Εργασία 1

Β. Αναγνώριση τύπων γυαλιού με βάση τη χημική τους σύσταση

1. Προετοιμασία των δεδομένων

Σκοπός της εργασίας είναι η αξιολόγηση μοντέλων τα οποία κατηγοριοποιούν μετρήσεις διαφόρων χημικών στοιχείων σε 6 τύπους γυαλιού. Τα δεδομένα αυτά είχαν συγκεντρωθεί με σκοπό να μπορεί να αναγνωριστεί ο τύπος του γυαλιού όταν αυτό συλλέγεται από τόπους εγκλήματος έτσι ωστέ να μπορεί να χρησιμοποιηθεί ως αποδεικτικό στοιχείο.

Παρακάτω βλέπουμε τις εκδόσεις της python και των βιβλιοθηκών που χρησιμοποιήθηκαν στην εργασία.

In [1]:
```
import matplotlib
import seaborn as sns
import pandas as pd
import numpy as np
import sklearn
import sys

np.random.seed(0)

print('Python version:', sys.version)
print('scikit-learn version:', sklearn.__version__)
print('pandas version:', pd.__version__)
print('numpy version:', np.__version__)
print('matplotlib version:', matplotlib.__version__)
print('seaborn version:', sns.__version__)
```

```
Python version: 3.7.9 (default, Aug 31 2020, 17:10:11) [MSC v.1916 64 bit (AMD6
4)]
scikit-learn version: 0.23.2
pandas version: 1.1.3
numpy version: 1.19.2
matplotlib version: 3.3.2
seaborn version: 0.11.0
```

Τα δεδομένα βρίσκονται στο αρχείο glass.data τα οποία διαβάζονται και αποθηκεύονται σε ένα pandas dataframe.

In [2]:
```
import numpy as np
import urllib.request
import os

np.random.seed(0)

url = 'https://archive.ics.uci.edu/ml/machine-learning-databases/glass/glass.data
filename = 'glass.data'

if not os.path.exists(filename):
    print('Downloading file...')
    urllib.request.urlretrieve(url, filename)
    print('Done.')

names = ("Id", "RI", "Na", "Mg", "Al", "Si", "K", "Ca", "Ba", "Fe", "Type")
df = pd.read_csv(filename, names=names)
```

Παρακάτω βλέπουμε τα 5 πρώτα παραδείγματα.

In [3]:
```
df.head()
```

Out[3]:

	Id	RI	Na	Mg	Al	Si	K	Ca	Ba	Fe	Type
0	1	1.52101	13.64	4.49	1.10	71.78	0.06	8.75	0.0	0.0	1
1	2	1.51761	13.89	3.60	1.36	72.73	0.48	7.83	0.0	0.0	1
2	3	1.51618	13.53	3.55	1.54	72.99	0.39	7.78	0.0	0.0	1
3	4	1.51766	13.21	3.69	1.29	72.61	0.57	8.22	0.0	0.0	1
4	5	1.51742	13.27	3.62	1.24	73.08	0.55	8.07	0.0	0.0	1

Ακολουθεί περιγραφή των διαφόρων χαρακτηριστικών.

In [4]:
```
%%html
<style>
table {float:left}
</style>
```

Id	Attribute	Description
1	Id	Id number: 1 to 214
2	RI	refractive index
3	Na	Sodium (unit measurement: weight percent in corresponding oxide, as are attributes 4-10)
4	Mg	Magnesium
5	Al	Aluminum
6	Si	Silicon
7	K	Potassium

Id	Attribute	Description
8	Ca	Calcium
9	Ba	Barium
10	Fe	Iron
11	Type	Type of glass: (class attribute)

Ακολουθεί περιγραφή των κλάσεων. Η 4η κλάση δεν χρησιμοποιείται.

Class	Description
1	building_windows_float_processed
2	building_windows_non_float_processed
3	vehicle_windows_float_processed
4	vehicle_windows_non_float_processed (none in this database)
5	containers
6	tableware
7	headlamps

Όλα τα χαρακτηριστικά είναι πραγματικοί αριθμοί εκτός από το Id και τη μεταβλητή στόχο Type οι οποίοι είναι ακέραιοι. Παρατηρούμε ότι δεν υπάρχουν τιμές που λείπουν.

In [5]:
```
df.info()
```

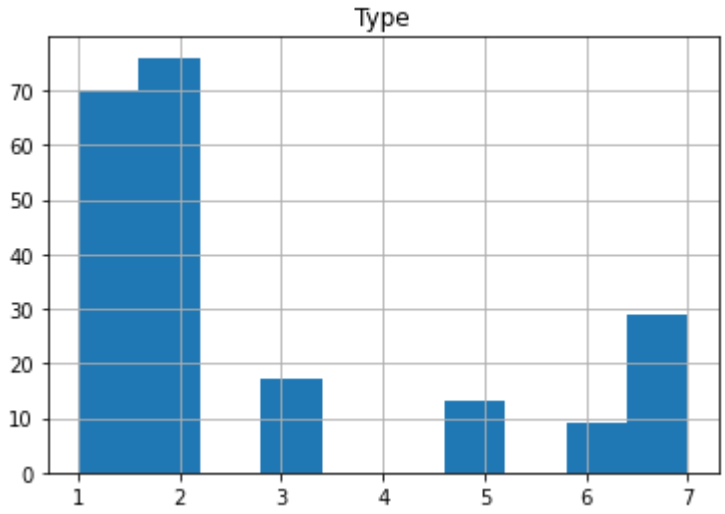
```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 214 entries, 0 to 213
Data columns (total 11 columns):
 #   Column  Non-Null Count  Dtype  
---  ------  --------------  -----  
 0   Id      214 non-null    int64  
 1   RI      214 non-null    float64
 2   Na      214 non-null    float64
 3   Mg      214 non-null    float64
 4   Al      214 non-null    float64
 5   Si      214 non-null    float64
 6   K       214 non-null    float64
 7   Ca      214 non-null    float64
 8   Ba      214 non-null    float64
 9   Fe      214 non-null    float64
 10  Type    214 non-null    int64  
dtypes: float64(9), int64(2)
memory usage: 18.5 KB
```

Βγάζουμε εκτός του dataframe το Id γιατί είναι απλώς ένας αύξων αριθμός και δεν προσφέρει κάποια χρήσιμη πληροφορία για την κατηγοριοποίηση

