ML_SP22_Project_2 (Classical Machine Learning Model Building)

Due Date: 5/2 23:59 pm

In [2]:
```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
import warnings
warnings.filterwarnings('ignore')
```

In [3]:
```
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LogisticRegression
from sklearn import svm
from sklearn.ensemble import RandomForestClassifier
from sklearn.tree import DecisionTreeClassifier
from sklearn.metrics import classification_report,confusion_matrix,accuracy_score
```

In [4]:
```
# include your Project 1 Decision Tree Model as well
from DT_Iman_Toussi import DecisionTreeModel
```

Original dataset was based on

https://archive.ics.uci.edu/ml/datasets/wine+quality

Attribute Information: For more information, read [Cortez et al., 2009]. Input variables (based on physicochemical tests): 1 - fixed acidity 2 - volatile acidity 3 - citric acid 4 - residual sugar 5 - chlorides 6 - free sulfur dioxide 7 - total sulfur dioxide 8 - density 9 - pH 10 - sulphates 11 - alcohol Output variable (based on sensory data): 12 - quality (score between 0 and 10)

However, we will be using a slightly modified version of the dataset as follow

In [5]:
```
df = pd.read_csv("wine-tasting.csv")
df.head()
```

Out[5]:

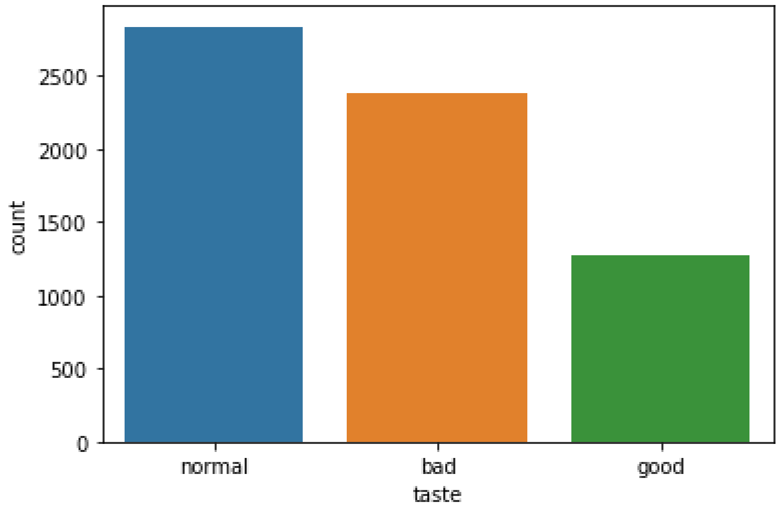
	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	sulphates	alcohol	type	pHValue	taste
0	7.0	0.27	0.36	20.7	0.045	45.0	170.0	1.0010	0.45	8.8	white	very acidic	normal
1	6.3	0.30	0.34	1.6	0.049	14.0	132.0	0.9940	0.49	9.5	white	quite acidic	normal
2	8.1	0.28	0.40	6.9	0.050	30.0	97.0	0.9951	0.44	10.1	white	quite acidic	normal
3	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956	0.40	9.9	white	very acidic	normal
4	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956	0.40	9.9	white	very acidic	normal

In [6]:

```
sns.countplot(x='taste',data=df)
```

Out[6]:

```
<AxesSubplot:xlabel='taste', ylabel='count'>
```

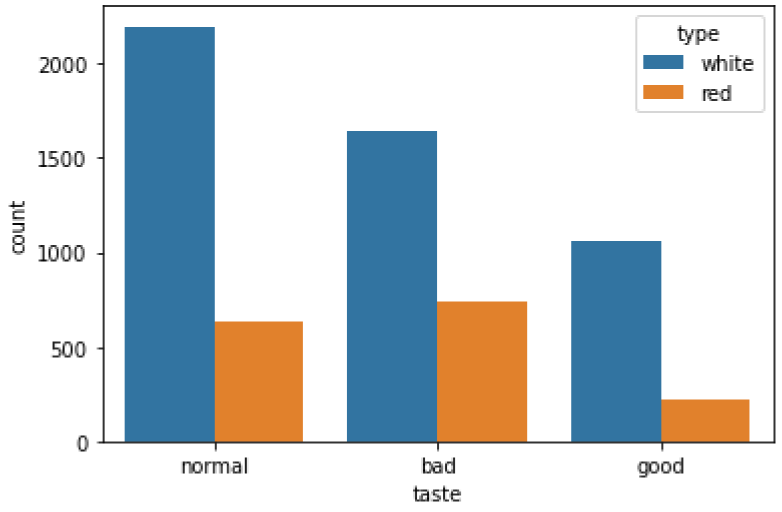


In [7]:

```
sns.countplot(x='taste', hue='type', data=df)
```

Out[7]:

```
<AxesSubplot:xlabel='taste', ylabel='count'>
```



Your task in this Project is to build the best predictive model to predict if a wine will be of good taste (ie we do not care if it is normal or bad taste, just good vs not good taste)

You should follow the usual best practice in building models such as

- EDA (chekcing missing values, removing outliers)
- performed basic exploration of relationship, with plots and graphs
- separated data set into training and testing
- setup dummy variables to take care categorical variables
- normalize numerical features if needed
- tried at least three (one of them is your own decision tree) models and checked their model performance
- performed cross-validations (f1-score)

You should have also done the following

- Try at least 3 models you have learned in class such as Logistic, Decision Tree, Random Forecast.
- Compare the sklearn Decision Tree with your own Decision Tree implementation results
- Include at least one ensemble models
- Identify out of all those you have tried, which one is the best model.

And answer the following questions based on what you observe from your model building process

- For the best fitted model, does it work better for the Red wine or White wine or similar
- Can ensemble methods improve your models?
- Whether the categorical variable pH Value is important or not. If it is important, and you need to make a prediction for one instance where the pH value is missing, how would you proceed?

