification
# https://towardsdatascience.com/decision-trees-how-to-draw-them-on-paper-e2597af497f0
# https://www.kdnuggets.com/2020/01/decision-tree-algorithm-explained.html

from sklearn.tree import DecisionTreeClassifier
DTclassifier = DecisionTreeClassifier(max_leaf_nodes=20)
DTclassifier.fit(X_train, y_train)

y_pred = DTclassifier.predict(X_test)

print(classification_report(y_test, y_pred))
print(confusion_matrix(y_test, y_pred))

from sklearn.metrics import accuracy_score
DTAcc = accuracy_score(y_pred,y_test)
print('Decision Tree accuracy is: {:.2f}%'.format(DTAcc*100))
```

```
              precision    recall  f1-score   support

       drugA       0.50      1.00      0.67         5
       drugB       0.75      1.00      0.86         3
       drugC       0.67      1.00      0.80         4
       drugX       0.80      0.89      0.84        18
       drugY       0.90      0.60      0.72        30

    accuracy                           0.77        60
   macro avg       0.72      0.90      0.78        60
weighted avg       0.81      0.77      0.76        60

[[ 5  0  0  0  0]
 [ 0  3  0  0  0]
 [ 0  0  4  0  0]
 [ 0  0  0 16  2]
 [ 5  1  2  4 18]]
```

```
Decision Tree accuracy is: 76.67%
```

[55]:
```
# If we were to work with varying the number of nodes

scoreListDT = []
for i in range(2,50):
    DTclassifier = DecisionTreeClassifier(max_leaf_nodes=i)
    DTclassifier.fit(X_train, y_train)
    scoreListDT.append(DTclassifier.score(X_test, y_test))

plt.plot(range(2,50), scoreListDT)
plt.xticks(np.arange(2,50,5))
plt.xlabel("Leaf")
plt.ylabel("Score")
plt.show()
DTAccMax = max(scoreListDT)
print("DT Acc Max {:.2f}%".format(DTAccMax*100))
```



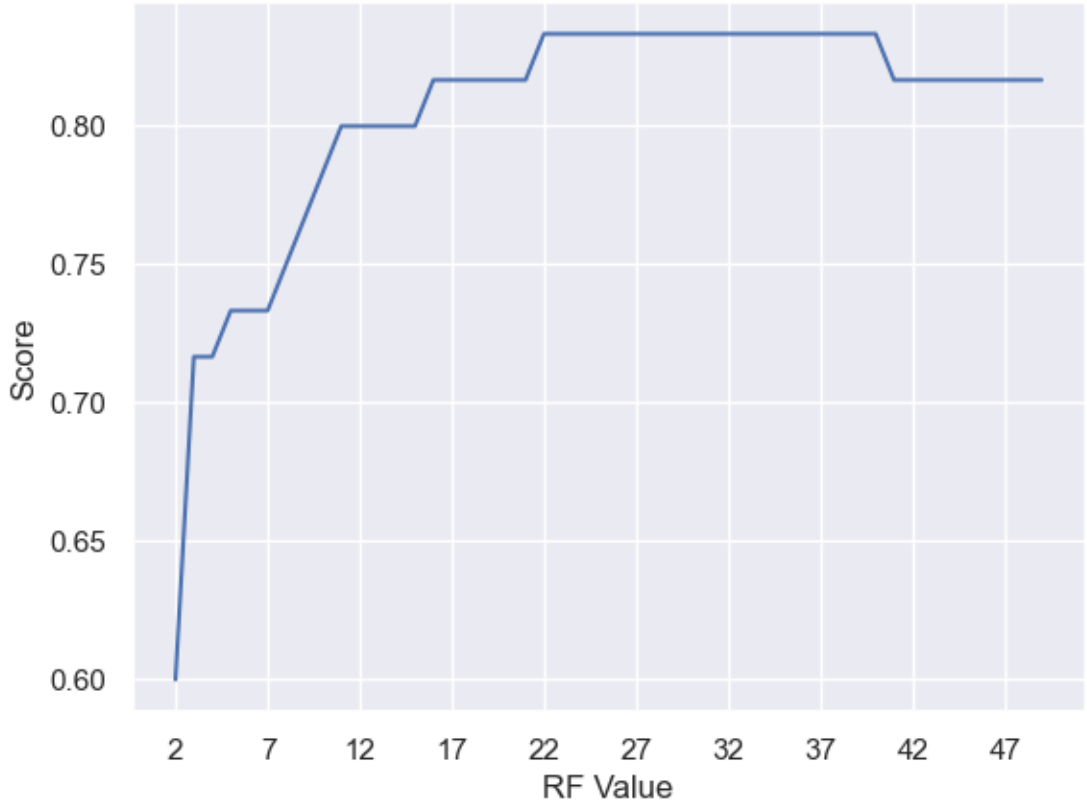