In [6]:
```
df.drop(labels='Id', axis=1, inplace=True)
```

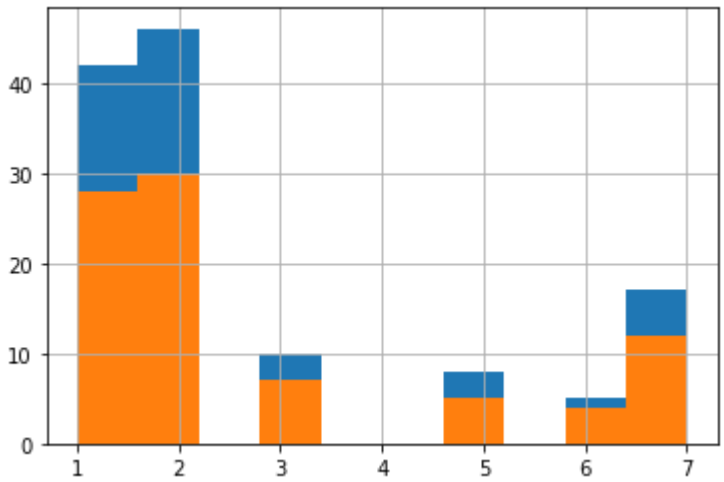
Το παρακάτω ιστόγραμμα μας δείχνει ότι οι κλάσεις των ψηφίων δεν είναι ζυγισμένες.

In [7]:
```
import matplotlib.pyplot as plt

df.hist(column='Type')
plt.show()
```



Το dataset χωρίζεται σε train set (60%) και test set (40%) χρησιμοποιώντας την συνάρτηση StratifiedShuffleSplit η οποία μας εξασφαλίζει οτι η κατανομή στα δυο set θα είναι ίδια ως προς τη μεταβλητή στόχο.

In [8]:
```
from sklearn import model_selection

split = model_selection.StratifiedShuffleSplit(n_splits=1, test_size=0.4, random_

for train_index, test_index in split.split(df, df['Type']):
    df_train = df.loc[train_index]
    df_test = df.loc[test_index]

df_train_x = df_train.drop('Type', axis=1)
df_train_y = df_train['Type']
df_test_x = df_test.drop('Type', axis=1)
df_test_y = df_test['Type']

df_train_y.hist()
df_test_y.hist()
plt.show()
```



Παρακάτω βλέπουμε κάποια στατιστικά δεδομένα για τις ανέξαρτητες μεταβλητές και την εξαρτημένη μεταβλητή Type.

In [9]:
```
df_train.describe()
```

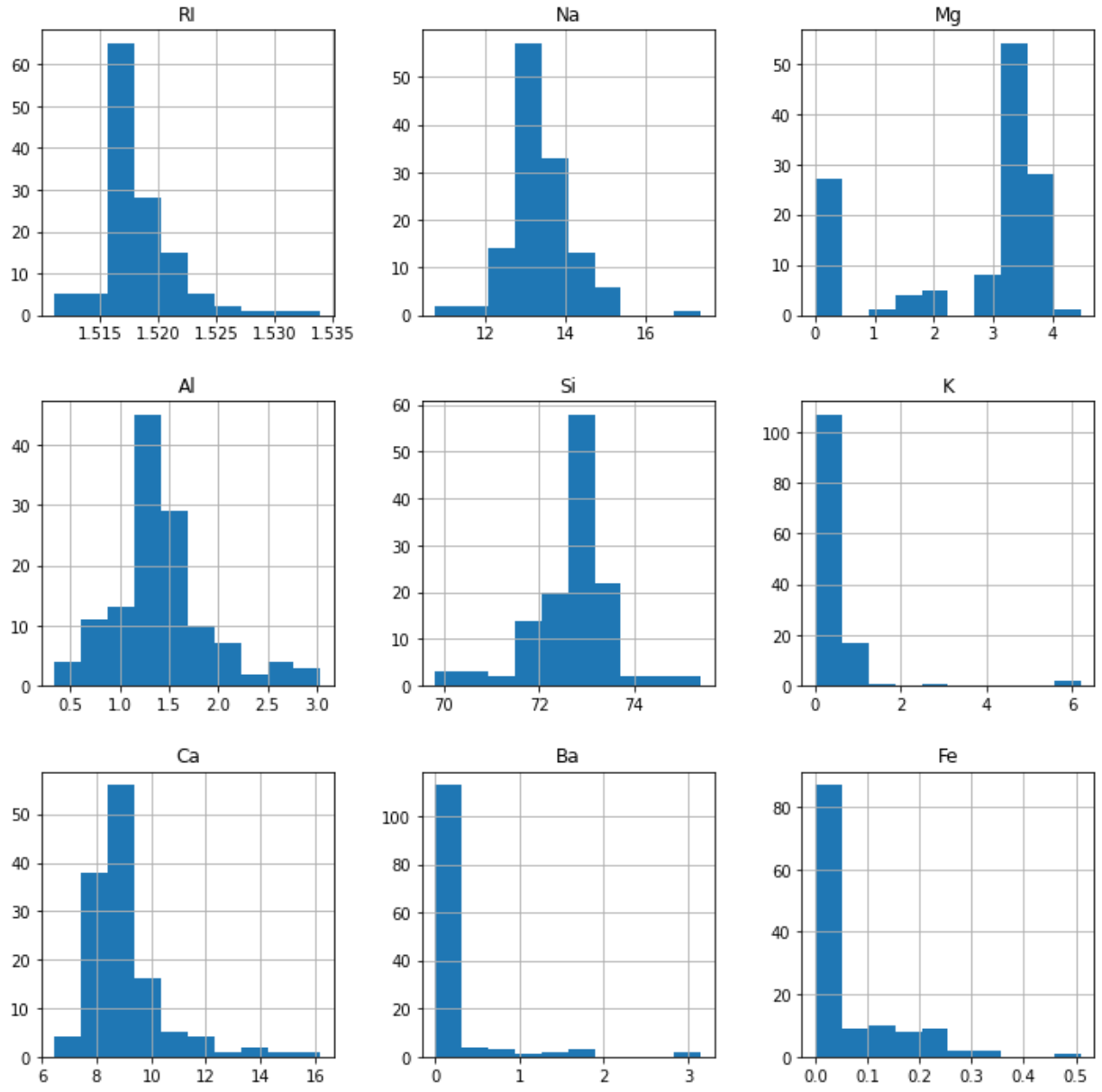
Out[9]:

	RI	Na	Mg	Al	Si	K	Ca	
count	128.000000	128.000000	128.00000	128.000000	128.000000	128.000000	128.000000	128.000
mean	1.518346	13.347344	2.63375	1.434531	72.693672	0.532500	9.016641	0.159
std	0.003189	0.792129	1.46517	0.494346	0.832269	0.791642	1.401949	0.503
min	1.511150	10.730000	0.00000	0.340000	69.810000	0.000000	6.470000	0.000
25%	1.516525	12.885000	1.83250	1.190000	72.330000	0.137500	8.317500	0.000
50%	1.517720	13.210000	3.45500	1.335000	72.845000	0.560000	8.605000	0.000
75%	1.518985	13.702500	3.58250	1.620000	73.102500	0.600000	9.200000	0.000
max	1.533930	17.380000	4.49000	3.040000	75.410000	6.210000	16.190000	3.150