1.) EDA

In [8]:
```
df.describe()
```

Out[8]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	sulphates	alcohol
count	6497.000000	6498.000000	6498.000000	6498.000000	6498.000000	6498.000000	6498.000000	6498.000000	6498.000000	6498.000000
mean	7.215307	0.339657	0.318650	5.442659	0.056038	30.523853	115.745691	0.996135	0.531251	10.492156
std	1.296434	0.164625	0.145313	4.757664	0.035032	17.748427	56.517576	0.116587	0.148801	1.192964
min	3.800000	0.080000	0.000000	0.600000	0.009000	1.000000	6.000000	0.987110	0.220000	8.000000
25%	6.400000	0.230000	0.250000	1.800000	0.038000	17.000000	77.125000	0.992340	0.430000	9.500000
50%	7.000000	0.290000	0.310000	3.000000	0.047000	29.000000	118.000000	0.994890	0.510000	10.300000
75%	7.700000	0.400000	0.390000	8.100000	0.065000	41.000000	156.000000	0.996990	0.600000	11.300000
max	15.900000	1.580000	1.660000	65.800000	0.611000	289.000000	440.000000	10.389800	2.000000	14.900000

In [9]:
```
df.shape
```

Out[9]:
```
(6498, 13)
```

In [10]:
```
df.isnull().sum()
```

Out[10]:
```
fixed acidity          1
volatile acidity       0
citric acid            0
residual sugar         0
chlorides              0
free sulfur dioxide    0
```

```
total sulfur dioxide    0
density                 0
sulphates               0
alcohol                 0
type                    0
pHValue                 0
taste                   0
dtype: int64
```

Remove missing data rows

In [11]:
```
df = df.dropna()
```

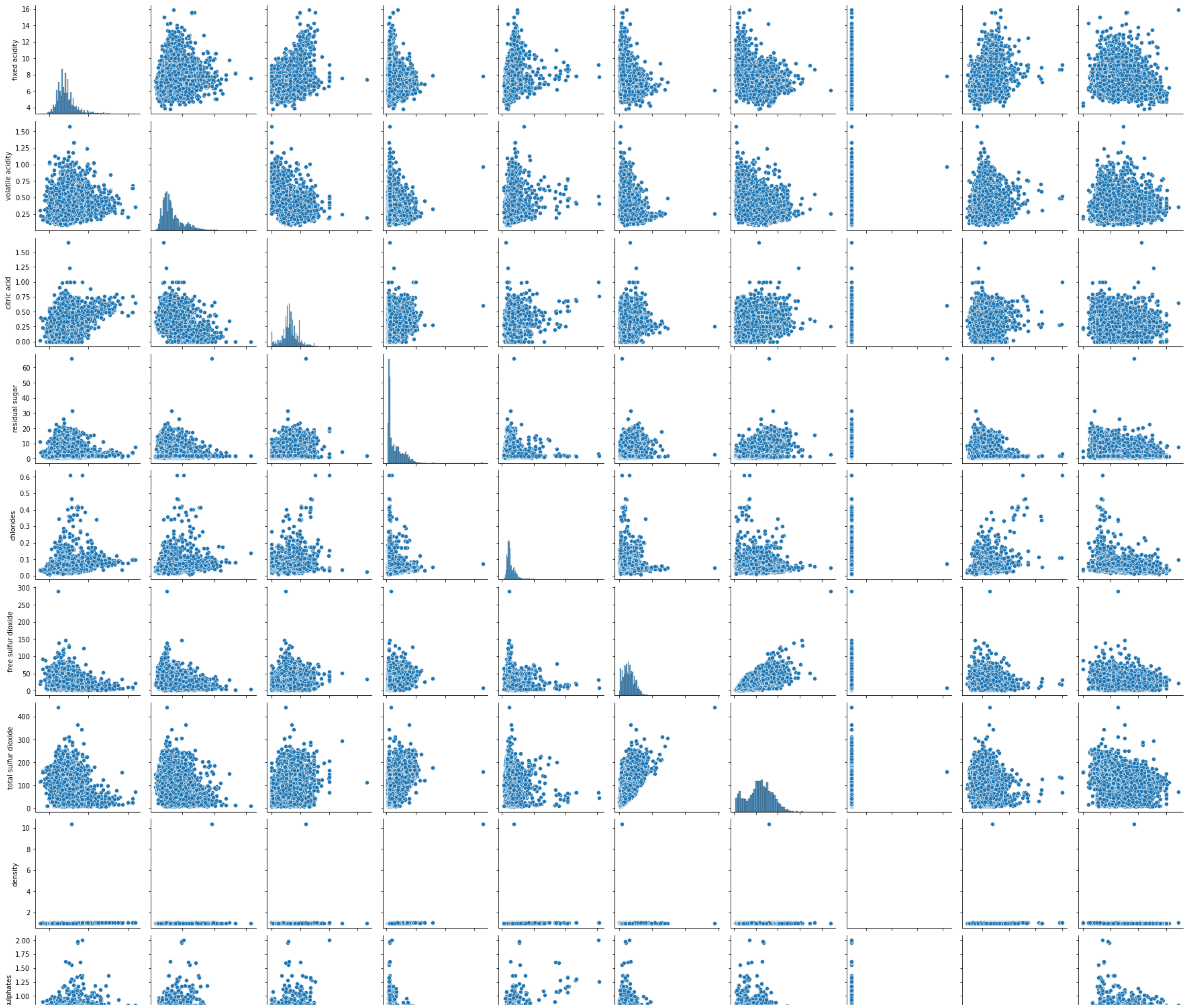
In [12]:
```
df.isnull().any()
```

Out[12]:
```
fixed acidity           False
volatile acidity        False
citric acid             False
residual sugar          False
chlorides               False
free sulfur dioxide     False
total sulfur dioxide    False
density                 False
sulphates               False
alcohol                 False
type                    False
pHValue                 False
taste                   False
dtype: bool
```

