Feature Selection

September 5, 2022

1 Exercício 7

Victor Emanuel Perticarrari Osório

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

from sklearn.tree import DecisionTreeClassifier, plot_tree, export_text,␣
 ↪export_graphviz
from sklearn.ensemble import ExtraTreesClassifier, RandomForestClassifier
from sklearn.feature_selection import SelectFromModel, SelectKBest, chi2,␣
 ↪SequentialFeatureSelector
from sklearn.metrics import classification_report, confusion_matrix,␣
 ↪make_scorer, precision_score, get_scorer_names
from sklearn.model_selection import cross_val_score, train_test_split
from sklearn.linear_model import RidgeCV, LogisticRegression

from sklearn.preprocessing import MinMaxScaler, StandardScaler, LabelEncoder
from sklearn.decomposition import PCA

import matplotlib.pyplot as plt
import seaborn as sns

import warnings
warnings.filterwarnings('ignore')
```

2 A) Seleção de atributos e redução de dimensionalidade

2.1 1.Carregando Dataset

Lendo dataset a considerando a categoria como números

[2]:
```
dfGeneDrug = pd.read_csv('gene-drug-test.csv').set_index('name')
dfGeneDrug['Category'] = pd.Categorical(dfGeneDrug['Category'])
dfGeneDrug['Code'] = dfGeneDrug['Category'].cat.codes

dfGeneDrug
```

[2]:

name	Mitomycin	Porfiromycin	Carmustine_(BCNU)	Chlorozotocin	Clomesone	\
ABCA1	-0.005728	-0.010251	0.213157	0.255619	0.087824	
ABCA2	-0.044587	0.043600	-0.107541	0.002564	0.057564	
ABCA4	0.018894	0.097074	0.212427	-0.041018	0.213042	
ABCA5	-0.010097	-0.050817	-0.201478	-0.119905	-0.300130	
ABCA7	0.022397	0.069963	-0.091184	-0.145500	-0.137955	
…	…	…	…	…	…	
VDAC3	-0.067146	-0.110991	-0.007510	0.000456	0.057175	
VIAAT	-0.017425	0.003690	-0.199145	-0.057808	-0.274055	
VIAATb	-0.132056	-0.078568	-0.117847	-0.215210	-0.271793	
VTN	0.062329	0.083597	0.012069	0.123423	0.177653	
XT3	-0.088552	-0.071734	-0.000497	0.046212	-0.046280	

name	Lomustine_(CCNU)	Mitozolamide	PCNU	Semustine_(MeCCNU)	\
ABCA1	0.302058	0.175523	0.164136	0.177113	
ABCA2	0.047830	-0.088138	0.029925	-0.034347	
ABCA4	0.057218	0.087730	0.093837	0.139256	
ABCA5	-0.154843	-0.171674	-0.210085	-0.132950	
ABCA7	-0.138202	-0.109726	-0.110401	-0.126757	
…	…	…	…	…	
VDAC3	0.157436	0.006010	0.121504	-0.030282	
VIAAT	-0.220356	-0.056733	-0.157432	-0.134191	
VIAATb	-0.107600	-0.203604	-0.208581	-0.250593	
VTN	0.028369	0.122214	0.061530	0.160445	
XT3	0.081984	0.055162	-0.082070	-0.002011	

name	Asaley	…	Taxol_analog_9	Taxol_analog_10	Taxol_analog_11	\
ABCA1	0.355767	…	0.124049	0.009704	-0.052499	
ABCA2	0.068064	…	-0.011423	0.060266	0.109640	
ABCA4	0.132200	…	0.146479	0.061052	-0.032011	
ABCA5	-0.181702	…	0.074752	0.153693	0.143052	
ABCA7	-0.112074	…	0.190451	0.222634	0.167930	
…	…	…	…	…	…	
VDAC3	-0.159701	…	0.111908	0.213902	0.297173	
VIAAT	-0.148598	…	-0.074962	-0.152942	-0.197705	
VIAATb	-0.039191	…	-0.098141	-0.035195	-0.049813	
VTN	0.023510	…	-0.119578	-0.081854	-0.158878	
XT3	0.031663	…	-0.024405	-0.059185	-0.024037	

name	Geldanamycin	3-Hydropicolinaldehyde-thiosemicarbazone	\
ABCA1	0.074925	0.318216	
ABCA2	0.099574	0.093316	
ABCA4	0.127430	-0.028956	

```
ABCA5       0.079874                                    -0.233601
ABCA7       0.091479                                    -0.099894
…              …                                          …
VDAC3       0.118500                                    -0.026009
VIAAT      -0.132760                                    -0.014061
VIAATb     -0.020701                                     0.018523
VTN        -0.094915                                    -0.021906
XT3        -0.012944                                     0.117066

        5-Hydroxypicolinaldehyde-thiosemicarbazone  Inosine-glycodialdehyde  \
name
ABCA1                                     0.182131                -0.065994
ABCA2                                     0.220406                 0.134427
ABCA4                                    -0.046351                 0.101048
ABCA5                                    -0.265675                -0.148781
ABCA7                                     0.046425                 0.054116
…                                            …                        …
VDAC3                                     0.018550                 0.082448
VIAAT                                    -0.008111                -0.149030
VIAATb                                   -0.051314                 0.039436
VTN                                       0.059610                -0.155153
XT3                                       0.183880                 0.035084

        Gemcitabine     Category  Code
name
ABCA1      0.121245  Transporter     5
ABCA2      0.154513  Transporter     5
ABCA4      0.011623  Transporter     5
ABCA5     -0.126315  Transporter     5
ABCA7      0.031716  Transporter     5
…             …          …   …
VDAC3     -0.000955      Channel     1
VIAAT      0.034586  Transporter     5
VIAATb    -0.020127  Transporter     5
VTN       -0.034415  Transporter     5
XT3        0.032701  Transporter     5