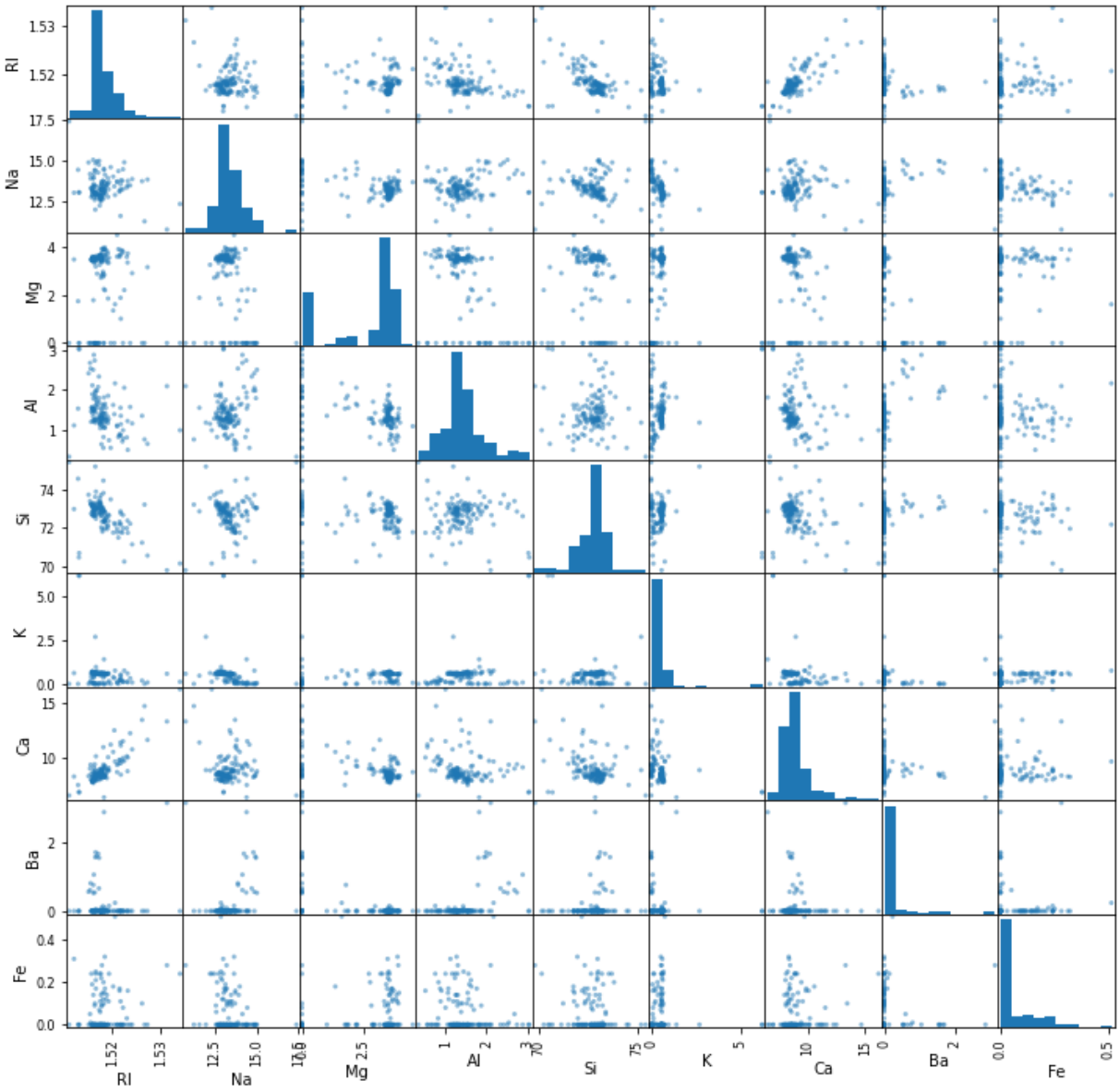
Ακολουθούν ιστογράμματα των χαρακτηριστικών και το scatter matrix.

In [10]:
```
df_train_x.hist(figsize=(12, 12))
plt.plot()
```

Out[10]: []



In [11]:
```
pd.plotting.scatter_matrix(df_train_x, figsize=(12, 12))
plt.show()
```



To train set και το test set αποθηκεύονται σε numpy arrays.

In [12]:
```
x_train = df_train_x.to_numpy()
y_train = df_train_y.to_numpy()
x_test = df_test_x.to_numpy()
y_test = df_test_y.to_numpy()

print('x_train.shape =', x_train.shape)
print('y_train.shape =', y_train.shape)
print('x_test.shape =', x_test.shape)
print('y_test.shape =', y_test.shape)
```

```
x_train.shape = (128, 9)
y_train.shape = (128,)
x_test.shape = (86, 9)
y_test.shape = (86,)
```

2. Μείωση διαστάσεων

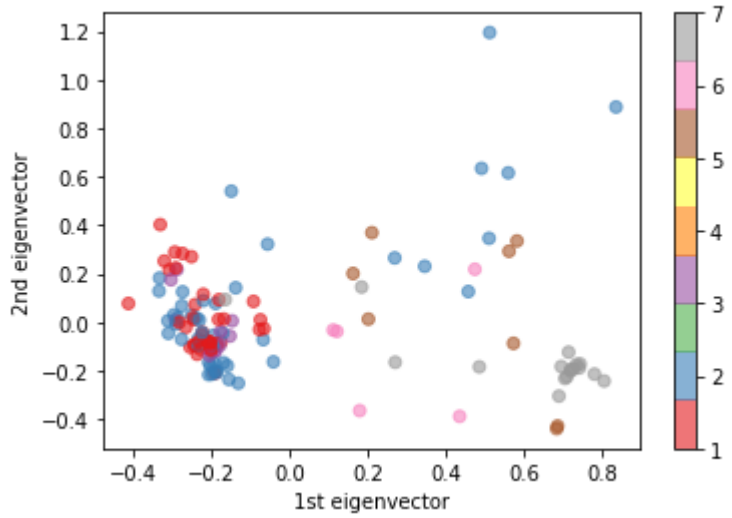
Εφαρμόζεται κανονικοποίηση και μείωση των διαστάσεων με την τεχνική PCA διατηρώντας το 90% της διασποράς.