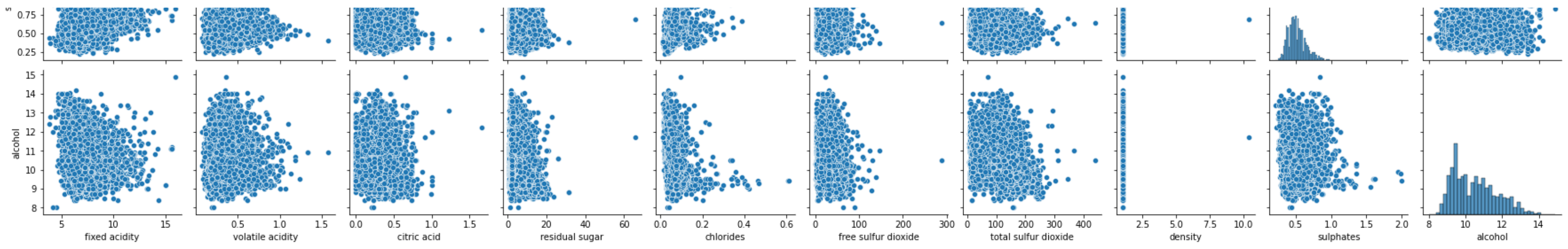
Check and remove outliers

In [13]:
```
sns.pairplot(data = df)
```

Out[13]:
```
<seaborn.axisgrid.PairGrid at 0x14e9718f610>
```

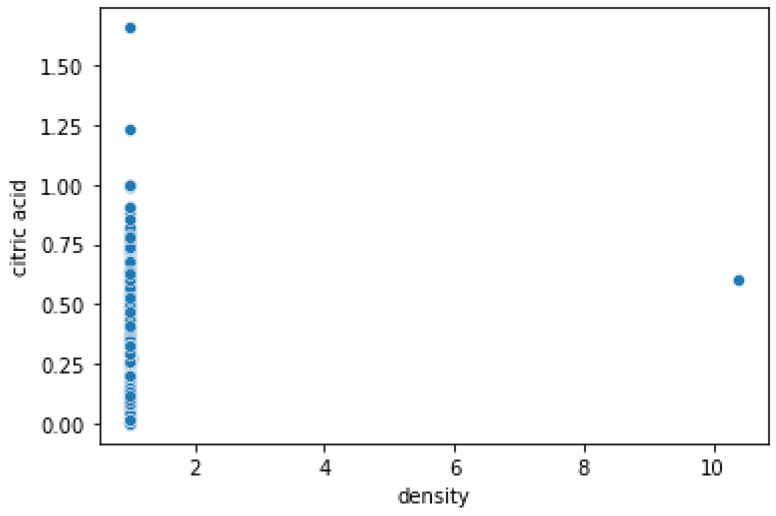


fixed acidity
volatile acidity
citric acid
residual sugar
chlorides
free sulfur dioxide
total sulfur dioxide
density
ulphates



In [14]:
```
sns.scatterplot(x ='density', y='citric acid', data=df)
```

Out[14]:
```
<AxesSubplot:xlabel='density', ylabel='citric acid'>
```

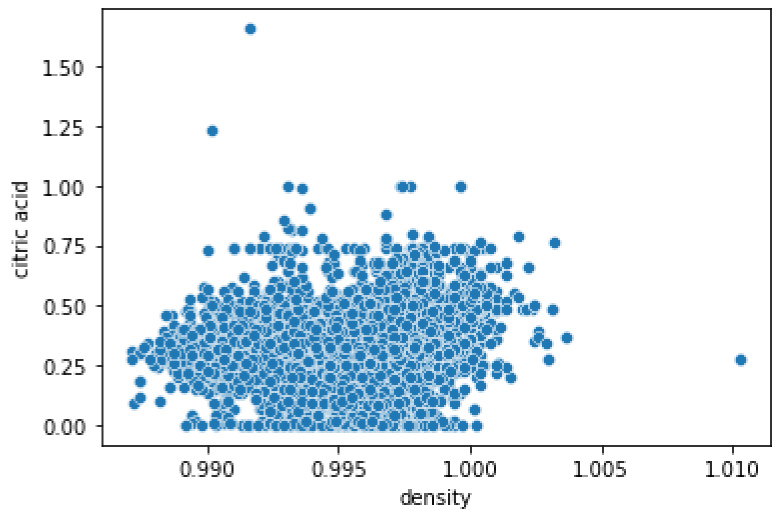


There is an outlier for density that must be removed

In [15]:
```
df = df[df['density'] < 10]
```

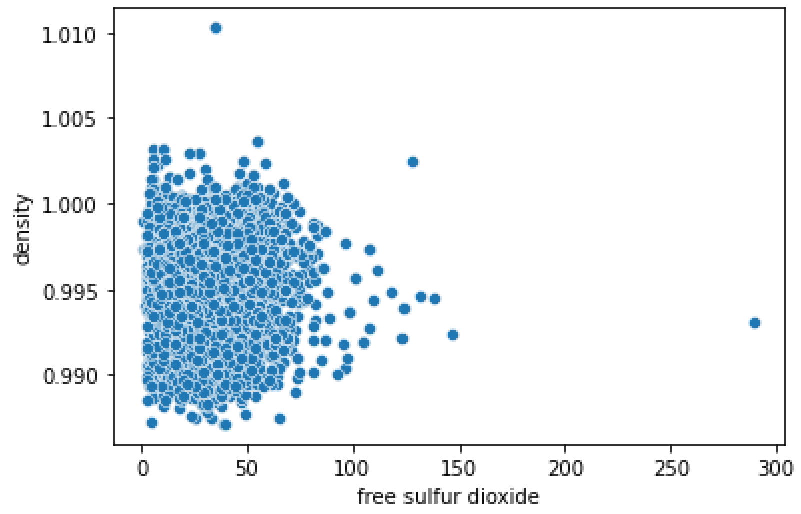
In [16]:
```
sns.scatterplot(x ='density', y='citric acid', data=df)
```