```
DT Acc Max 78.33%
```

[56]:
```
# Random Forest - ensemble of decision trees - Each individual tree in the␣
 ↪random forest spits out a class prediction and the class with the most votes␣
 ↪becomes our model's prediction
# https://towardsdatascience.com/understanding-random-forest-58381e0602d2

from sklearn.ensemble import RandomForestClassifier

RFclassifier = RandomForestClassifier(max_leaf_nodes=30)
RFclassifier.fit(X_train, y_train)

y_pred = RFclassifier.predict(X_test)

print(classification_report(y_test, y_pred))
print(confusion_matrix(y_test, y_pred))

from sklearn.metrics import accuracy_score
RFAcc = accuracy_score(y_pred,y_test)
print('Random Forest accuracy is: {:.2f}%'.format(RFAcc*100))
```

```
              precision    recall  f1-score   support

       drugA       0.62      1.00      0.77         5
       drugB       0.75      1.00      0.86         3
       drugC       0.67      1.00      0.80         4
       drugX       0.82      1.00      0.90        18
       drugY       1.00      0.67      0.80        30

    accuracy                           0.83        60
   macro avg       0.77      0.93      0.83        60
weighted avg       0.88      0.83      0.83        60

[[ 5  0  0  0  0]
 [ 0  3  0  0  0]
 [ 0  0  4  0  0]
 [ 0  0  0 18  0]
 [ 3  1  2  4 20]]
Random Forest accuracy is: 83.33%
```

[57]:
```
# Iterate through different numbers of trees

scoreListRF = []
for i in range(2,50):
    RFclassifier = RandomForestClassifier(n_estimators = 1000, random_state =␣
 ↪1, max_leaf_nodes=i)
    RFclassifier.fit(X_train, y_train)
    scoreListRF.append(RFclassifier.score(X_test, y_test))
```

```
plt.plot(range(2,50), scoreListRF)
plt.xticks(np.arange(2,50,5))
plt.xlabel("RF Value")
plt.ylabel("Score")
plt.show()
RFAccMax = max(scoreListRF)
print("RF Acc Max {:.2f}%".format(RFAccMax*100))
```




```
RF Acc Max 83.33%
```

[58]:
```
# Compare all the models

compare = pd.DataFrame({'Model': ['Logistic Regression', 'K Neighbors', 'K␣
 ↪Neighbors Max', 'SVM', 'Categorical NB', 'Gaussian NB', 'Decision Tree',␣
 ↪'Decision Tree Max', 'Random Forest', 'Random Forest Max'],
                        'Accuracy': [LRAcc*100, KNAcc*100, KNAccMax*100,␣
 ↪SVCAcc*100, NBAcc1*100, NBAcc2*100, DTAcc*100, DTAccMax*100, RFAcc*100,␣
 ↪RFAccMax*100]})
compare.sort_values(by='Accuracy', ascending=False)
```

[58]:

	Model	Accuracy
0	Logistic Regression	83.333333
3	SVM	83.333333
8	Random Forest	83.333333
9	Random Forest Max	83.333333
4	Categorical NB	81.666667
2	K Neighbors Max	80.000000
7	Decision Tree Max	78.333333
6	Decision Tree	76.666667
1	K Neighbors	73.333333
5	Gaussian NB	70.000000

[59]:
```
# Now we need to get the predicted output

pred_lr = NBclassifier1.predict(X_test)
prediction = pd.DataFrame({'Sex_F': X_test.loc[:,"Sex_F"],
                           'Sex_M': X_test.loc[:,"Sex_M"],
                           'BP_HIGH': X_test.loc[:,"BP_HIGH"],
                           'BP_LOW': X_test.loc[:,"BP_LOW"],
                           'BP_NORMAL': X_test.loc[:,"BP_NORMAL"],
                           'Cholesterol_HIGH': X_test.loc[:,"Cholesterol_HIGH"],
                           'Cholesterol_NORMAL': X_test.loc[:
 ↪,"Cholesterol_NORMAL"],
                           'Age_binned_<20s': X_test.loc[:,"Age_binned_<20s"],
                           'Age_binned_20s': X_test.loc[:,"Age_binned_20s"],
                           'Age_binned_30s': X_test.loc[:,"Age_binned_30s"],
                           'Age_binned_40s': X_test.loc[:,"Age_binned_40s"],
                           'Age_binned_50s': X_test.loc[:,"Age_binned_50s"],
                           'Age_binned_60s': X_test.loc[:,"Age_binned_60s"],
                           'Age_binned_>60s': X_test.loc[:,"Age_binned_>60s"],
                           'Na_to_K_binned_<10': X_test.loc[:
 ↪,"Na_to_K_binned_<10"],
                           'Na_to_K_binned_10-20': X_test.loc[:
 ↪,"Na_to_K_binned_10-20"],
                           'Na_to_K_binned_20-30': X_test.loc[:
 ↪,"Na_to_K_binned_20-30"],
                           'Na_to_K_binned_>30': X_test.loc[:
 ↪,"Na_to_K_binned_>30"],'DrugType': pred_lr})
```

[60]:
```
# Sex
prediction['Sex_F'] = prediction['Sex_F'].replace([1, 0],['Female', 'Male'])