In [13]:
```
from sklearn import decomposition
from sklearn import preprocessing

scaler = preprocessing.MinMaxScaler()
x_train_scaled = scaler.fit_transform(x_train)

pca = decomposition.PCA(n_components=0.9, svd_solver='full', random_state=0)
x_train_reduced = pca.fit_transform(x_train_scaled)

print('x_train.shape', x_train.shape)
print('x_train_reduced.shape =', x_train_reduced.shape)
```

```
x_train.shape (128, 9)
x_train_reduced.shape = (128, 5)
```

Η διαδικάσια αυτή γίνεται μόνο για την απεικόνιση των παραδειγμάτων στο επίπεδο των δυο πρώτων ιδιοδιανυσμάτων. Αργότερα εφαρμόζεται μέσω pipeline.

In [14]:
```
plt.scatter(x_train_reduced[:, 0], x_train_reduced[:, 1], c=y_train, cmap='Set1',
plt.xlabel('1st eigenvector')
plt.ylabel('2nd eigenvector')
plt.colorbar()
plt.show()
```



3. Αξιολόγηση μοντέλων

3.1 Περιγραφή της διαδικασίας

Επιλέγεται να γίνει αξιολόγηση των μοντέλων για την αναζήτηση των βέλτιστων παραμέτρων με την τεχνική της διασταυρωμένης επικύρωσης επειδή τα παραδείγματα είναι λίγα. Για την αξιολόγηση επιλέγεται η μετρική F1 επειδή οι κλάσεις δεν είναι ζυγισμένες. Η συνάρτηση GridSearchCV εφαρμόζει k-fold cross-validation με k=5 και stratified shuffle split. Μετά απο κάθε split εφαρμόζεται κανονικοποίηση με τον MinMaxScaler, PCA και εκπαίδευση του μοντέλου. Αυτά τα 3 βήματα ομαδοποιούνται σε ένα pipeline. Όταν τελειώσει η διαδικασία του grid search δημιουργείται ένα διάγραμμα για το πώς αλλάζει το μέσο F1 ($\pm$std) στο train set και στο validation set καθώς αλλάζει μια παράμετρος και ένα αντίστοιχο διάγραμμα για τον χρόνο εκπαίδευσης. Στο τέλος εκπαιδεύεται το βέλτιστο μοντέλο εκ νέου σε ολόκληρο το train set και αξιολογείται στο test set.

In [15]:
```
def plot_grid_search(search, baseline_score_val, param1, param2=None, xscale='lir
    param1_key = 'model__' + param1

    if param2 is None:
        x = [x['model__' + param1] for x in search.cv_results_['params']]
        mean_train_score = search.cv_results_['mean_train_score']
        mean_test_score = search.cv_results_['mean_test_score']
        mean_fit_time = search.cv_results_['mean_fit_time']
        std_train_score = search.cv_results_['std_train_score']
        std_test_score = search.cv_results_['std_test_score']
        std_fit_time = search.cv_results_['std_fit_time']
    else:
        param2_key = 'model__' + param2
        x = []
        mean_train_score = []
        mean_test_score = []
        mean_fit_time = []
        std_train_score = []
        std_test_score = []
        std_fit_time = []
        val2 = search.best_params_[param2_key]
        all_mean_train_score = search.cv_results_['mean_train_score']
        all_mean_test_score = search.cv_results_['mean_test_score']
        all_mean_fit_time = search.cv_results_['mean_fit_time']
        all_std_train_score = search.cv_results_['std_train_score']
        all_std_test_score = search.cv_results_['std_test_score']
        all_std_fit_time = search.cv_results_['std_fit_time']

        for i, params in enumerate(search.cv_results_['params']):
            if params[param2_key] == val2:
                x.append(params[param1_key])
                mean_train_score.append(all_mean_train_score[i])
                mean_test_score.append(all_mean_test_score[i])
                mean_fit_time.append(all_mean_fit_time[i])
                std_train_score.append(all_std_train_score[i])
                std_test_score.append(all_std_test_score[i])
                std_fit_time.append(all_std_fit_time[i])

        mean_train_score = np.array(mean_train_score)
        mean_test_score = np.array(mean_test_score)
        mean_fit_time = np.array(mean_fit_time)
        std_train_score = np.array(std_train_score)
        std_test_score = np.array(std_test_score)
        std_fit_time = np.array(std_fit_time)

    baseline_score = np.full(len(x), baseline_score_val)

    if param2 is None:
        plt.title('Score')
    else:
        if val2 is isinstance(val2, float):
            plt.title('Score for ' + param2 + ' = ' + "{:.4f}".format(val2))
        else:
            plt.title('Score for ' + param2 + ' = ' + str(val2))
    plt.plot(x, mean_train_score, label='Train')
    plt.fill_between(x, mean_train_score-std_train_score, mean_train_score+std_tr
```

```
    plt.plot(x, mean_test_score, label='Validation')
    plt.fill_between(x, mean_test_score-std_test_score, mean_test_score+std_test_
    plt.plot(x, baseline_score, label='Baseline', linestyle='dotted')
    plt.xscale(xscale)
    plt.xlabel(param1)
    plt.ylabel('F1')
    plt.legend()
    plt.show()

    plt.title('Training time')
    plt.plot(x, mean_fit_time)
    plt.fill_between(x, mean_fit_time-std_fit_time, mean_fit_time+std_fit_time, a
    plt.xscale('log')
    plt.xlabel(param1)
    plt.ylabel('Time (sec)')
    plt.show()
```

In [16]:
```
final_results = []

def evaluate_model(search, classifier_str):
    y_pred = search.predict(x_test)
    y_train_pred = search.predict(x_train)

    train_f1 = metrics.f1_score(y_train, y_train_pred, average='micro')
    test_f1 = metrics.f1_score(y_test, y_pred, average='micro')

    print('Training time = {} sec'.format(search.refit_time_))
    print('Accuracy =', metrics.accuracy_score(y_test, y_pred))
    print('Precision =', metrics.precision_score(y_test, y_pred, average='micro')
    print('Recall =', metrics.recall_score(y_test, y_pred, average='micro'))
    print('F1 =', test_f1)
    print('Train F1 =', train_f1)

    confusion_matrix = metrics.confusion_matrix(y_test, y_pred, labels=range(1, 8
    labels = [str(x) for x in range(1, 8)]
    sns.heatmap(confusion_matrix, cmap="Oranges", annot=True,
                xticklabels=labels, yticklabels=labels)
    plt.title('Confusion matrix')
    plt.show()

    correct_indices = np.where(y_test == y_pred)[0]
    incorrect_indices = np.where(y_test != y_pred)[0]

    for i in correct_indices[:1]:
        print('Example of correct classification (y_pred = {}, y_test = {})'.form
        print(df_test_x.iloc[i])
    print()
    for i in incorrect_indices[:1]:
        print('Example of misclassification (y_pred = {}, y_test = {})'.format(y_
        print(df_test_x.iloc[i])

    best_params_str = ''
    for param, value in search.best_params_.items():
        if best_params_str != '':
            best_params_str += ', '
        if param.startswith('model__'):
            best_params_str += param[len('model__'):]
        else:
            best_params_str += param
        best_params_str += ' = '
        if isinstance(value, float):
            best_params_str += '{:.4f}'.format(value)
        else:
            best_params_str += str(value)

    res = {
        'Classifier': classifier_str,
        'Parameters': best_params_str,
        'Train F1': "{:.4f}".format(train_f1),
        'Test F1': "{:.4f}".format(test_f1),
        'Training Time (sec)': "{:.4f}".format(search.refit_time_)
    }
    final_results.append(res)
```