Out[16]:
```
<AxesSubplot:xlabel='density', ylabel='citric acid'>
```



```
In [17]: sns.scatterplot(x ='free sulfur dioxide', y='density', data=df)
```

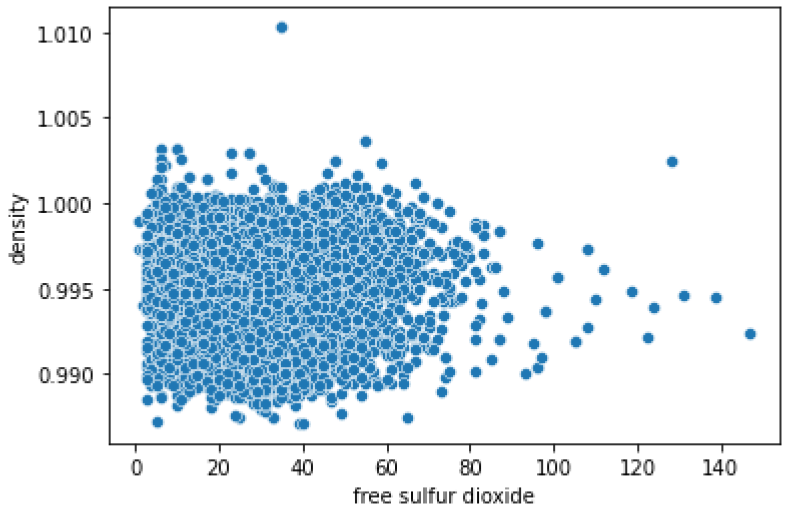
```
Out[17]: <AxesSubplot:xlabel='free sulfur dioxide', ylabel='density'>
```



There is an outlier for free sulfur dioxide that must be removed

```
In [18]: df = df[df['free sulfur dioxide'] < 250]
In [19]: sns.scatterplot(x ='free sulfur dioxide', y='density', data=df)
```

```
Out[19]: <AxesSubplot:xlabel='free sulfur dioxide', ylabel='density'>
```



```
In [20]: df.corr()
```

Out[20]:

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	sulphates	alcohol
fixed acidity	1.000000	0.218944	0.324362	-0.114369	0.298154	-0.285474	-0.329223	0.465745	0.299651	-0.095535
volatile acidity	0.218944	1.000000	-0.379693	-0.206276	0.377241	-0.357050	-0.416051	0.267452	0.225698	-0.038279
citric acid	0.324362	-0.379693	1.000000	0.140427	0.038839	0.136874	0.195992	0.093324	0.055957	-0.010799
residual sugar	-0.114369	-0.206276	0.140427	1.000000	-0.131610	0.418628	0.501973	0.539397	-0.190352	-0.365992
chlorides	0.298154	0.377241	0.038839	-0.131610	1.000000	-0.197650	-0.280196	0.367670	0.395599	-0.257022
free sulfur dioxide	-0.285474	-0.357050	0.136874	0.418628	-0.197650	1.000000	0.722035	0.030785	-0.193115	-0.182701
total sulfur dioxide	-0.329223	-0.416051	0.195992	0.501973	-0.280196	0.722035	1.000000	0.031688	-0.277253	-0.266578
density	0.465745	0.267452	0.093324	0.539397	0.367670	0.030785	0.031688	1.000000	0.261579	-0.700986
sulphates	0.299651	0.225698	0.055957	-0.190352	0.395599	-0.193115	-0.277253	0.261579	1.000000	-0.003197

	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	sulphates	alcohol
alcohol	-0.095535	-0.038279	-0.010799	-0.365992	-0.257022	-0.182701	-0.266578	-0.700986	-0.003197	1.000000

reset index

In [21]:
```
df = df.reset_index()
df.tail()
```

Out[21]:

	index	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	sulphates	alcohol	type	pHValue	taste
6490	6493	6.2	0.600	0.08	2.0	0.090	32.0	44.0	0.99490	0.58	10.5	red	midly acidic	bad
6491	6494	5.9	0.550	0.10	2.2	0.062	39.0	51.0	0.99512	0.76	11.2	red	midly acidic	normal
6492	6495	6.3	0.510	0.13	2.3	0.076	29.0	40.0	0.99574	0.75	11.0	red	midly acidic	normal
6493	6496	5.9	0.645	0.12	2.0	0.075	32.0	44.0	0.99547	0.71	10.2	red	midly acidic	bad
6494	6497	6.0	0.310	0.47	3.6	0.067	18.0	42.0	0.99549	0.66	11.0	red	quite acidic	normal

2.) Setup dummy variables for categorical variables

In [22]:
```
df['type'].unique()
```

Out[22]:
```
array(['white', 'red'], dtype=object)
```

In [23]:
```
df['pHValue'].unique()
```

Out[23]:
```
array(['very acidic', 'quite acidic', 'extremly acidic', 'midly acidic',
       'acidic', 'lightly acidic'], dtype=object)
```

```
In [24]: df['taste'].unique()
```

```
Out[24]: array(['normal', 'bad', 'good'], dtype=object)
```

Now, we create dummy variables for the above categorical variables

```
In [25]: df_dummies = pd.get_dummies(df, columns = ['type', 'pHValue', 'taste'])
```

```
In [26]: df_dummies.head()
```