[732 rows x 121 columns]
```

2.1.1 Vendo correlação entre colunas

O próximo passo é ver a correlação entre as colunas, quanto mais próximo de 1, maior a correlação. Colunas com correlação alta podem indicar colunas que podem ser descartados.

[3]:
```
corr = dfGeneDrug.corr()
corr
```

[3]:

	Mitomycin	Porfiromycin	\
Mitomycin	1.000000	0.902602	
Porfiromycin	0.902602	1.000000	
Carmustine_(BCNU)	0.456340	0.370992	
Chlorozotocin	0.392093	0.233868	
Clomesone	0.549755	0.502399	
…	…	…	
3-Hydropicolinaldehyde-thiosemicarbazone	0.383983	0.369012	
5-Hydroxypicolinaldehyde-thiosemicarbazone	0.441555	0.425478	
Inosine-glycodialdehyde	0.038879	0.146733	
Gemcitabine	0.556483	0.545793	
Code	0.044154	0.056343	

	Carmustine_(BCNU)	Chlorozotocin	\
Mitomycin	0.456340	0.392093	
Porfiromycin	0.370992	0.233868	
Carmustine_(BCNU)	1.000000	0.522208	
Chlorozotocin	0.522208	1.000000	
Clomesone	0.715443	0.726280	
…	…	…	
3-Hydropicolinaldehyde-thiosemicarbazone	0.368214	0.499847	
5-Hydroxypicolinaldehyde-thiosemicarbazone	0.546623	0.415818	
Inosine-glycodialdehyde	0.517120	-0.149108	
Gemcitabine	0.388289	0.442967	
Code	0.006737	-0.017678	

	Clomesone	Lomustine_(CCNU)	\
Mitomycin	0.549755	0.340960	
Porfiromycin	0.502399	0.265006	
Carmustine_(BCNU)	0.715443	0.745182	
Chlorozotocin	0.726280	0.586364	
Clomesone	1.000000	0.656543	
…	…	…	
3-Hydropicolinaldehyde-thiosemicarbazone	0.488716	0.466478	
5-Hydroxypicolinaldehyde-thiosemicarbazone	0.547287	0.510055	
Inosine-glycodialdehyde	0.172895	0.417781	
Gemcitabine	0.468424	0.379310	
Code	-0.026582	-0.011139	

	Mitozolamide	PCNU	\
Mitomycin	0.622375	0.582913	
Porfiromycin	0.526877	0.479945	
Carmustine_(BCNU)	0.653678	0.719003	
Chlorozotocin	0.831874	0.775605	
Clomesone	0.793993	0.863937	
…	…	…	
3-Hydropicolinaldehyde-thiosemicarbazone	0.421311	0.469974	

5-Hydroxypicolinaldehyde-thiosemicarbazone	0.475257	0.511323
Inosine-glycodialdehyde	0.012877	0.118856
Gemcitabine	0.483398	0.541830
Code	0.018413	-0.047352

	Semustine_(MeCCNU)	Asaley	…	\
Mitomycin	0.430202	0.306406	…	
Porfiromycin	0.447188	0.240346	…	
Carmustine_(BCNU)	0.750335	0.686311	…	
Chlorozotocin	0.481568	0.494786	…	
Clomesone	0.725378	0.529508	…	
…	…	…	…	
3-Hydropicolinaldehyde-thiosemicarbazone	0.283867	0.522614	…	
5-Hydroxypicolinaldehyde-thiosemicarbazone	0.418922	0.612888	…	
Inosine-glycodialdehyde	0.270457	0.463499	…	
Gemcitabine	0.244664	0.453511	…	
Code	0.030725	-0.045232	…	

	Taxol_analog_8	Taxol_analog_9	\
Mitomycin	0.203923	0.280435	
Porfiromycin	0.137871	0.316153	
Carmustine_(BCNU)	0.329907	0.519078	
Chlorozotocin	0.010823	0.018646	
Clomesone	0.094238	0.241603	
…	…	…	
3-Hydropicolinaldehyde-thiosemicarbazone	0.112923	-0.004479	
5-Hydroxypicolinaldehyde-thiosemicarbazone	0.092636	0.187779	
Inosine-glycodialdehyde	0.463399	0.508514	
Gemcitabine	0.020493	0.008276	
Code	0.097788	0.044620	

	Taxol_analog_10	Taxol_analog_11	\
Mitomycin	0.325142	0.231929	
Porfiromycin	0.281367	0.267427	
Carmustine_(BCNU)	0.477727	0.225274	
Chlorozotocin	0.071617	-0.136422	
Clomesone	0.202812	0.019360	
…	…	…	
3-Hydropicolinaldehyde-thiosemicarbazone	0.011351	-0.132539	
5-Hydroxypicolinaldehyde-thiosemicarbazone	0.245686	0.057764	
Inosine-glycodialdehyde	0.493748	0.462697	
Gemcitabine	0.027095	-0.124626	
Code	0.036523	0.080787	

	Geldanamycin	\
Mitomycin	0.163517	
Porfiromycin	0.178115	

```
Carmustine_(BCNU)                                0.486130
Chlorozotocin                                   -0.032953
Clomesone                                        0.173263
…                                                     …
3-Hydropicolinaldehyde-thiosemicarbazone        -0.010993
5-Hydroxypicolinaldehyde-thiosemicarbazone       0.252290
Inosine-glycodialdehyde                          0.678485
Gemcitabine                                     -0.133829
Code                                             0.019303

                                                 3-Hydropicolinaldehyde-
thiosemicarbazone  \
Mitomycin
0.383983
Porfiromycin
0.369012
Carmustine_(BCNU)
0.368214
Chlorozotocin
0.499847
Clomesone
0.488716
…
…
3-Hydropicolinaldehyde-thiosemicarbazone
1.000000
5-Hydroxypicolinaldehyde-thiosemicarbazone
0.772269
Inosine-glycodialdehyde
0.081629
Gemcitabine
0.738221
Code
0.060458