3.2 Dummy Classifier

Ο Dummy Classifier χρησιμοποίεται ως ένα απλό baseline για τη σύγκριση με τα άλλα μοντέλα. Επιλέγει πάντα την πιο συχνή ετικέτα στο train set.

In [17]:
```
from sklearn import dummy
from sklearn import metrics
from sklearn import pipeline
from time import time

model = dummy.DummyClassifier(strategy='most_frequent', random_state=0)
pipe = pipeline.Pipeline([('scaler', scaler), ('pca', pca), ('model', model)])

t1 = time()
pipe.fit(x_train, y_train)
t2 = time()
y_pred = pipe.predict(x_test)
y_train_pred = pipe.predict(x_train)

train_f1 = metrics.f1_score(y_train, y_train_pred, average='micro')
dummy_f1 = metrics.f1_score(y_test, y_pred, average='micro')

print('Training time = {} sec'.format(t2 - t1))
print('Accuracy =', metrics.accuracy_score(y_test, y_pred))
print('Precision =', metrics.precision_score(y_test, y_pred, average='micro'))
print('Recall =', metrics.recall_score(y_test, y_pred, average='micro'))
print('F1 =', dummy_f1)
print('Train F1 =', train_f1)

res = {
    'Classifier': 'Dummy Classifier',
    'Parameters': "strategy = 'most_frequent'",
    'Train F1': "{:.4f}".format(train_f1),
    'Test F1': "{:.4f}".format(dummy_f1),
    'Training Time (sec)': "{:.4f}".format(t2 - t1)
}
final_results.append(res)
```

```
Training time = 0.001994609832763672 sec
Accuracy = 0.3488372093023256
Precision = 0.3488372093023256
Recall = 0.3488372093023256
F1 = 0.3488372093023256
Train F1 = 0.359375
```

3.3 Linear SVM

Ακολουθεί βελτιστοποίηση του SVM classifier με linear kernel ως προς την παράμετρο C. Το C είναι η παράμετρος αντιστάθμισης μεταξύ της προσπάθειας για μέγιστο περιθώριο μεταξύ των κλάσεων και για ελάχιστο αριθμό λαθών.

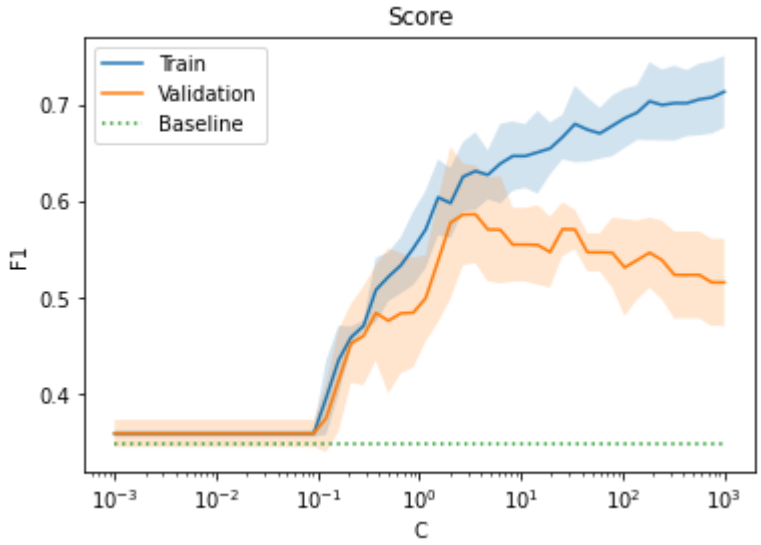
$$Loss = \mathbf{w}^T\mathbf{w} + C\sum_{k=1}^{R}\varepsilon_k$$

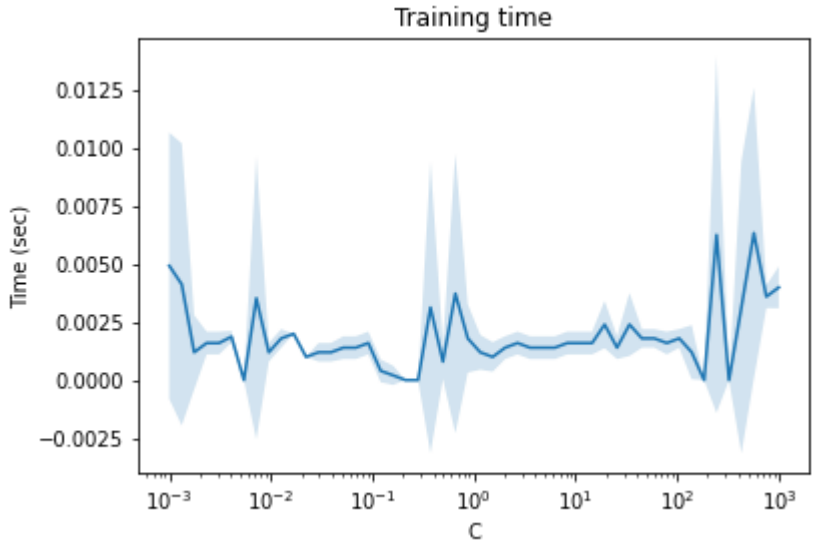
Kernel: $K(\mathbf{x}, \mathbf{x}') = \langle \mathbf{x}, \mathbf{x}' \rangle$