Out[26]:

	index	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	sulphates	...	type_white	pHValue_acidic	pHValue_extremly acidic	pH
0	0	7.0	0.27	0.36	20.7	0.045	45.0	170.0	1.0010	0.45	...	1	0	0	
1	1	6.3	0.30	0.34	1.6	0.049	14.0	132.0	0.9940	0.49	...	1	0	0	
2	2	8.1	0.28	0.40	6.9	0.050	30.0	97.0	0.9951	0.44	...	1	0	0	
3	3	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956	0.40	...	1	0	0	
4	4	7.2	0.23	0.32	8.5	0.058	47.0	186.0	0.9956	0.40	...	1	0	0	

5 rows × 22 columns

deal with the 'good' values of taste

```
In [27]: df['taste_good'] = df['taste'].apply(lambda x: 1 if x == 'taste_good' else 0)
```

```
In [28]: numerical_features = ['fixed acidity', 'volatile acidity', 'citric acid', 'residual sugar', 'chlorides', 'free sulfur dic
         categorical_features = ['type', 'pHValue', 'taste']
```

```
In [29]: numerical_df = df[numerical_features + ['taste_good']]
```

3.) Separate data set into training and testing

In [27]:

```
df_dummies.corr()
```

Out[27]:

	index	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	sulphates	...	type_white	pH
index	1.000000	0.246827	0.488407	-0.223172	-0.259495	0.356644	-0.363024	-0.598139	0.175603	0.359147	...	-0.746197	
fixed acidity	0.246827	1.000000	0.218944	0.324362	-0.114369	0.298154	-0.285474	-0.329223	0.465745	0.299651	...	-0.486764	
volatile acidity	0.488407	0.218944	1.000000	-0.379693	-0.206276	0.377241	-0.357050	-0.416051	0.267452	0.225698	...	-0.654099	
citric acid	-0.223172	0.324362	-0.379693	1.000000	0.140427	0.038839	0.136874	0.195992	0.093324	0.055957	...	0.187334	
residual sugar	-0.259495	-0.114369	-0.206276	0.140427	1.000000	-0.131610	0.418628	0.501973	0.539397	-0.190352	...	0.352168	
chlorides	0.356644	0.298154	0.377241	0.038839	-0.131610	1.000000	-0.197650	-0.280196	0.367670	0.395599	...	-0.512739	
free sulfur dioxide	-0.363024	-0.285474	-0.357050	0.136874	0.418628	-0.197650	1.000000	0.722035	0.030785	-0.193115	...	0.478433	
total sulfur dioxide	-0.598139	-0.329223	-0.416051	0.195992	0.501973	-0.280196	0.722035	1.000000	0.031688	-0.277253	...	0.701632	
density	0.175603	0.465745	0.267452	0.093324	0.539397	0.367670	0.030785	0.031688	1.000000	0.261579	...	-0.398677	
sulphates	0.359147	0.299651	0.225698	0.055957	-0.190352	0.395599	-0.193115	-0.277253	0.261579	1.000000	...	-0.487463	
alcohol	0.114004	-0.095535	-0.038279	-0.010799	-0.365992	-0.257022	-0.182701	-0.266578	-0.700986	-0.003197	...	0.032884	
type_red	0.746197	0.486764	0.654099	-0.187334	-0.352168	0.512739	-0.478433	-0.701632	0.398677	0.487463	...	-1.000000	
type_white	-0.746197	-0.486764	-0.654099	0.187334	0.352168	-0.512739	0.478433	0.701632	-0.398677	-0.487463	...	1.000000	
pHValue_acidic	0.051466	-0.110103	0.065555	-0.111843	-0.064461	0.019114	-0.033032	-0.055557	0.009662	0.084907	...	-0.078088	
pHValue_extremly acidic	-0.062751	0.115290	-0.106524	0.112443	0.131643	-0.025511	0.021553	0.047448	0.007432	-0.076027	...	0.118720	
pHValue_lightly acidic	0.013335	-0.052481	0.024254	-0.039810	-0.027271	-0.010312	-0.015744	-0.013228	-0.014195	0.009150	...	-0.026751	
pHValue_midly acidic	0.115132	-0.145294	0.176548	-0.220909	-0.146730	0.039435	-0.085980	-0.155940	0.030841	0.111682	...	-0.204593	

	index	fixed acidity	volatile acidity	citric acid	residual sugar	chlorides	free sulfur dioxide	total sulfur dioxide	density	sulphates	...	type_white	pH
pHValue_quite acidic	0.087573	-0.061052	0.074517	-0.084791	-0.132411	0.003225	-0.095304	-0.119712	-0.025916	0.074427	...	-0.139005	
pHValue_very acidic	-0.143490	0.126447	-0.151852	0.200619	0.176933	-0.019506	0.149500	0.211385	0.000506	-0.129019	...	0.231515	
taste_bad	0.043634	0.067597	0.267939	-0.075453	0.034516	0.182057	-0.048729	0.046646	0.275429	-0.035841	...	-0.116670	
taste_good	-0.069130	-0.049484	-0.151638	0.054575	-0.063866	-0.161772	0.016046	-0.050862	-0.279098	0.034113	...	0.087574	
taste_normal	0.012995	-0.026036	-0.138862	0.029590	0.017638	-0.047282	0.034496	-0.004570	-0.044000	0.007492	...	0.043200	

22 rows × 22 columns

In [32]:
```
X = df_dummies.drop('taste_good', axis='columns')
Y = df_dummies['taste_good']
X_train, X_test, Y_train, Y_test = train_test_split(X, Y, test_size=0.20, random_state=101)
```

4.) Build models and check their model performance

Build a logistic regression first

In [33]:
```
model1 = LogisticRegression()
model1.fit(X_train, Y_train)
```

Out[33]:
```
LogisticRegression()
```

In [34]:
```
predictions = model1.predict(X_test)
```

In [35]:
```
print(classification_report(Y_test,predictions))
print(accuracy_score(Y_test, predictions))
```

```
              precision    recall  f1-score   support
```

```
           0       0.96      0.97      0.97      1071
           1       0.87      0.82      0.84       228

    accuracy                           0.95      1299
   macro avg       0.92      0.90      0.91      1299
weighted avg       0.95      0.95      0.95      1299

0.9468822170900693
```

With logistic regression, we get an f1-score of 84%!