                                                 5-Hydroxypicolinaldehyde-
thiosemicarbazone  \
Mitomycin
0.441555
Porfiromycin
0.425478
Carmustine_(BCNU)
0.546623
Chlorozotocin
0.415818
Clomesone
0.547287
```

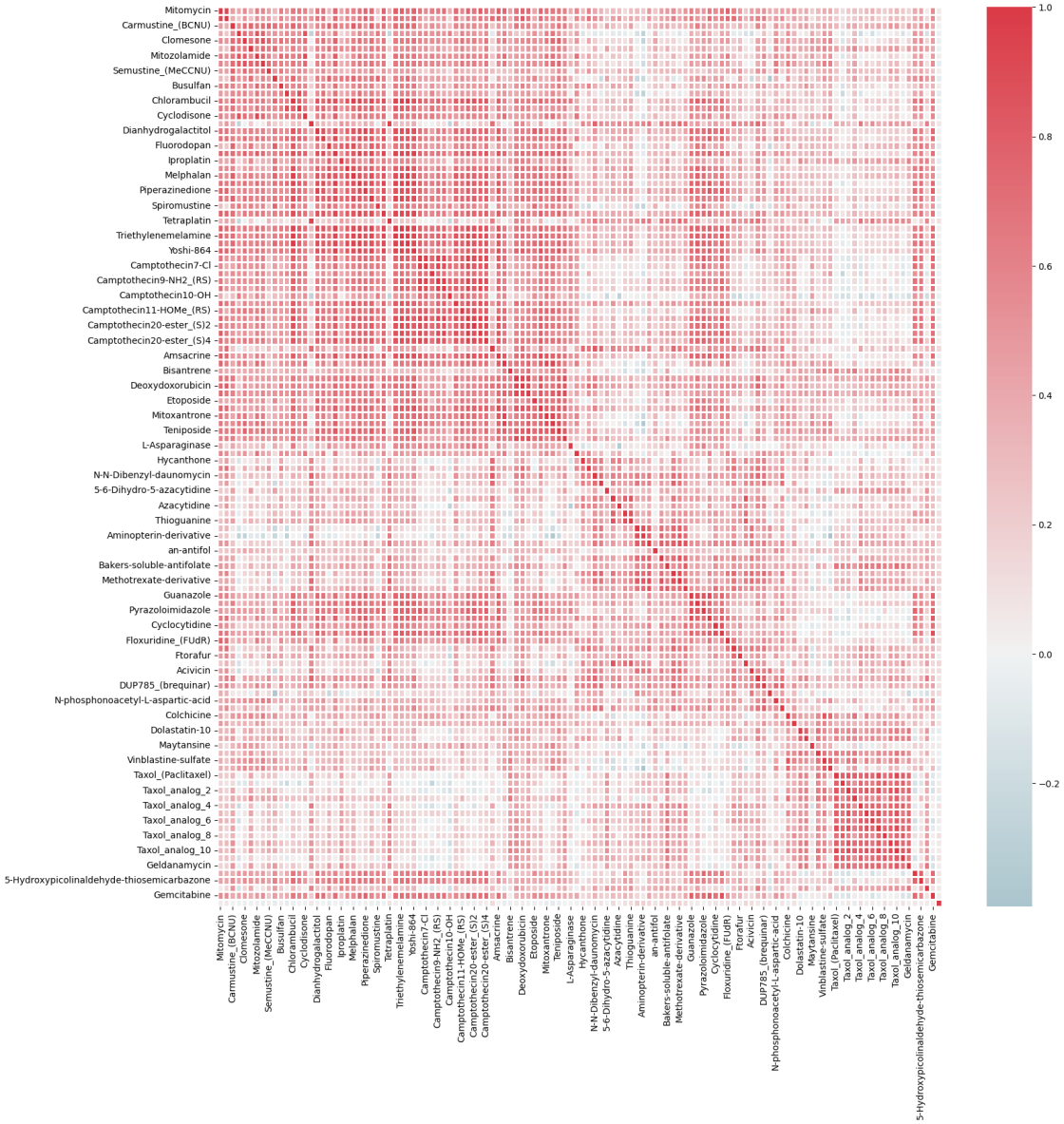
```
…
…
3-Hydropicolinaldehyde-thiosemicarbazone
0.772269
5-Hydroxypicolinaldehyde-thiosemicarbazone
1.000000
Inosine-glycodialdehyde
0.343972
Gemcitabine
0.589509
Code
0.023963
```

	Inosine-glycodialdehyde	\
Mitomycin	0.038879	
Porfiromycin	0.146733	
Carmustine_(BCNU)	0.517120	
Chlorozotocin	-0.149108	
Clomesone	0.172895	
…	…	
3-Hydropicolinaldehyde-thiosemicarbazone	0.081629	
5-Hydroxypicolinaldehyde-thiosemicarbazone	0.343972	
Inosine-glycodialdehyde	1.000000	
Gemcitabine	0.103356	
Code	0.039775	

	Gemcitabine	Code
Mitomycin	0.556483	0.044154
Porfiromycin	0.545793	0.056343
Carmustine_(BCNU)	0.388289	0.006737
Chlorozotocin	0.442967	-0.017678
Clomesone	0.468424	-0.026582
…	…	…
3-Hydropicolinaldehyde-thiosemicarbazone	0.738221	0.060458
5-Hydroxypicolinaldehyde-thiosemicarbazone	0.589509	0.023963
Inosine-glycodialdehyde	0.103356	0.039775
Gemcitabine	1.000000	0.031913
Code	0.031913	1.000000

[120 rows x 120 columns]

[4]:
```
f, ax = plt.subplots(figsize=(18, 18))
cmap = sns.diverging_palette(220, 10, as_cmap=True)
heatmap = sns.heatmap(corr, cmap=cmap, center=0.0, vmax=1, linewidths=1, ax=ax)
```



2.2 Baseline

Para criar o baseline vamos primeiro normalizar os dados usando MinMaxScaler. E depois todas as validações serão feitas usando os valores padrão para `DecisionTreeClassifier`

[5]:
```
scaler = MinMaxScaler()
dfGeneDrug[dfGeneDrug.columns.difference(['Category', 'Code'])] = scaler.
  ↪fit_transform(dfGeneDrug[dfGeneDrug.columns.difference(['Category',␣
  ↪'Code'])])
dfGeneDrug
```

[5]:

name	Mitomycin	Porfiromycin	Carmustine_(BCNU)	Chlorozotocin	Clomesone
ABCA1	0.447080	0.501244	0.732737	0.783864	0.534845
ABCA2	0.391110	0.572022	0.375981	0.440372	0.498302
ABCA4	0.482542	0.642305	0.731925	0.381214	0.686058
ABCA5	0.440787	0.447926	0.271482	0.274136	0.066351
ABCA7	0.487588	0.606672	0.394177	0.239393	0.262193
…	…	…	…	…	…
VDAC3	0.358619	0.368838	0.487259	0.437511	0.497833
VIAAT	0.430232	0.519566	0.274078	0.358424	0.097839
VIAATb	0.265128	0.411453	0.364516	0.144770	0.100571
VTN	0.545102	0.624592	0.509039	0.604423	0.643323
XT3	0.327787	0.420435	0.495061	0.499619	0.372901

name	Lomustine_(CCNU)	Mitozolamide	PCNU	Semustine_(MeCCNU)
ABCA1	0.819563	0.721087	0.678801	0.776177
ABCA2	0.529071	0.394485	0.519215	0.511973
ABCA4	0.539797	0.612337	0.595210	0.728878
ABCA5	0.297487	0.291007	0.233826	0.388775
ABCA7	0.316502	0.367744	0.352356	0.396513
…	…	…	…	…
VDAC3	0.654312	0.511108	0.628108	0.517051
VIAAT	0.222629	0.433387	0.296434	0.387225
VIAATb	0.351469	0.251455	0.235615	0.241788
VTN	0.506834	0.655052	0.556795	0.755351
XT3	0.568097	0.571993	0.386045	0.552374

name	Asaley	…	Taxol_analog_9	Taxol_analog_10	Taxol_analog_11
ABCA1	0.895434	…	0.680105	0.612274	0.499645
ABCA2	0.603944	…	0.521421	0.670323	0.695612
ABCA4	0.668924	…	0.706378	0.671225	0.524407
ABCA5	0.350890	…	0.622361	0.777583	0.735995
ABCA7	0.421434	…	0.757883	0.856731	0.766063
…	…	…	…	…	…
VDAC3	0.373181	…	0.665883	0.846706	0.922270
VIAAT	0.384430	…	0.446997	0.425548	0.324144
VIAATb	0.495277	…	0.419846	0.560728	0.502891
VTN	0.558804	…	0.394737	0.507161	0.371071
XT3	0.567063	…	0.506216	0.533186	0.534045

name	Geldanamycin	3-Hydropicolinaldehyde-thiosemicarbazone
ABCA1	0.616894	0.924229
ABCA2	0.642648	0.640220
ABCA4	0.671752	0.485812