In [18]:
```
from sklearn import svm

model = svm.SVC(kernel='linear')
pipe = pipeline.Pipeline([('scaler', scaler), ('pca', pca), ('model', model)])

param_grid = {
    'model__C': np.logspace(-3, 3)
}

search = model_selection.GridSearchCV(pipe, param_grid, n_jobs=-1, scoring='f1_mi
search.fit(x_train, y_train)

print('Best F1 =', search.best_score_)
print('Best params =', search.best_params_)
```

```
Best F1 = 0.5861538461538462
Best params = {'model__C': 3.5564803062231287}
```

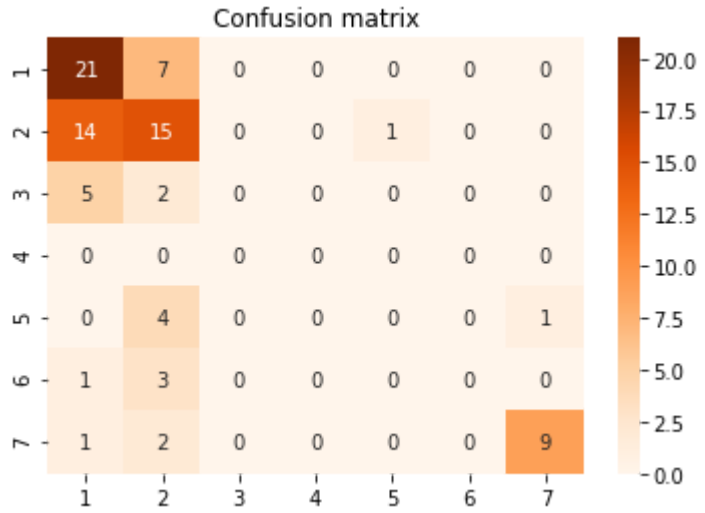
In [19]:
```
plot_grid_search(search, dummy_f1, 'C', xscale='log')
```





In [20]:
```
evaluate_model(search, 'Linear SVM')
```

```
Training time = 0.0009975433349609375 sec
Accuracy = 0.5232558139534884
Precision = 0.5232558139534884
Recall = 0.5232558139534884
F1 = 0.5232558139534884
Train F1 = 0.609375
```




```
Example of correct classification (y_pred = 1, y_test = 1)
RI     1.5172
Na    13.3800
Mg     3.5000
Al     1.1500
Si    72.8500
K      0.5000
Ca     8.4300
Ba     0.0000
Fe     0.0000
Name: 24, dtype: float64

Example of misclassification (y_pred = 2, y_test = 5)
RI     1.52151
Na    11.03000
Mg     1.71000
Al     1.56000
Si    73.44000
K      0.58000
Ca    11.62000
Ba     0.00000
Fe     0.00000
Name: 166, dtype: float64
```

3.4 Polynomial SVM

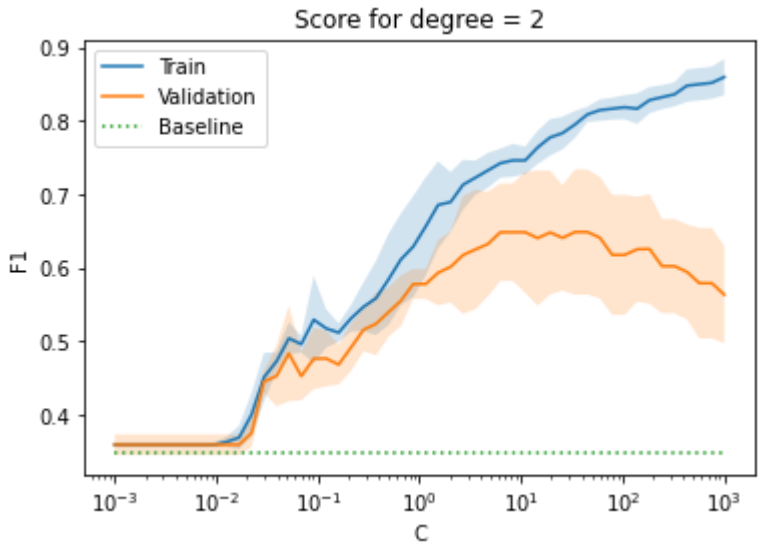
Ακολουθεί βελτιστοποίηση του SVM classifier με polynomial kernel ως προς τις παραμέτρους C και degree. Το degree είναι ο βαθμός του πολυωνύμου.

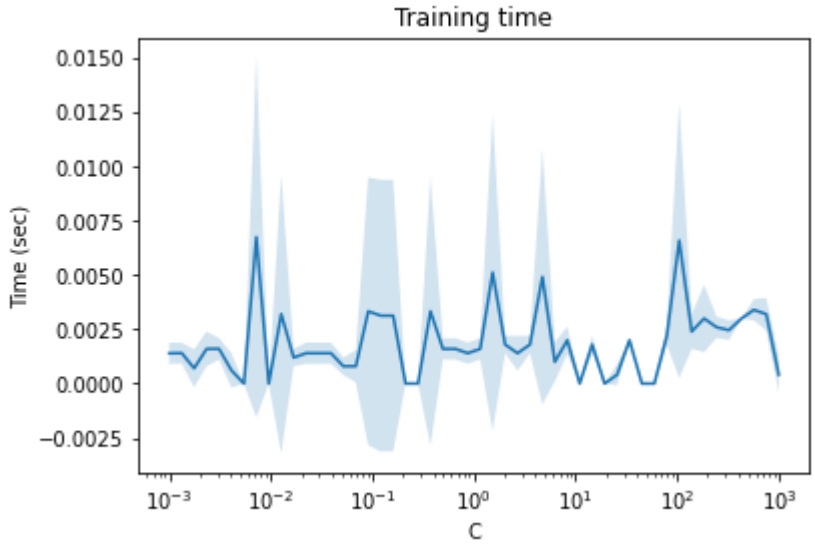
Kernel: $K(\mathbf{x}, \mathbf{x}') = (\gamma\langle \mathbf{x}, \mathbf{x}' \rangle + r)^d$

In [21]:
```
model = svm.SVC(kernel='poly')
pipe = pipeline.Pipeline([('scaler', scaler), ('pca', pca), ('model', model)])

param_grid = {
    'model__C': np.logspace(-3, 3),
    'model__degree': np.arange(2, 5)
}

search = model_selection.GridSearchCV(pipe, param_grid, n_jobs=-1, scoring='f1_mi
search.fit(x_train, y_train)

print('Best F1 =', search.best_score_)
print('Best params =', search.best_params_)
```

```
Best F1 = 0.6486153846153846
Best params = {'model__C': 33.9322177189533, 'model__degree': 2}
```

