In [1]:

```python
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
from sklearn import neighbors, datasets, tree, linear_model, metrics
from sklearn.model_selection import cross_val_score, train_test_split
import itertools
from itertools import permutations
from sklearn.metrics import recall_score
from sklearn.model_selection import GridSearchCV
import warnings
warnings.filterwarnings('ignore')
```

1. Data Import & Cleaning

In [3]:

```python
#1. Import Data
data =  pd.read_csv('wdbc.data', sep=",",header=None)
data.head()
```

Out[3]:

	0	1	2	3	4	5	6	7	8	9	...	22	23	24	25	26	27	28
0	842302	M	17.99	10.38	122.80	1001.0	0.11840	0.27760	0.3001	0.14710	...	25.38	17.33	184.60	2019.0	0.1622	0.6656	0.7119
1	842517	M	20.57	17.77	132.90	1326.0	0.08474	0.07864	0.0869	0.07017	...	24.99	23.41	158.80	1956.0	0.1238	0.1866	0.2416
2	84300903	M	19.69	21.25	130.00	1203.0	0.10960	0.15990	0.1974	0.12790	...	23.57	25.53	152.50	1709.0	0.1444	0.4245	0.4504
3	84348301	M	11.42	20.38	77.58	386.1	0.14250	0.28390	0.2414	0.10520	...	14.91	26.50	98.87	567.7	0.2098	0.8663	0.6869
4	84358402	M	20.29	14.34	135.10	1297.0	0.10030	0.13280	0.1980	0.10430	...	22.54	16.67	152.20	1575.0	0.1374	0.2050	0.4000

5 rows × 32 columns

In [4]:

```python
#2. Fix the column names
features=['radius','texture','perimeter','area','smoothness','compactness','concavity','concave points'
,'symmetry','fractal dimension']
atr=['mean','standard error','largest']
column1 = ['ID','Diagnosis']
column2 = list(itertools.product(features,atr))
for i in range(len(column2)):
    column2[i]='-'.join(column2[i])
column1.extend(column2)
data.columns=column1
data.head(3)
```

Out[4]:

	ID	Diagnosis	radius-mean	radius-standard error	radius-largest	texture-mean	texture-standard error	texture-largest	perimeter-mean	perimeter-standard error	...	concavity-largest	concave points-mean	concave points-standard error
0	842302	M	17.99	10.38	122.8	1001.0	0.11840	0.27760	0.3001	0.14710	...	25.38	17.33	184.6
1	842517	M	20.57	17.77	132.9	1326.0	0.08474	0.07864	0.0869	0.07017	...	24.99	23.41	158.8
2	84300903	M	19.69	21.25	130.0	1203.0	0.10960	0.15990	0.1974	0.12790	...	23.57	25.53	152.5

3 rows × 32 columns

In [5]:

```python
#3. Data Describtion: there's no NA value within the dataframe
data.isna().sum()
data.describe()
```

Out[5]:

	ID	radius-mean	radius-standard error	radius-largest	texture-mean	texture-standard error	texture-largest	perimeter-mean	perimeter-standard error	perimeter-largest	...	(
count	5.690000e+02	569.000000	569.000000	569.000000	569.000000	569.000000	569.000000	569.000000	569.000000	569.000000	...	5
mean	3.037183e+07	14.127292	19.289649	91.969033	654.889104	0.096360	0.104341	0.088799	0.048919	0.181162	...	
std	1.250206e+08	3.524049	4.301036	24.298981	351.914129	0.014064	0.052813	0.079720	0.038803	0.027414	...	
min	8.670000e+03	6.981000	9.710000	43.790000	143.500000	0.052630	0.019380	0.000000	0.000000	0.106000	...	
25%	8.692180e+05	11.700000	16.170000	75.170000	420.300000	0.086370	0.064920	0.029560	0.020310	0.161900	...	
50%	9.060240e+05	13.370000	18.840000	86.240000	551.100000	0.095870	0.092630	0.061540	0.033500	0.179200	...	
75%	8.813129e+06	15.780000	21.800000	104.100000	782.700000	0.105300	0.130400	0.130700	0.074000	0.195700	...	
max	9.113205e+08	28.110000	39.280000	188.500000	2501.000000	0.163400	0.345400	0.426800	0.201200	0.304000	...	