#BP
prediction['BP_HIGH'] = prediction['BP_HIGH'].replace([1, 0],['High',''])
prediction['BP_LOW'] = prediction['BP_LOW'].replace([1, 0],['Low', ''])
prediction['BP_NORMAL'] = prediction['BP_NORMAL'].replace([1, 0],['Normal', ''])
```

```
prediction['BP_HIGH'] = np.where((prediction['BP_HIGH'] == ''),␣
 ↪prediction['BP_LOW'], prediction['BP_HIGH'])
prediction['BP_HIGH'] = np.where((prediction['BP_HIGH'] == ''),␣
 ↪prediction['BP_NORMAL'], prediction['BP_HIGH'])

#Cholestrol
prediction['Cholesterol_HIGH'] = prediction['Cholesterol_HIGH'].replace([1,␣
 ↪0],['High', 'Normal'])

#Age_binned
prediction['Age_binned_<20s'] = prediction['Age_binned_<20s'].replace([1,␣
 ↪0],['<20s',''])
prediction['Age_binned_20s'] = prediction['Age_binned_20s'].replace([1,␣
 ↪0],['20s',''])
prediction['Age_binned_30s'] = prediction['Age_binned_30s'].replace([1,␣
 ↪0],['30s',''])
prediction['Age_binned_40s'] = prediction['Age_binned_40s'].replace([1,␣
 ↪0],['40s',''])
prediction['Age_binned_50s'] = prediction['Age_binned_50s'].replace([1,␣
 ↪0],['50s',''])
prediction['Age_binned_60s'] = prediction['Age_binned_60s'].replace([1,␣
 ↪0],['60s',''])
prediction['Age_binned_>60s'] = prediction['Age_binned_>60s'].replace([1,␣
 ↪0],['>60s',''])

prediction['Age_binned_<20s'] = np.where((prediction['Age_binned_<20s'] == ''),␣
 ↪prediction['Age_binned_20s'], prediction['Age_binned_<20s'])
prediction['Age_binned_<20s'] = np.where((prediction['Age_binned_<20s'] == ''),␣
 ↪prediction['Age_binned_30s'], prediction['Age_binned_<20s'])
prediction['Age_binned_<20s'] = np.where((prediction['Age_binned_<20s'] == ''),␣
 ↪prediction['Age_binned_40s'], prediction['Age_binned_<20s'])
prediction['Age_binned_<20s'] = np.where((prediction['Age_binned_<20s'] == ''),␣
 ↪prediction['Age_binned_50s'], prediction['Age_binned_<20s'])
prediction['Age_binned_<20s'] = np.where((prediction['Age_binned_<20s'] == ''),␣
 ↪prediction['Age_binned_60s'], prediction['Age_binned_<20s'])
prediction['Age_binned_<20s'] = np.where((prediction['Age_binned_<20s'] == ''),␣
 ↪prediction['Age_binned_>60s'], prediction['Age_binned_<20s'])

#Na to K
prediction['Na_to_K_binned_<10'] = prediction['Na_to_K_binned_<10'].replace([1,␣
 ↪0],['<10',''])
prediction['Na_to_K_binned_10-20'] = prediction['Na_to_K_binned_10-20'].
 ↪replace([1, 0],['10-20',''])
prediction['Na_to_K_binned_20-30'] = prediction['Na_to_K_binned_20-30'].
 ↪replace([1, 0],['20-30',''])
```

```
prediction['Na_to_K_binned_>30'] = prediction['Na_to_K_binned_>30'].replace([1,␣
↪0],['>30s',''])

prediction['Na_to_K_binned_<10'] = np.where((prediction['Na_to_K_binned_<10']␣
↪== ''), prediction['Na_to_K_binned_10-20'], prediction['Na_to_K_binned_<10'])
prediction['Na_to_K_binned_<10'] = np.where((prediction['Na_to_K_binned_<10']␣
↪== ''), prediction['Na_to_K_binned_20-30'], prediction['Na_to_K_binned_<10'])
prediction['Na_to_K_binned_<10'] = np.where((prediction['Na_to_K_binned_<10']␣
↪== ''), prediction['Na_to_K_binned_>30'], prediction['Na_to_K_binned_<10'])