```
ABCA5       0.622065                                    0.227380
ABCA7       0.634190                                    0.396229
…              …                                         …
VDAC3       0.662422                                    0.489532
VIAAT       0.399906                                    0.504621
VIAATb      0.516985                                    0.545768
VTN         0.439446                                    0.494714
XT3         0.525089                                    0.670211

        5-Hydroxypicolinaldehyde-thiosemicarbazone  Inosine-glycodialdehyde  \
name
ABCA1                                     0.710535                 0.490417
ABCA2                                     0.757766                 0.687806
ABCA4                                     0.428586                 0.654932
ABCA5                                     0.157937                 0.408882
ABCA7                                     0.543072                 0.608710
…                                            …                        …
VDAC3                                     0.508674                 0.636613
VIAAT                                     0.475774                 0.408636
VIAATb                                    0.422462                 0.594252
VTN                                       0.559342                 0.402606
XT3                                       0.712693                 0.589965

        Gemcitabine     Category  Code
name
ABCA1      0.598000  Transporter     5
ABCA2      0.640517  Transporter     5
ABCA4      0.457902  Transporter     5
ABCA5      0.281614  Transporter     5
ABCA7      0.483580  Transporter     5
…             …           …   …
VDAC3      0.441826      Channel     1
VIAAT      0.487249  Transporter     5
VIAATb     0.417325  Transporter     5
VTN        0.399064  Transporter     5
XT3        0.484840  Transporter     5

[732 rows x 121 columns]
```

[6]:
```
X = dfGeneDrug.iloc[:,:-2]
y = dfGeneDrug['Code']

dfGeneDrug_train, dfGeneDrug_test = train_test_split(dfGeneDrug, test_size=0.2,␣
 ↪stratify=dfGeneDrug['Code'])

X_test = dfGeneDrug_test.iloc[:,:-2]
y_test = dfGeneDrug_test['Code']
```

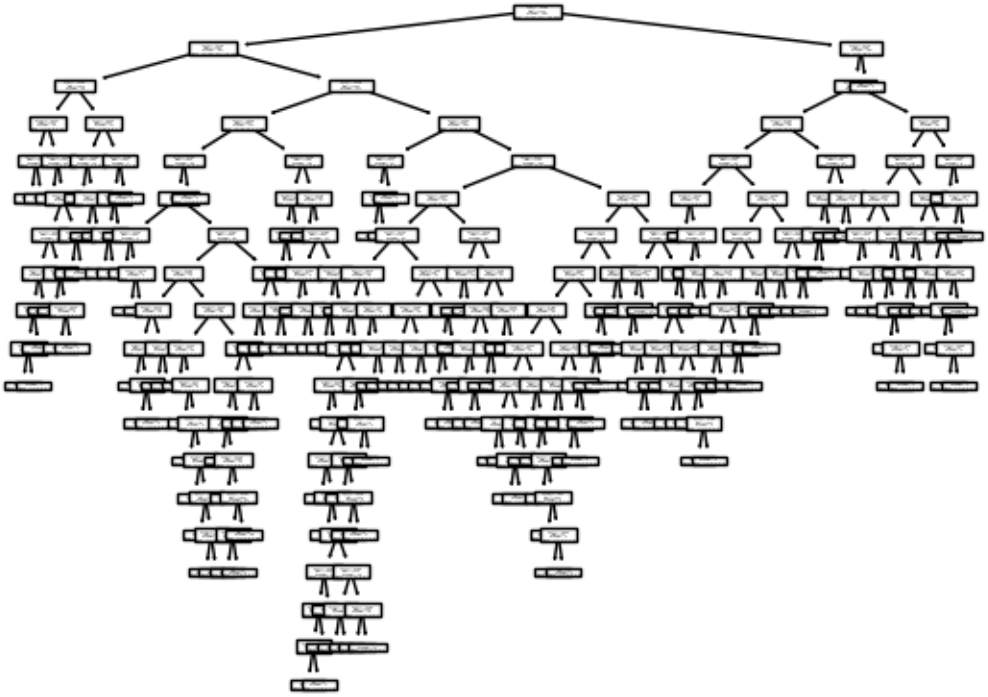
```
X_train = dfGeneDrug_train.iloc[:,:-2]
y_train = dfGeneDrug_train['Code']

feature_names = dfGeneDrug.columns[:-2]


print("Train: {} Test: {}".format(dfGeneDrug_train.shape, dfGeneDrug_test.
 ↪shape))
```