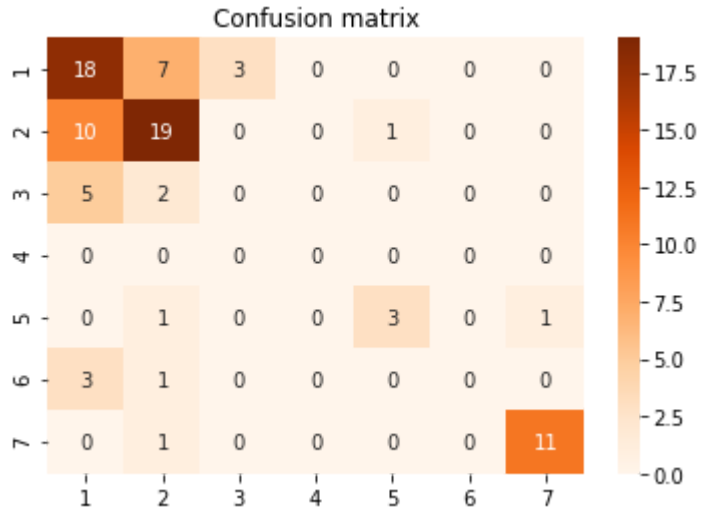
In [22]:
```
plot_grid_search(search, dummy_f1, 'C', param2='degree', xscale='log')
```





In [23]:
```
evaluate_model(search, 'Polynomial SVM')
```

```
Training time = 0.0 sec
Accuracy = 0.5930232558139535
Precision = 0.5930232558139535
Recall = 0.5930232558139535
F1 = 0.5930232558139535
Train F1 = 0.765625
```




```
Example of correct classification (y_pred = 5, y_test = 5)
RI     1.52151
Na    11.03000
Mg     1.71000
Al     1.56000
Si    73.44000
K      0.58000
Ca    11.62000
Ba     0.00000
Fe     0.00000
Name: 166, dtype: float64

Example of misclassification (y_pred = 1, y_test = 3)
RI     1.51643
Na    12.16000
Mg     3.52000
Al     1.35000
Si    72.89000
K      0.57000
Ca     8.53000
Ba     0.00000
```

```
Fe     0.00000
Name: 149, dtype: float64
```

3.5 RBF SVM

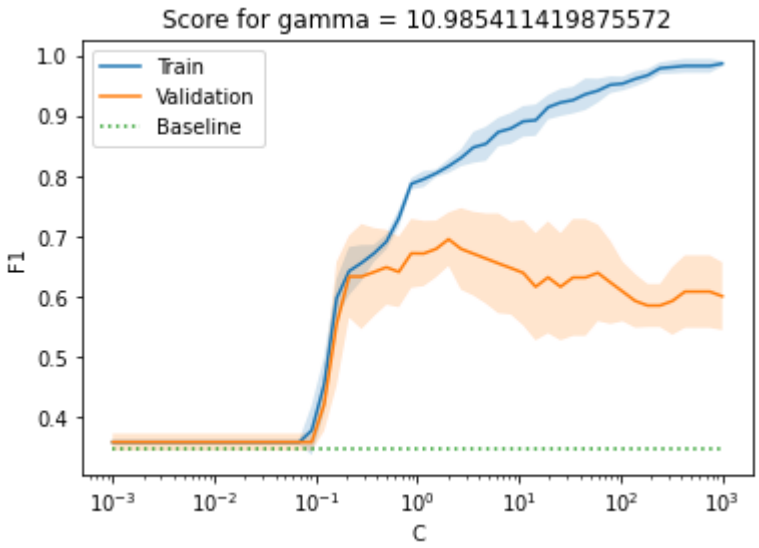
Ακολουθεί βελτιστοποίηση του SVM classifier με rbf kernel ως προς τις παραμέτρους C και gamma. Το gamma δείχνει πόσο μακριά φτάνει η επιρροή ενός παραδείγματος.

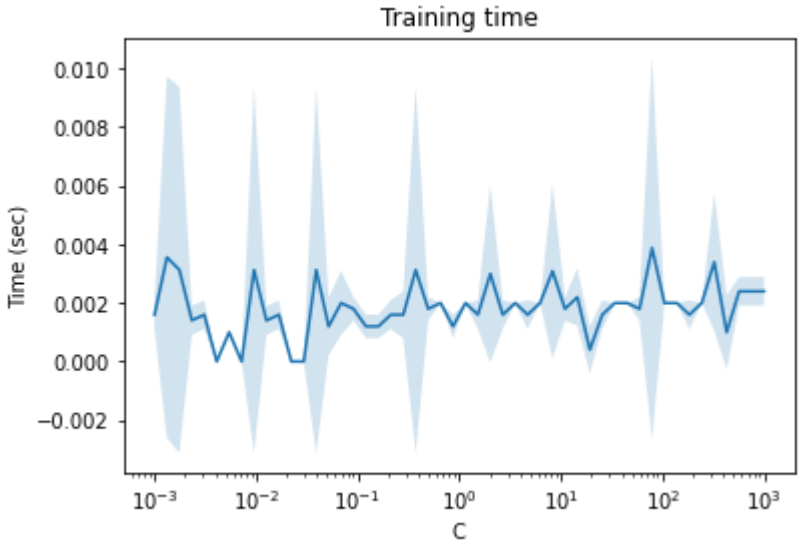
Kernel: $K(\mathbf{x}, \mathbf{x}') = e^{-\gamma||\mathbf{x}-\mathbf{x}'||^2}$

In [24]:
```
model = svm.SVC(kernel='rbf')
pipe = pipeline.Pipeline([('scaler', scaler), ('pca', pca), ('model', model)])

param_grid = {
    'model__C': np.logspace(-3, 3),
    'model__gamma': np.logspace(-3, 3)
}

search = model_selection.GridSearchCV(pipe, param_grid, n_jobs=-1, scoring='f1_mi
search.fit(x_train, y_train)

print('Best F1 =', search.best_score_)
print('Best params =', search.best_params_)
```

```
Best F1 = 0.6953846153846154
Best params = {'model__C': 2.023589647725158, 'model__gamma': 10.98541141987557
2}
```

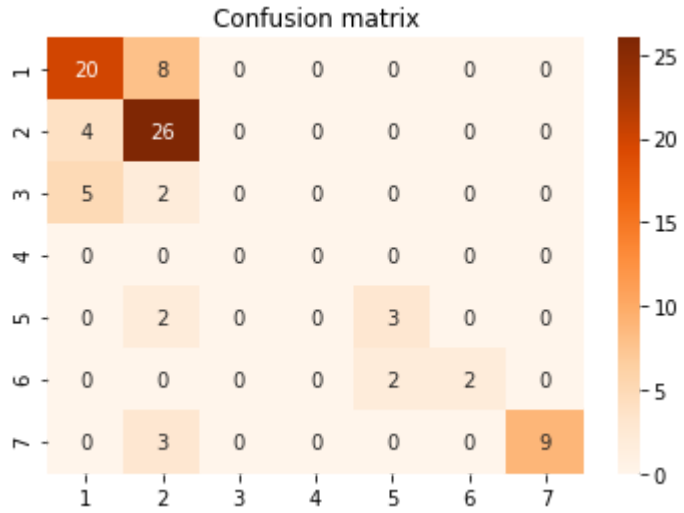
In [25]:
```
plot_grid_search(search, dummy_f1, 'C', param2='gamma', xscale='log')
```