# Drop columns
prediction = prediction.drop(['Sex_M', 'BP_LOW', 'BP_NORMAL',␣
↪'Cholesterol_NORMAL', 'Age_binned_20s', 'Age_binned_30s',
                'Age_binned_40s', 'Age_binned_50s', 'Age_binned_60s',␣
↪'Age_binned_>60s',
               'Na_to_K_binned_10-20', 'Na_to_K_binned_20-30',␣
↪'Na_to_K_binned_>30'], axis = 1)
```

[61]:
```
# Rename columns name
new_name = {'Sex_F': 'Sex', 'BP_HIGH': 'BP', 'Cholesterol_HIGH': 'Cholesterol',␣
↪'Age_binned_<20s': 'Age_binned',
          'Na_to_K_binned_<10': 'Na_to_K_binned'}
prediction.rename(columns=new_name, inplace=True)
```

[62]:
```
prediction.to_csv('prediction.csv', index=False)
predictioncsv = pd.read_csv('./prediction.csv')
predictioncsv.head()
```

[62]:

	Sex	BP	Cholesterol	Age_binned	Na_to_K_binned	DrugType
0	Male	Low	High	20s	<10	drugX
1	Female	Normal	High	20s	10-20	drugX
2	Male	Low	High	40s	20-30	drugY
3	Male	High	Normal	20s	>30s	drugY
4	Male	Normal	High	20s	20-30	drugY

[63]:
```
predictioncsv
```

[63]:

	Sex	BP	Cholesterol	Age_binned	Na_to_K_binned	DrugType
0	Male	Low	High	20s	<10	drugX
1	Female	Normal	High	20s	10-20	drugX
2	Male	Low	High	40s	20-30	drugY
3	Male	High	Normal	20s	>30s	drugY
4	Male	Normal	High	20s	20-30	drugY
5	Female	Low	Normal	20s	10-20	drugX
6	Female	Normal	High	20s	<10	drugX
7	Female	Low	Normal	30s	10-20	drugX
8	Male	Low	High	40s	10-20	drugC

9	Male	Normal	Normal	50s	<10	drugX
10	Male	High	Normal	20s	10-20	drugA
11	Female	High	Normal	<20s	20-30	drugY
12	Female	High	Normal	20s	20-30	drugY
13	Male	Low	Normal	30s	10-20	drugX
14	Male	High	High	60s	10-20	drugB
15	Male	Low	High	40s	10-20	drugC
16	Female	High	Normal	60s	>30s	drugY
17	Female	Normal	High	>60s	20-30	drugY
18	Male	Low	Normal	30s	10-20	drugX
19	Male	High	Normal	30s	10-20	drugA
20	Female	High	Normal	30s	10-20	drugA
21	Male	Normal	High	60s	10-20	drugX
22	Female	Normal	Normal	60s	<10	drugX
23	Female	Low	Normal	30s	10-20	drugX
24	Female	Low	Normal	30s	>30s	drugY
25	Female	Normal	High	30s	10-20	drugX
26	Female	Normal	High	60s	10-20	drugX
27	Female	Normal	Normal	50s	20-30	drugY
28	Male	Normal	High	30s	20-30	drugY
29	Female	Normal	Normal	50s	10-20	drugX
30	Male	Low	Normal	60s	10-20	drugX
31	Female	Low	High	20s	10-20	drugC
32	Male	High	Normal	40s	<10	drugA
33	Female	Normal	Normal	40s	<10	drugX
34	Male	Low	Normal	40s	>30s	drugY
35	Male	High	Normal	60s	20-30	drugY
36	Female	Normal	High	30s	<10	drugX
37	Female	Low	High	60s	10-20	drugC
38	Female	High	Normal	30s	10-20	drugA
39	Male	Normal	High	20s	10-20	drugX
40	Female	High	High	40s	20-30	drugY
41	Male	High	High	20s	10-20	drugA
42	Male	High	High	30s	>30s	drugY
43	Female	Low	Normal	60s	10-20	drugX
44	Female	Low	Normal	50s	20-30	drugY
45	Male	Low	Normal	40s	<10	drugX
46	Male	Normal	High	60s	10-20	drugX
47	Male	Low	Normal	20s	20-30	drugY
48	Female	High	Normal	30s	10-20	drugA
49	Male	High	Normal	>60s	10-20	drugB
50	Female	Normal	High	20s	20-30	drugY
51	Female	High	Normal	50s	10-20	drugB
52	Female	High	High	<20s	>30s	drugY
53	Female	High	High	50s	20-30	drugY
54	Male	Low	High	20s	<10	drugX
55	Female	Low	High	30s	>30s	drugY

```
56  Female  Normal      Normal       <20s           <10    drugX
57  Female  Normal        High        30s         10-20    drugX
58  Female  Normal        High       >60s         20-30    drugY
59    Male    High      Normal        60s         10-20    drugB
```

[ ]:
```
# We have our output of a 30% split in testing hence 60 rows out of 200␣
↪original dataset
```