```
Train: (585, 121) Test: (147, 121)
```

[7]:
```
## print("Possível scores: {}".format(get_scorer_names()))
```

[8]:
```
tree_model = DecisionTreeClassifier(random_state=0).fit(X_train, y_train)

f1_score  = cross_val_score(tree_model, X_test, y_test, cv=5,␣
 ↪scoring='f1_macro').mean() * 100
print("F1 Score: {0:2.2f}%".format(f1_score))
print("Nós: {} Profundidade: {}".format(tree_model.get_n_leaves(), tree_model.
 ↪get_depth()))


plot_tree(tree_model)
plt.show()
```

```
F1 Score: 13.46%
Nós: 174 Profundidade: 18
```

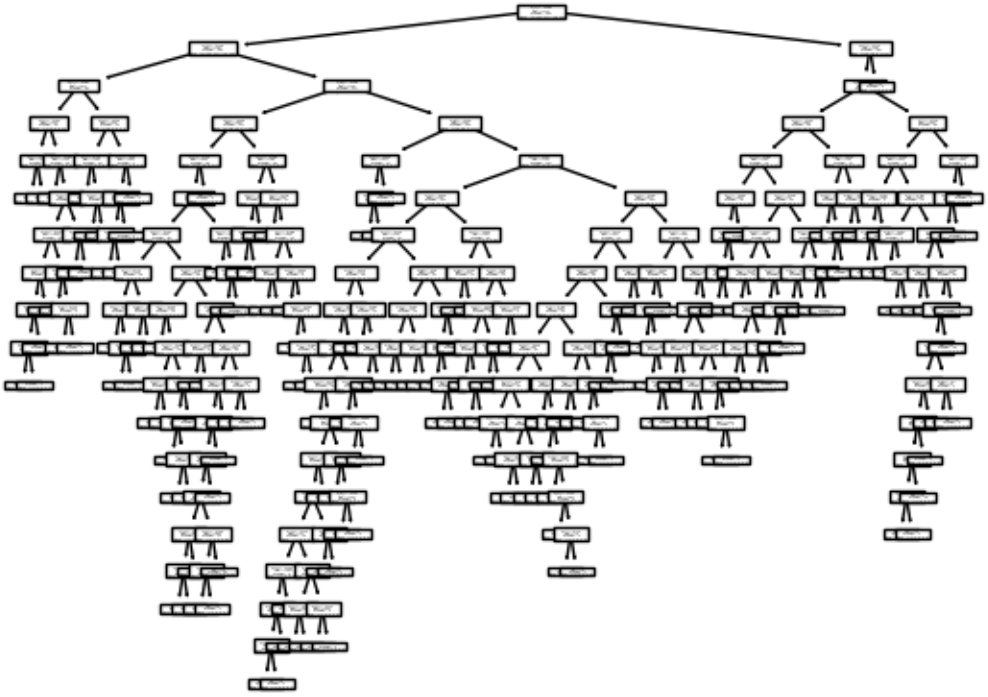


2.3 1. Usando *Seleção de features baseadas em modelo*

[9]:
```
select_model = SelectFromModel(tree_model, prefit=True)
X_train_new = select_model.transform(X_train)
X_test_new = select_model.transform(X_test)
print("Old shape: {} New shape: {}".format(X_train.shape, X_train_new.shape))

reduced_model = DecisionTreeClassifier(random_state=0).fit(X_train_new, y_train)

f1_score  = cross_val_score(reduced_model, X_test_new, y_test, cv=5,␣
 ↪scoring='f1_macro').mean() * 100
print("F1 Score: {0:2.2f}%".format(f1_score))
print("Nós: {} Profundidade: {}".format(reduced_model.get_n_leaves(),␣
 ↪reduced_model.get_depth()))
print("Colunas selecionadas: {}".format(feature_names[select_model.
 ↪get_support()]))

plot_tree(reduced_model)
plt.show()
```

```
Old shape: (585, 119) New shape: (585, 50)
F1 Score: 20.66%
Nós: 177 Profundidade: 18
```

```
Colunas selecionadas: Index(['Mitomycin', 'Asaley', 'Diaminocyclohexyl-Pt-II',
       'Diaziridinylbenzoquinone', 'Iproplatin', 'Camptothecin9-MeO',
       'Camptothecin11-formyl_(RS)', 'Amonafide', 'Amsacrine', 'Daunorubicin',
       'Mitoxantrone', 'Teniposide', 'L-Asparaginase', 'Hycanthone',
       'Morpholino-adriamycin', 'N-N-Dibenzyl-daunomycin',
       '5-6-Dihydro-5-azacytidine', 'alpha-2-Deoxythioguanosine',
       'Azacytidine', 'beta-2-Deoxythioguanosine', 'Aminopterin-derivative',
       'Aminopterin-derivative2', 'Methotrexate', 'Methotrexate-derivative',
       'Trimetrexate', 'Hydroxyurea', 'Floxuridine_(FUdR)',
       'Fluorouracil_(5FU)', 'Ftorafur', 'Thiopurine_(6MP)',
       'Dichloroallyl-lawsone', 'DUP785_(brequinar)', 'L-Alanosine',
       'N-phosphonoacetyl-L-aspartic-acid', 'Colchicine', 'Dolastatin-10',
       'Halichondrin_B', 'Maytansine', 'Trityl-cysteine',
       'Vinblastine-sulfate', 'Vincristine-sulfate', 'Taxol_analog_1',
       'Taxol_analog_6', 'Taxol_analog_7', 'Taxol_analog_9', 'Taxol_analog_11',
       'Geldanamycin', '3-Hydropicolinaldehyde-thiosemicarbazone',
       '5-Hydroxypicolinaldehyde-thiosemicarbazone', 'Gemcitabine'],
      dtype='object')
```



2.4 2. Usando *Seleção baseada em importância*

[10]:
```
ridge = RidgeCV().fit(X, y)

importance = np.abs(ridge.coef_)
threshold = np.sort(importance)[-5] + 0.1

sfm = SelectFromModel(ridge, threshold=threshold).fit(X, y)
X_train_new = sfm.transform(X_train)
X_test_new = sfm.transform(X_test)
print("Old shape: {} New shape: {}".format(X_train.shape, X_train_new.shape))

reduced_model = DecisionTreeClassifier(random_state=0).fit(X_train_new, y_train)

f1_score  = cross_val_score(reduced_model, X_test_new, y_test, cv=5,␣
 ↪scoring='f1_macro').mean() * 100
print("F1 Score: {0:2.2f}%".format(f1_score))
print("Nós: {} Profundidade: {}".format(reduced_model.get_n_leaves(),␣
 ↪reduced_model.get_depth()))
print("Colunas selecionadas: {}".format(feature_names[sfm.get_support()]))