8 rows × 31 columns

2. Performance Metric

Given that the consequence of not identifying maligant case is also serious, I want to also take **Recall** into account and therefore choose the **F-measure(maligant)** as our performance matric.

3. Decision Tree

- I am going to tune the **max_depth** hyper-parameter to see the effect of underfitting and overfitting.
- I will split **10%** of the data out as my test data.

In [6]:

```python
target=np.where(data['Diagnosis']=='M',1,0)
features=data.iloc[:,2:]
X_train, X_test, y_train, y_test=train_test_split(features,target, test_size=0.2,random_state=99)
```

Here, I try to use **cross vaidation and grid search** to find the best hyperparameter for Decision Tree model.

In [7]:

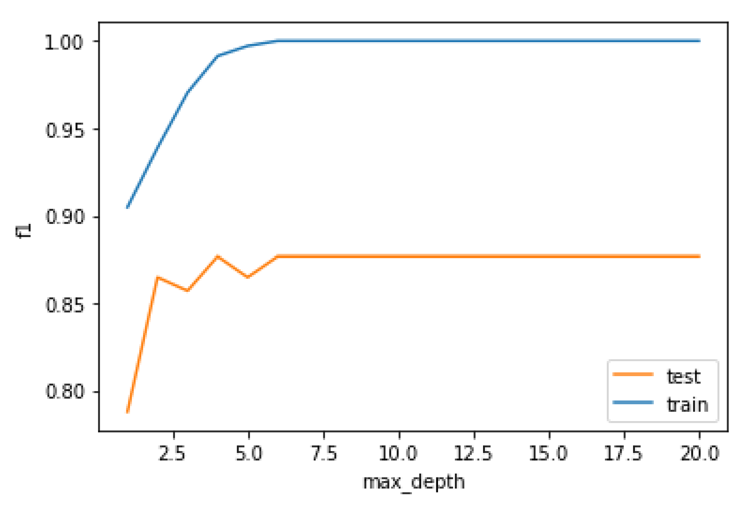
```python
param_grid = {'criterion':['gini','entropy'],'max_depth':list(range(1,21))}
grid = GridSearchCV(tree.DecisionTreeClassifier(random_state=10), param_grid, cv = 10, scoring = 'f1')
grid.fit(X_train,y_train)
print ("Best Model's F1-Positive Score on Train Data: {}%".format(round(grid.best_score_*100,2)))
print ("With CV grid search, I found the best hyperparameter is criterion={} and max_depth={}.".format(
grid.best_params_['criterion'],grid.best_params_['max_depth']))
print("Prediction F1-Positive Score on Test Data: {}%".format(round(metrics.f1_score(y_test, grid.predi
ct(X_test))*100,2)))
```

```
Best Model's F1-Positive Score on Train Data: 93.26%
With CV grid search, I found the best hyperparameter is criterion=entropy and max_depth=4.
Prediction F1-Positive Score on Test Data: 87.67%
```

In [11]:

```python
f1_train=[]
f1_test=[]
for i in range(1,21):
    clf = tree.DecisionTreeClassifier(criterion=grid.best_params_['criterion'],max_depth =i,random_stat
e=10)
    clf.fit(X_train,y_train)
    f1_train.append(metrics.f1_score(y_train,clf.predict(X_train)))
    f1_test.append(metrics.f1_score(y_test,clf.predict(X_test)))

max_depth=list(range(1,21))
line1, =plt.plot(max_depth,f1_train,label='train')
line2, =plt.plot(max_depth,f1_test,label='test')
plt.xlabel("max_depth")
plt.ylabel("f1")
plt.legend((line2, line1), ('test', 'train'))
plt.show()
```



Given that when **max_depth<3**, both train and test data do not perform too well, so the model is probably **underfitting**. On the other hand, when the max_depth is smaller than 10, there isn't apparent pattern of overfitting.

4. Logistic Regression

- I am going to tune the hyper parameter **C (the inverse of regularization strength)** to see the effect of underfitting and overfitting. The smaller the c is the the more intense the regularization is.
- I will also split **10%** of the data out as my test data

Here, I try to use **cross vaidation and grid search** to find the best hyperparameter for Logistic Regression model.