Building a decision tree

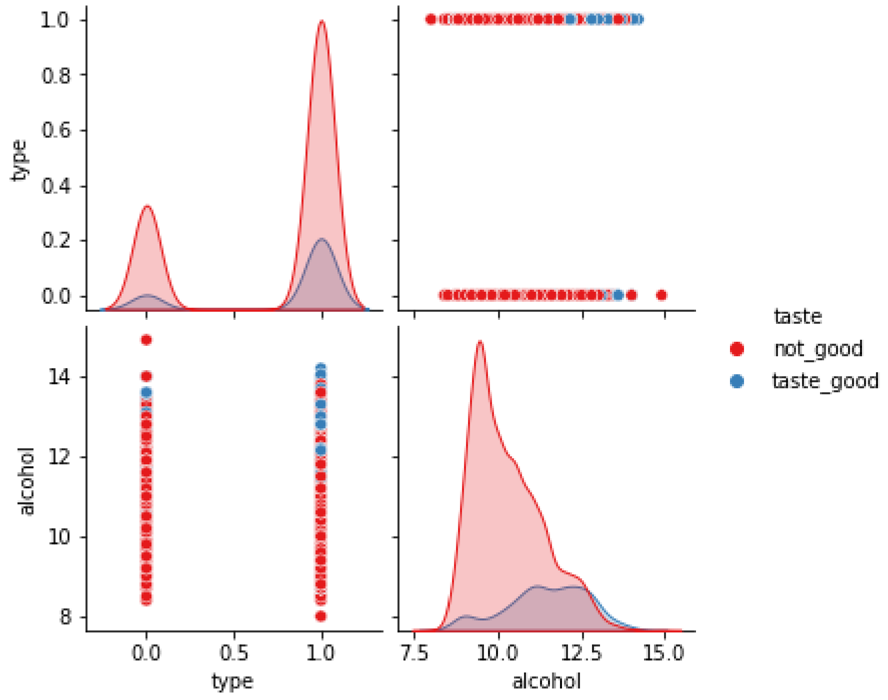
In [54]:
```
tree_df = df[['taste', 'type', 'alcohol']]
tree_df['taste'] = df_dummies['taste_good'].apply(lambda x: 'taste_good' if x == 1 else 'not_good')
tree_df['type'] = df['type'].apply(lambda x: 1 if x == 'white' else 0)
```

In [55]:
```
tree_df
```

Out[55]:

	taste	type	alcohol
0	not_good	1	8.8
1	not_good	1	9.5
2	not_good	1	10.1
3	not_good	1	9.9
4	not_good	1	9.9
...	...	...	...
6490	not_good	0	10.5
6491	not_good	0	11.2
6492	not_good	0	11.0
6493	not_good	0	10.2
6494	not_good	0	11.0

6495 rows × 3 columns

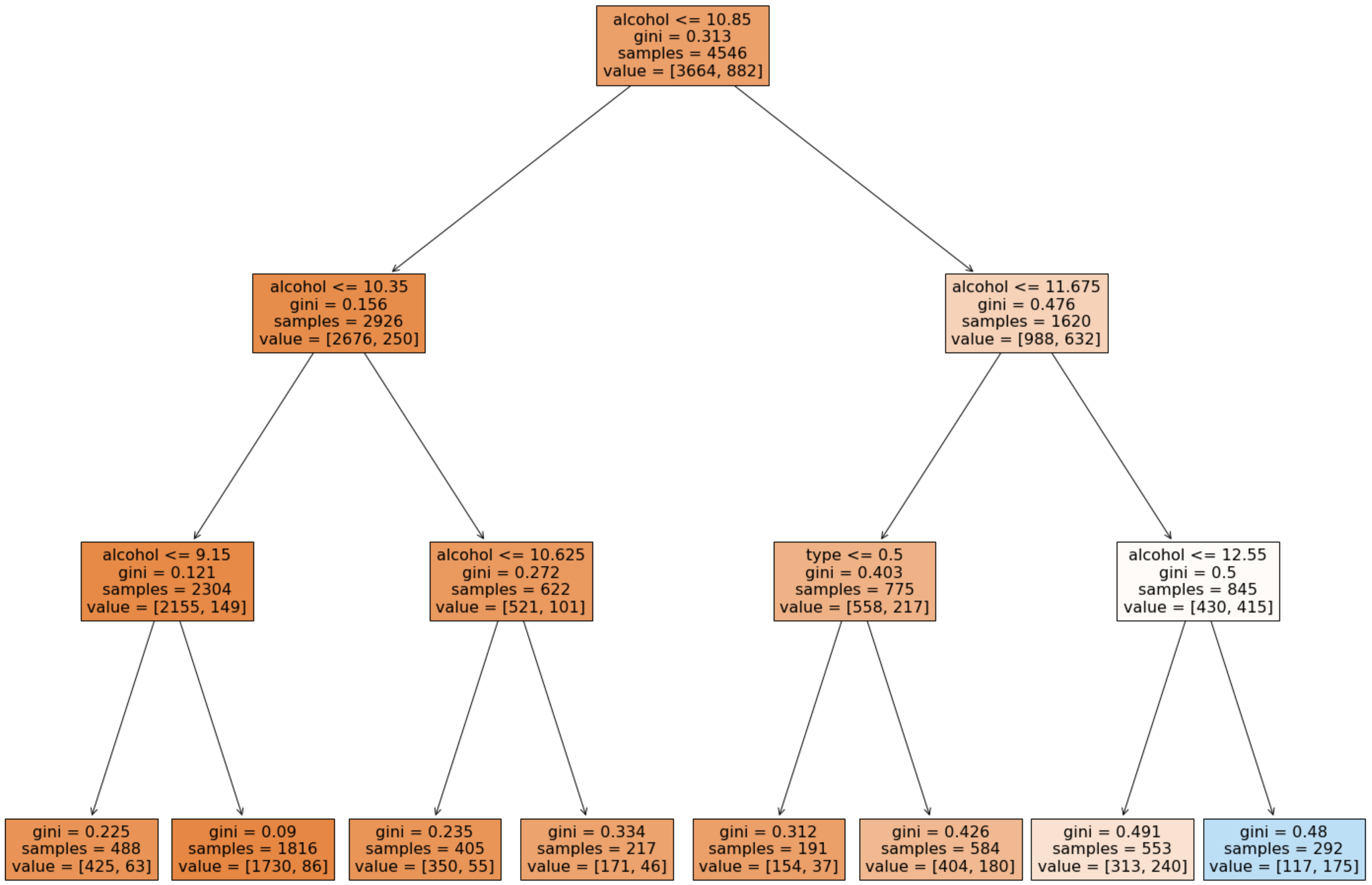
In [56]:
```
sns.pairplot(tree_df, hue='taste',palette='Set1')
```
Out[56]:
```
<seaborn.axisgrid.PairGrid at 0x14eab8d82b0>
```