plot_tree(reduced_model)
plt.show()
```

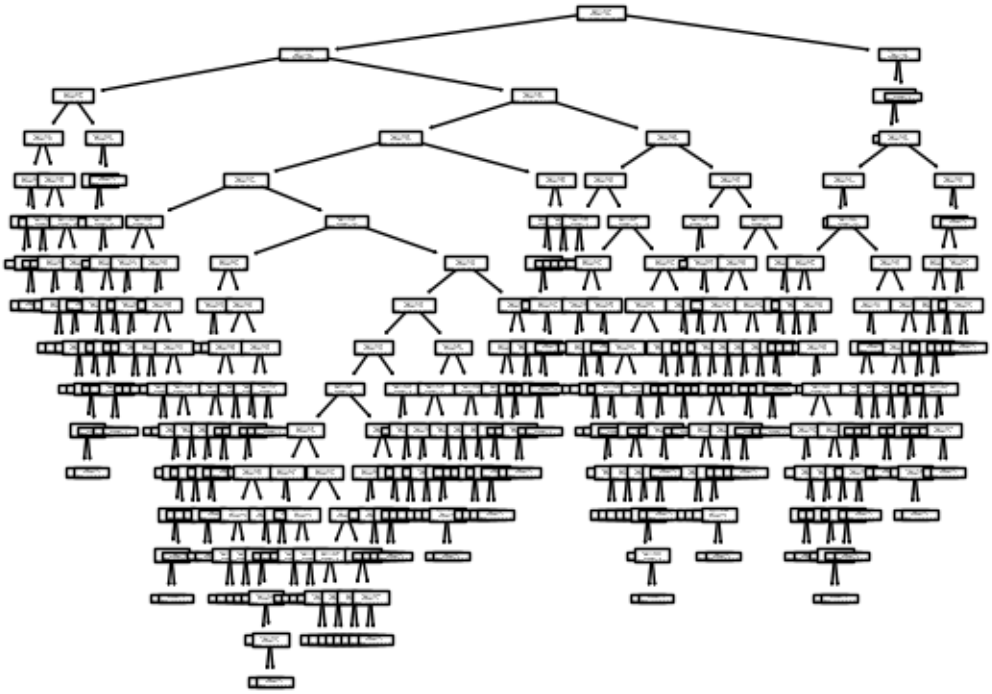
```
Old shape: (585, 119) New shape: (585, 1)
F1 Score: 19.29%
Nós: 413 Profundidade: 26
Colunas selecionadas: Index(['Maytansine'], dtype='object')
```

2.5 3. Usando *Seleção de features univariada*

[11]:
```
selector = SelectKBest(chi2).fit(X, y)
X_train_new = selector.transform(X_train)
X_test_new = selector.transform(X_test)
print("Old shape: {} New shape: {}".format(X_train.shape, X_train_new.shape))

reduced_model = DecisionTreeClassifier(random_state=0).fit(X_train_new, y_train)

f1_score  = cross_val_score(reduced_model, X_test_new, y_test, cv=5,␣
 ↪scoring='f1_macro').mean() * 100
print("F1 Score: {0:2.2f}%".format(f1_score))
print("Nós: {} Profundidade: {}".format(reduced_model.get_n_leaves(),␣
 ↪reduced_model.get_depth()))
print("Colunas selecionadas: {}".format(feature_names[selector.get_support()]))

plot_tree(reduced_model)
plt.show()
```

```
Old shape: (585, 119) New shape: (585, 10)
F1 Score: 12.76%
Nós: 220 Profundidade: 16
Colunas selecionadas: Index(['L-Asparaginase', 'Hycanthone',
```

```
'alpha-2-Deoxythioguanosine',
       'Thioguanine', 'Aminopterin', 'Aminopterin-derivative', 'an-antifol2',
       'Methotrexate', 'Methotrexate-derivative', 'Thiopurine_(6MP)'],
      dtype='object')
```



2.6 4. Usando *Seletor Sequencial*

[12]:
```
selector = SequentialFeatureSelector(tree_model, n_features_to_select=10).
 ↪fit(X, y)
X_train_new = selector.transform(X_train)
X_test_new = selector.transform(X_test)

print("Old shape: {} New shape: {}".format(X_train.shape, X_train_new.shape))

reduced_model = DecisionTreeClassifier(random_state=0).fit(X_train_new, y_train)

f1_score  = cross_val_score(reduced_model, X_test_new, y_test, cv=5,␣
 ↪scoring='f1_macro').mean() * 100
print("F1 Score: {0:2.2f}%".format(f1_score))
print("Nós: {} Profundidade: {}".format(reduced_model.get_n_leaves(),␣
 ↪reduced_model.get_depth()))
print("Colunas selecionadas: {}".format(feature_names[selector.get_support()]))
```

```
plot_tree(reduced_model)
plt.show()
```

```
Old shape: (585, 119) New shape: (585, 10)
F1 Score: 18.51%
Nós: 229 Profundidade: 23
Colunas selecionadas: Index(['Busulfan', 'Triethylenemelamine',
'Camptothecin9-MeO',
       'Camptothecin20-ester_(S)1', 'an-antifol2', 'Cytarabine_(araC)',
       'Pyrazofurin', 'Vincristine-sulfate', 'Taxol_(Paclitaxel)',
       'Taxol_analog_5'],
      dtype='object')
```

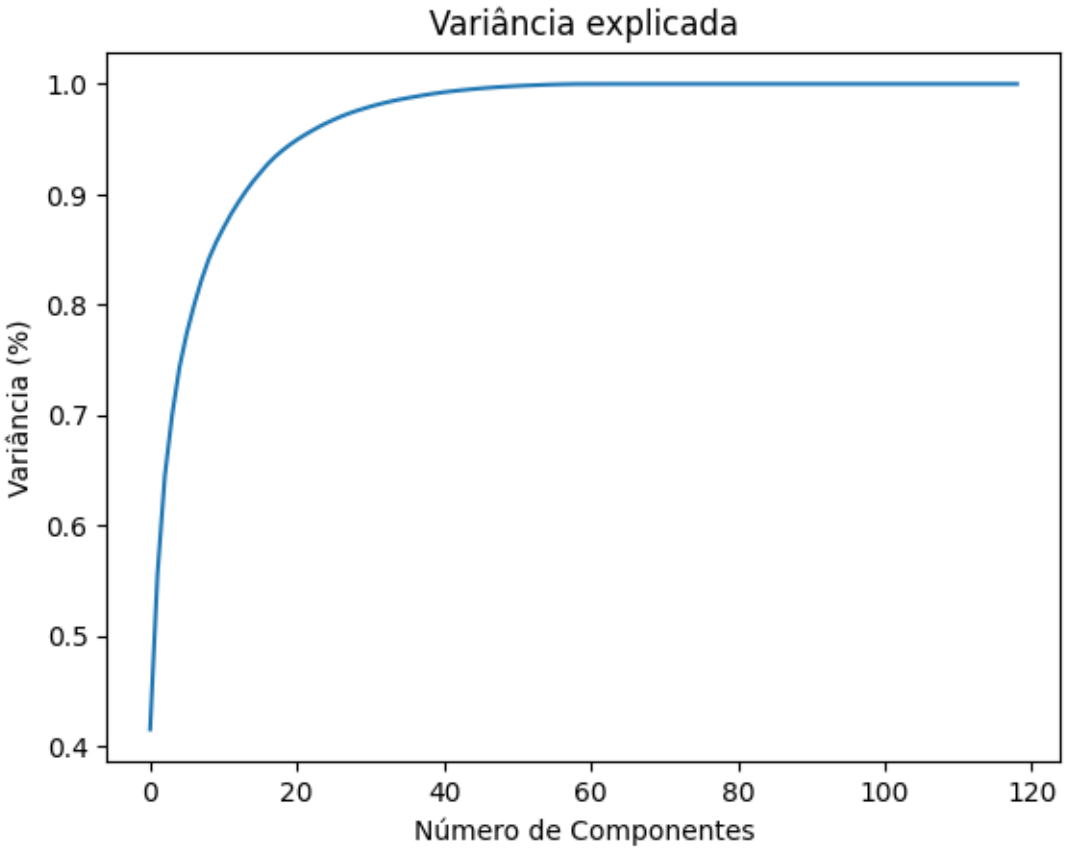
2.7 5. Usando PCA

[ ]:

2.7.1 PCA

[13]:
```
pca = PCA()
principal_components = pca.fit_transform(X)
plt.figure()
plt.plot(np.cumsum(pca.explained_variance_ratio_))
```