In [112]:

```python
normalized_features=(features-features.min())/(features.max()-features.min())
X_train, X_test, y_train, y_test=train_test_split(normalized_features,target, test_size=0.2,random_stat
e=99)
param_grid = {'C':[2,1.9,1.8,1.7,1.6,1.5,1.4,1.3,1.2,1.1,1,0.9,0.8,0.7,0.6,0.5,0.4,0.3,0.2,0.1]}
grid = GridSearchCV(linear_model.LogisticRegression(solver='saga',l1_ratio=0.5,random_state=10,penalty=
'elasticnet'), param_grid, cv = 10, scoring = 'f1')
grid.fit(X_train,y_train)
print ("Best Model's F1-Positive Score on Train Data: {}%".format(round(grid.best_score_*100,2)))
print ("With CV grid search, I found the best hyperparameter is C={}.".format(grid.best_params_['C']))
print("Prediction F1-Positive Score on Test Data: {}%".format(round(metrics.f1_score(y_test, grid.predi
ct(X_test))*100,2)))
```

```
Best Model's F1-Positive Score on Train Data: 95.8%
With CV grid search, I found the best hyperparameter is C=2.
Prediction F1-Positive Score on Test Data: 95.89%
```

With regularization, some features are discriminated and eventually have coefficeints equal to 0.

In [126]:

```python
best_model=grid.best_estimator_
best_model.coef_.T
```

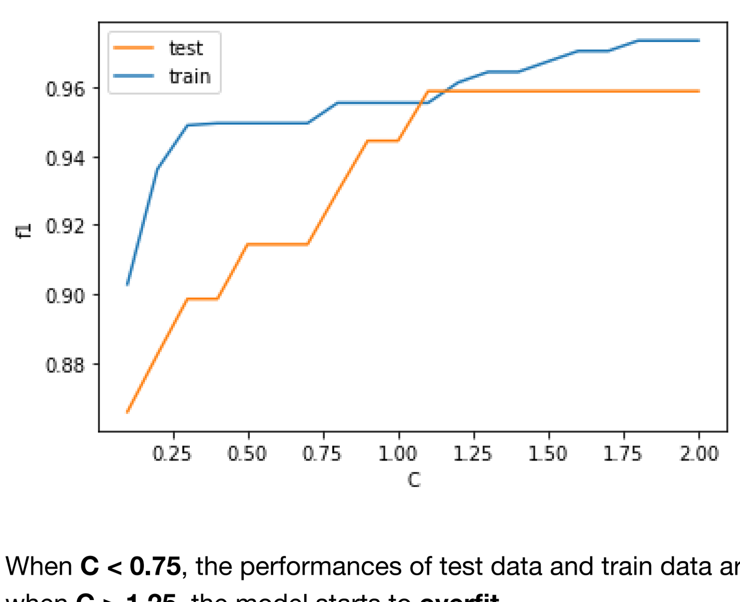
Out[126]:

```
array([[ 2.21502065],
       [ 2.43416955],
       [ 2.15692162],
       [ 1.86877042],
       [ 0.59736962],
       [ 0.        ],
       [ 1.53505621],
       [ 3.03442944],
       [ 0.11690881],
       [-0.7464025 ],
       [ 2.13051211],
       [ 0.        ],
       [ 1.44379433],
       [ 0.92521458],
       [ 0.        ],
       [-0.75434628],
       [ 0.        ],
       [ 0.        ],
       [ 0.        ],
       [-0.39040489],
       [ 3.16433488],
       [ 3.0140817 ],
       [ 2.8571796 ],
       [ 2.15333802],
       [ 2.54331356],
       [ 0.50021648],
       [ 1.32246731],
       [ 3.7510223 ],
       [ 1.76060078],
       [ 0.16839529]])
```

In [19]:

```python
f1_train=[]
f1_test=[]
for i in [2,1.9,1.8,1.7,1.6,1.5,1.4,1.3,1.2,1.1,1,0.9,0.8,0.7,0.6,0.5,0.4,0.3,0.2,0.1]:
    clf = linear_model.LogisticRegression(C=i,multi_class='ovr',solver='saga',l1_ratio=0.5,random_state
=10,penalty='elasticnet')
    clf.fit(X_train,y_train)
    f1_train.append(metrics.f1_score(y_train,clf.predict(X_train)))
    f1_test.append(metrics.f1_score(y_test,clf.predict(X_test)))

C=[2,1.9,1.8,1.7,1.6,1.5,1.4,1.3,1.2,1.1,1,0.9,0.8,0.7,0.6,0.5,0.4,0.3,0.2,0.1]
line1, =plt.plot(C,f1_train,label='train')
line2, =plt.plot(C,f1_test,label='test')
plt.xlabel("C")
plt.ylabel("f1")
plt.legend((line2, line1), ('test', 'train'))
plt.show()
```



When **C < 0.75**, the performances of test data and train data are both bad. Thus, the model is probably **underfitting**. On the other hand, when **C > 1.25**, the model starts to **overfit**.