In [62]:
```
features = tree_df.drop('taste', axis=1).columns
```
In [63]:
```
X = tree_df.drop('taste', axis=1)
Y = tree_df['taste']
X_train, X_test, Y_train, Y_test = train_test_split(X, Y, test_size=0.30)
```
In [64]:
```
model2 = DecisionTreeClassifier(max_depth=3)
model2.fit(X_train,Y_train)
```
Out[64]:
```
DecisionTreeClassifier(max_depth=3)
```

In [65]:
```
predictions = model2.predict(X_test)
print(confusion_matrix(Y_test,predictions))
print(classification_report(Y_test,predictions))
print(accuracy_score(Y_test, predictions))
```

```
[[1499   55]
 [ 317   78]]
              precision    recall  f1-score   support

    not_good       0.83      0.96      0.89      1554
  taste_good       0.59      0.20      0.30       395

    accuracy                           0.81      1949
   macro avg       0.71      0.58      0.59      1949
weighted avg       0.78      0.81      0.77      1949

0.8091328886608518
```

In [66]:
```
from sklearn import tree
fig = plt.figure(figsize=(25,20))
_ = tree.plot_tree(model2, feature_names = features, filled=True)
```



With decision tree, we get an f1-score of 30%

Building a random forest

In [69]:
```
rfc = RandomForestClassifier(n_estimators=100)
rfc.fit(X_train, Y_train)
```

Out[69]:
```
RandomForestClassifier()
```

In [70]:
```
rfc_pred = rfc.predict(X_test)
print(classification_report(Y_test, rfc_pred))
print(accuracy_score(Y_test, rfc_pred))
```

```
              precision    recall  f1-score   support

    not_good       0.83      0.97      0.89      1554
  taste_good       0.60      0.20      0.30       395

    accuracy                           0.81      1949
   macro avg       0.71      0.58      0.60      1949
weighted avg       0.78      0.81      0.77      1949

0.8106721395587481
```

Similarly with the decision tree, the random forest gives us an f1-score of 30%

5.) Make an ensemble model

We will make a bagging ensemble

In [73]:
```
from sklearn.ensemble import BaggingClassifier
bag_clf = BaggingClassifier(
    DecisionTreeClassifier(random_state=101), n_estimators=500,
    max_samples=100, bootstrap=True, random_state=42)
bag_clf.fit(X_train, Y_train)
Y_pred = bag_clf.predict(X_test)
```

In [75]:
```
print(accuracy_score(Y_test, Y_pred))
```

```
0.8086198050282196
```

```
In [78]: print(classification_report(Y_test, Y_pred))
```

```
              precision    recall  f1-score   support

    not_good       0.83      0.96      0.89      1554
  taste_good       0.58      0.21      0.31       395

    accuracy                           0.81      1949
   macro avg       0.70      0.59      0.60      1949
weighted avg       0.78      0.81      0.77      1949
```

The bagging ensemble method shows a slight improvement to the f1-score to 31%

6.) Questions

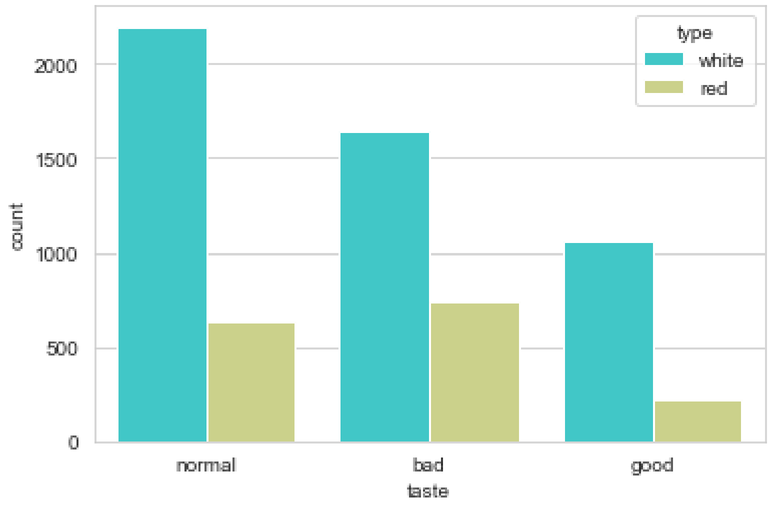
- Identify out of all those you have tried, which one is the best model

Out of all of the models, logistic regression turned out to have the best f1-scores of 84% while both the decision tree and random forest had an f1-score of 30%. Even the bagging ensemble was not able to come close to the logistic regression score.