```
plt.xlabel("Número de Componentes")
plt.ylabel("Variância (%)")
plt.title("Variância explicada")
plt.show()
```

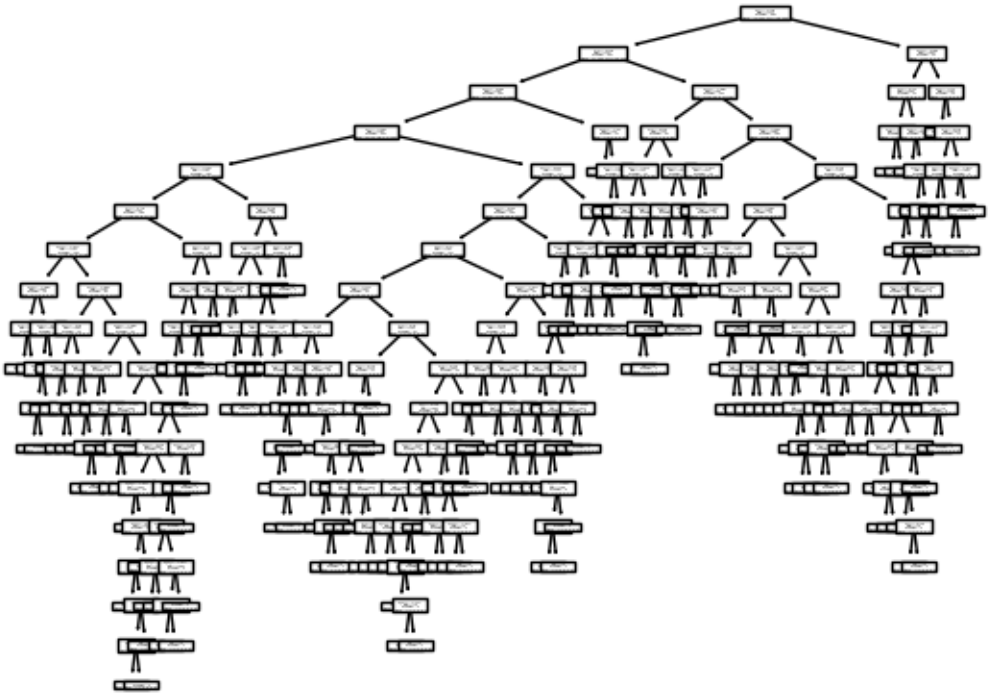


De acordo com o gráfico acima, se selecionarmos por volta de 19 features temos uma boa seleção de valores.

[14]:
```
pca = PCA(n_components=20).fit(X)
X_train_new = pca.transform(X_train)
X_test_new = pca.transform(X_test)

print("Old shape: {} New shape: {}".format(X_train.shape, X_train_new.shape))

reduced_model = DecisionTreeClassifier().fit(X_train_new, y_train)

f1_score  = cross_val_score(reduced_model, X_test_new, y_test, cv=5,␣
 ↪scoring='f1_weighted').mean() * 100
print("F1 Score: {0:2.2f}%".format(f1_score))
```

```
print("Nós: {} Profundidade: {}".format(reduced_model.get_n_leaves(),␣
 ↪reduced_model.get_depth()))

plot_tree(reduced_model)
plt.show()
```

```
Old shape: (585, 119) New shape: (585, 20)
F1 Score: 27.19%
Nós: 185 Profundidade: 17
```



2.8 Conclusões

Usando os valores padrão para `DecisionTreeClassifier` percebeu-se que houve um aumento da qualidade de acordo com o número de features selecionadas para alguns métodos. Esse dataset tem um conjunto ótimo de features em torno de 19 features. Usando o PCA temos um aumento significativo, mas ele não seleciona as features e sim cria um conjunto novo de features baseadas nas features originais.

AVISO Os valores de *F1 Score* são baseados em execuções anteriores.

Método	F1 Score	Análise
Baseline	18.03%	Base

Método	F1 Score	Análise
Modelo	16.35%	Como é baseado no baseline, o aumento foi pouco e depois apresentou redução. Provavel que esse aumento seja referente a remoção de ruídos.
RidgeCV	15.11%	Caiu a qualidade. Não é um bom seletor para esse modelo
Univariada	19.71%	A seleção basead no chi^2 apresentou um desempenho melhor por remover o erro do baseline. Selecionando as melhroes features
Sequencial	18.47%	A seleção sequencial apresentou um bom score, mas ficou abaixo do chi^2
PCA	23.79%	Melhor método de seleção de features.

3 B) Desafio

1. Considerando o que é pedido no desafio, faça um classificador utilizando Floresta Aleatória. Teste o desempenho utilizando todos os atributos disponíveis. Este será o seu baseline.
2. Utilize o PCA, bem como algumas técnicas de seleção de atributos e avalie se o desempenho de classificação melhorou em relação ao baseline.
3. Avalie criticamente se alguma estratégia de seleção de atributos ou o PCA deve ser considerada em novas propostas de modelos de classificação no contexto do desafio. Justifique a sua resposta

3.1 Baseline

Para criar o baseline escolhi o critério **entropia** por apresentar um score F1 melhor.

[15]:
```
X = dfGeneDrug.iloc[:,:-2]
y = dfGeneDrug['Code']

dfGeneDrug_train, dfGeneDrug_test = train_test_split(dfGeneDrug, test_size=0.2,␣
 ↪stratify=dfGeneDrug['Code'])