5. KNN

- I am going to tune the hyper-parameter **n-neighbors** to see the effect of overfitting and underfitting
- Given that the KNN method is built based on data and does not have a model, I am not going to split the data.

In [14]:

```python
normalized_features=(features-features.min())/(features.max()-features.min())
X_train, X_test, y_train, y_test=train_test_split(normalized_features,target, test_size=0.2,random_stat
e=99)
```

Here, I try to use **cross vaidation and grid search** to find the best hyperparameter for KNN model.

In [15]:

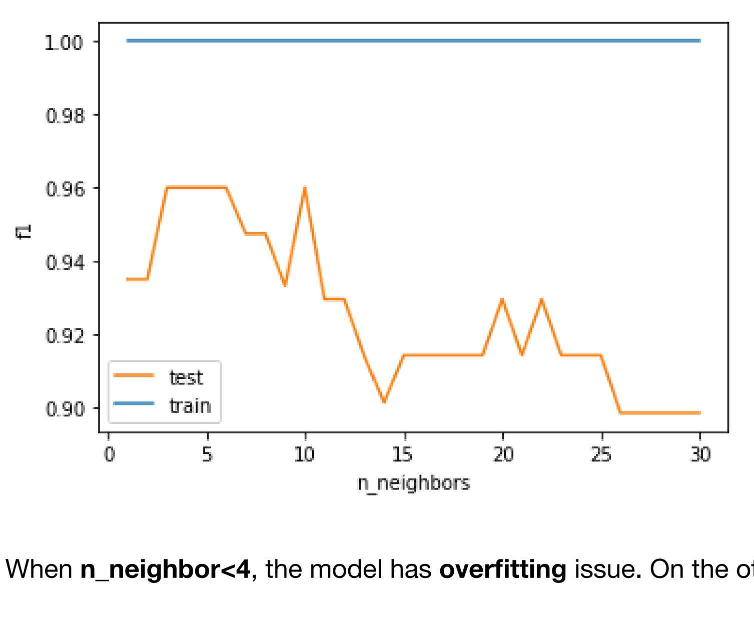
```python
k_range = list(range(1,31))
weight_options = ["uniform", "distance"]
param_grid={'n_neighbors':k_range,'weights':weight_options}
grid = GridSearchCV(neighbors.KNeighborsClassifier(), param_grid, cv = 10, scoring = 'f1')
grid.fit(X_train,y_train)
print ("Best Model's F1-Positive Score on Train Data: {}%".format(round(grid.best_score_*100,2)))
print ("With CV grid search, I found the best hyperparameter is weights={} and n_neighbors={}.".format(
grid.best_params_['weights'],grid.best_params_['n_neighbors']))
print("Prediction F1-Positive Score on Test Data: {}%".format(round(metrics.f1_score(y_test, grid.predi
ct(X_test))*100,2)))
```

```
Best Model's F1-Positive Score on Train Data: 95.78%
With CV grid search, I found the best hyperparameter is weights=distance and n_neighbors=12.
Prediction F1-Positive Score on Test Data: 92.96%
```

In [18]:

```python
f1_train=[]
f1_test=[]
for i in range(1,31):
    knn = neighbors.KNeighborsClassifier(i, weights=grid.best_params_['weights'])
    knn.fit(X_train,y_train)
    f1_train.append(metrics.f1_score(y_train,knn.predict(X_train)))
    f1_test.append(metrics.f1_score(y_test,knn.predict(X_test)))

n_neighbors=list(range(1,31))
line1, =plt.plot(n_neighbors,f1_train,label='train')
line2, =plt.plot(n_neighbors,f1_test,label='test')
plt.xlabel("n_neighbors")
plt.ylabel("f1")
plt.legend((line2, line1), ('test', 'train'))
plt.show()
```



When **n_neighbor<4**, the model has **overfitting** issue. On the other hand, when **n_neighbors > 10**, the model is underfitting for **test data.**