- For the best fitted model, does it work better for the Red wine or White wine or similar?

```
In [80]: sns.set_style('whitegrid')
         sns.countplot(x='taste',hue='type',data=df,palette='rainbow')
```

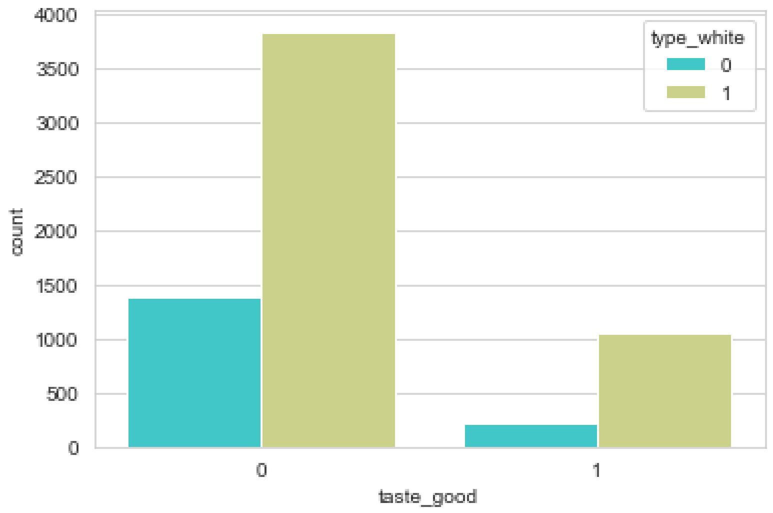
```
Out[80]: <AxesSubplot:xlabel='taste', ylabel='count'>
```



```
In [82]: df = df_dummies
```

```
In [83]: sns.set_style('whitegrid')
         sns.countplot(x='taste_good',hue='type_white',data=df,palette='rainbow')
```

```
Out[83]: <AxesSubplot:xlabel='taste_good', ylabel='count'>
```



In [89]:

```
X = df_dummies.drop('type_white', axis='columns')
Y = df_dummies['type_white']
X_train, X_test, Y_train, Y_test = train_test_split(X, Y, test_size=0.20, random_state=101)
model1 = LogisticRegression()
model1.fit(X_train, Y_train)
predictions = model1.predict(X_test)
```

In [90]:

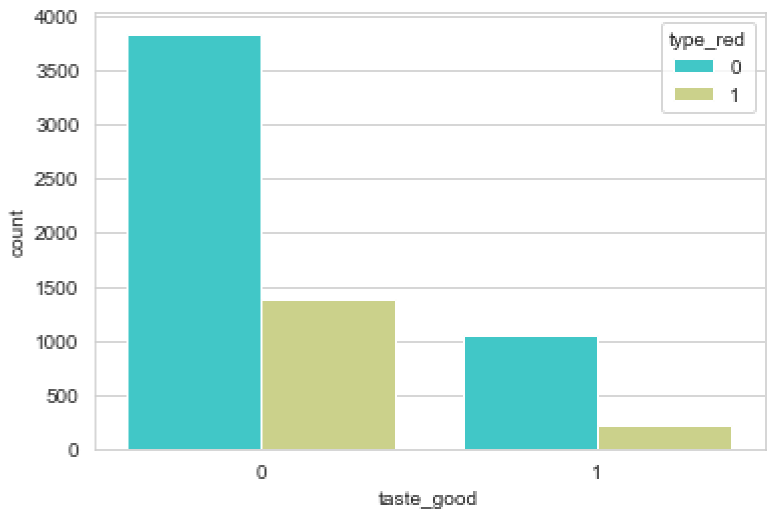
```
print(classification_report(Y_test,predictions))
print(accuracy_score(Y_test, predictions))
```

```
              precision    recall  f1-score   support

           0       0.99      0.98      0.98       312
           1       0.99      1.00      0.99       987

    accuracy                           0.99      1299
   macro avg       0.99      0.99      0.99      1299
weighted avg       0.99      0.99      0.99      1299

0.9923017705927637
```

In [85]:

```
sns.set_style('whitegrid')
sns.countplot(x='taste_good',hue='type_red',data=df,palette='rainbow')
```

```
Out[85]: <AxesSubplot:xlabel='taste_good', ylabel='count'>
```



```
In [91]:
X = df_dummies.drop('type_red', axis='columns')
Y = df_dummies['type_red']
X_train, X_test, Y_train, Y_test = train_test_split(X, Y, test_size=0.20, random_state=101)
model1 = LogisticRegression()
model1.fit(X_train, Y_train)
predictions = model1.predict(X_test)
```

```
In [92]:
print(classification_report(Y_test,predictions))
print(accuracy_score(Y_test, predictions))
```

```
              precision    recall  f1-score   support

           0       0.99      1.00      1.00       987
           1       0.99      0.98      0.99       312

    accuracy                           0.99      1299
   macro avg       0.99      0.99      0.99      1299
weighted avg       0.99      0.99      0.99      1299

0.993841416474211
```

The logistic regression model works similarly for both the red and white wines

- Can ensemble methods improve your models?

As seen from the bagging ensemble above, ensemble method will improve the models. However, it will only improve them by a very little amount

- Whether the categorical variable pH Value is important or not. If it is important, and you need to make a prediction for one instance where the pH value is missing, how would you proceed?

The categorical variable pH Value is not important when considering the taste of a wine. If there is an instance of a pH Value that is missing, the best option would to be to give it a normalized value.

```
In [ ]:
```