X_test = dfGeneDrug_test.iloc[:,:-2]
y_test = dfGeneDrug_test['Code']

X_train = dfGeneDrug_train.iloc[:,:-2]
y_train = dfGeneDrug_train['Code']
```

```
feature_names = dfGeneDrug.columns[:-2]


print("Train: {} Test: {}".format(dfGeneDrug_train.shape, dfGeneDrug_test.
 ↪shape))
```

```
Train: (585, 121) Test: (147, 121)
```

[16]:
```
c_parameter_values = [0.00005,
                      0.0001,
                      0.0002,
                      0.0005,
                      0.001,
                      0.0015,
                      0.002,
                      0.005,
                      0.01]
df = pd.DataFrame(columns=['min_impurity_decrease', 'f1-score'])
c_best_f1_score = float('-inf')
c_worst_f1_score = float('inf')
c_best_parameter = None
c_worst_parameter = None
c_best_model = None
c_worst_model = None
for input_parameter in c_parameter_values:
    model = DecisionTreeClassifier(min_impurity_decrease=input_parameter,␣
 ↪random_state=21)
    model.fit(X_train, y_train)

    f1_score = cross_val_score(reduced_model, X_test, y_test, cv=5,␣
 ↪scoring='f1_weighted').mean() * 100

    df = pd.concat([df, pd.DataFrame([{'min_impurity_decrease' :␣
 ↪input_parameter , 'f1-score' : f1_score}])])

    if f1_score > c_best_f1_score:
        c_best_f1_score = f1_score
        c_best_parameter = input_parameter
        c_best_model = model

    if f1_score < c_worst_f1_score:
        c_worst_f1_score = f1_score
        c_worst_parameter = input_parameter
        c_worst_model = model

print(df)
```

```
print("Melhor min_impurity_decrease: {}".format(c_best_parameter))
print("Pior min_impurity_decrease: {}".format(c_worst_parameter))
```

```
   min_impurity_decrease   f1-score
0                0.00005  32.849728
0                0.00010  28.982033
0                0.00020  30.241202
0                0.00050  28.326649
0                0.00100  27.043951
0                0.00150  29.985422
0                0.00200  31.460633
0                0.00500  31.739594
0                0.01000  30.188761
Melhor min_impurity_decrease: 5e-05
Pior min_impurity_decrease: 0.001
```

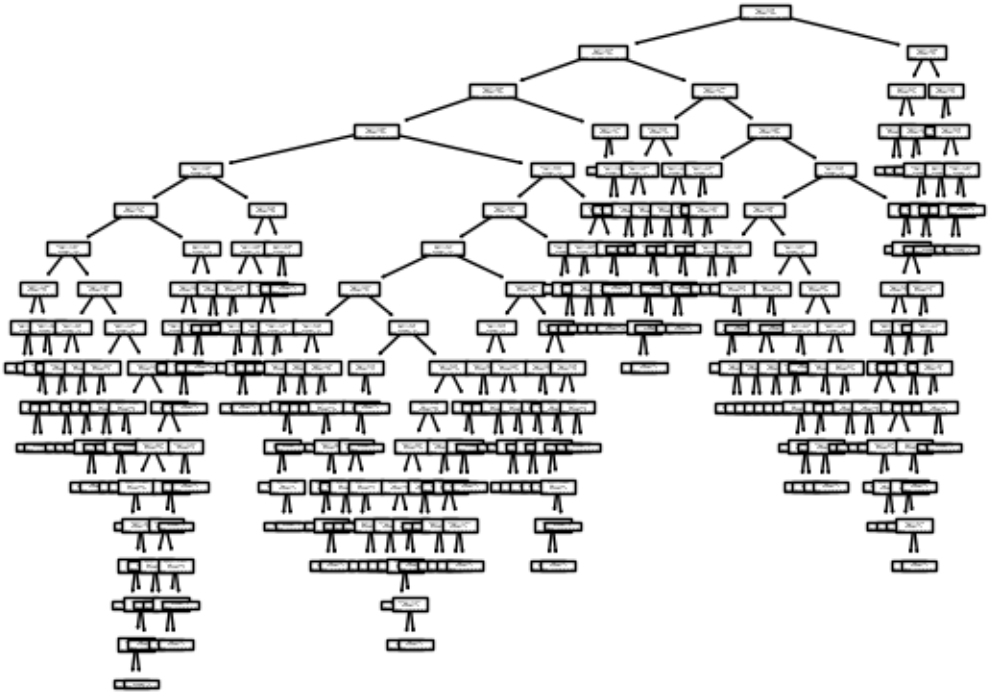
[17]:
```
rf_classifier = RandomForestClassifier(random_state=0, criterion="entropy",␣
 ↪min_impurity_decrease=0.01).fit(X_train, y_train)
f1_score  = cross_val_score(rf_classifier, X_test, y_test, cv=5,␣
 ↪scoring='f1_macro').mean() * 100
print("F1 Score: {0:2.2f}%".format(f1_score))
```

```
F1 Score: 13.79%
```

3.2 Usando PCA

[18]:
```
pca = PCA(n_components=20).fit(X)
X_train_new = pca.transform(X_train)
X_test_new = pca.transform(X_test)

print("Old shape: {} New shape: {}".format(X_train.shape, X_train_new.shape))

rf_classifier_red = RandomForestClassifier(random_state=0, criterion="entropy",␣
 ↪min_impurity_decrease=0.01).fit(X_train_new, y_train)

f1_score  = cross_val_score(reduced_model, X_test_new, y_test, cv=5,␣
 ↪scoring='f1_weighted').mean() * 100
print("F1 Score: {0:2.2f}%".format(f1_score))
print("Nós: {} Profundidade: {}".format(reduced_model.get_n_leaves(),␣
 ↪reduced_model.get_depth()))

plot_tree(reduced_model)
plt.show()
```

```
Old shape: (585, 119) New shape: (585, 20)
F1 Score: 26.81%
Nós: 185 Profundidade: 17
```



3.3 Análise

O PCA sempre apresenta um resultado positivo em relação aos outros métodos. Mas no contextos do desafio onde se deve escolher alguns métodos de análises química ele não deve ser levado em consideração pois os valores usados como features são uma função de todos os valores anteriores.

A ideia dessa análise é escolher qual é o conjunto de drogas deve ser utilizada contra o câncer, como ele não apresenta um subconjunto válido de opções, é um método inútil.