In [26]:
```
evaluate_model(search, 'RBF SVM')
```

```
Training time = 0.001970529556274414 sec
Accuracy = 0.6976744186046512
Precision = 0.6976744186046512
Recall = 0.6976744186046512
F1 = 0.6976744186046512
Train F1 = 0.8046875
```




```
Example of correct classification (y_pred = 5, y_test = 5)
RI     1.52151
Na    11.03000
Mg     1.71000
Al     1.56000
Si    73.44000
K      0.58000
Ca    11.62000
Ba     0.00000
Fe     0.00000
Name: 166, dtype: float64

Example of misclassification (y_pred = 1, y_test = 3)
RI     1.51643
Na    12.16000
Mg     3.52000
Al     1.35000
```

```
Si    72.89000
K      0.57000
Ca     8.53000
Ba     0.00000
Fe     0.00000
Name: 149, dtype: float64
```

3.6 Sigmoid SVM

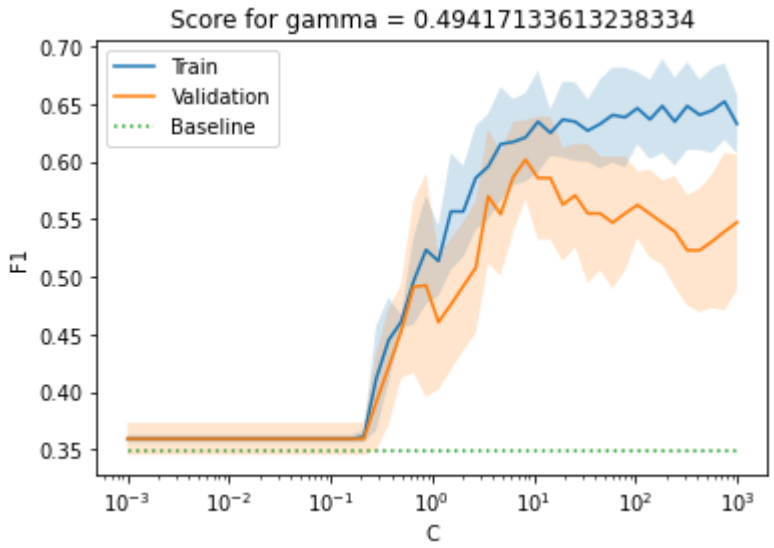
Ακολουθεί βελτιστοποίηση του SVM classifier με sigmoid kernel ως προς τις παραμέτρους C και gamma.

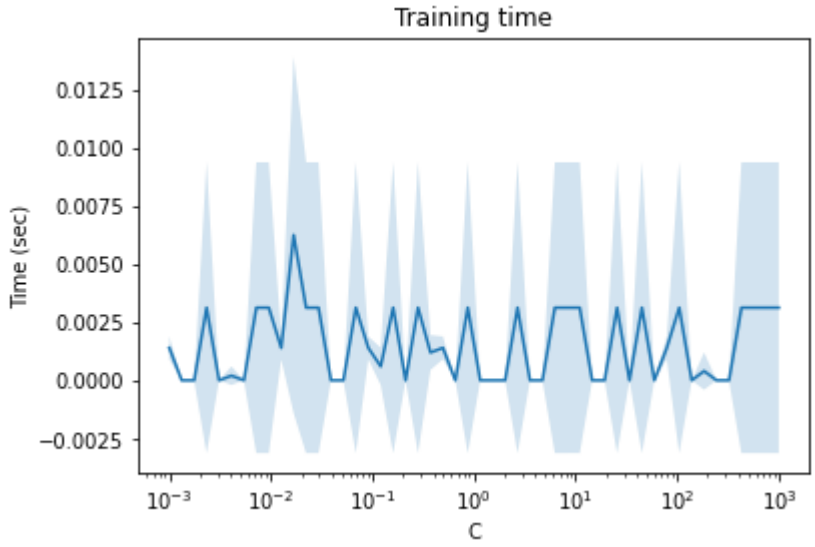
Kernel: $K(\mathbf{x}, \mathbf{x}') = tanh(\gamma\langle \mathbf{x}, \mathbf{x}' \rangle + r)$

In [27]:
```
model = svm.SVC(kernel='sigmoid')
pipe = pipeline.Pipeline([('scaler', scaler), ('pca', pca), ('model', model)])

param_grid = {
    'model__C': np.logspace(-3, 3),
    'model__gamma': np.logspace(-3, 3)
}

search = model_selection.GridSearchCV(pipe, param_grid, n_jobs=-1, scoring='f1_mi
search.fit(x_train, y_train)

print('Best F1 =', search.best_score_)
print('Best params =', search.best_params_)
```

```
Best F1 = 0.6018461538461539
Best params = {'model__C': 8.286427728546842, 'model__gamma': 0.494171336132383
34}
```

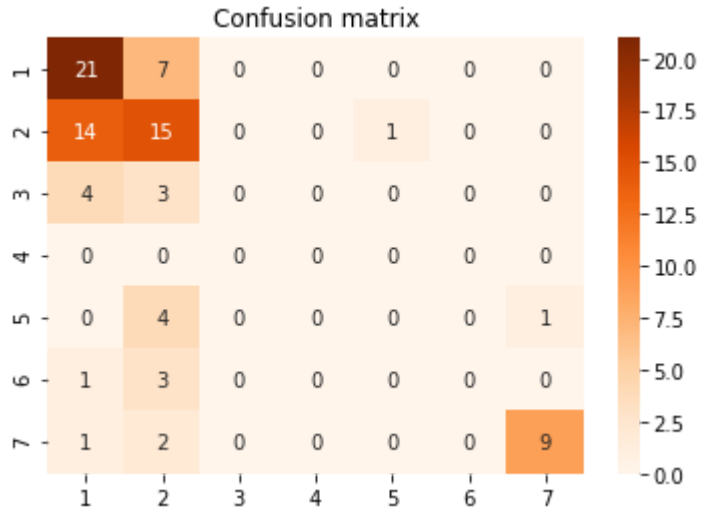
In [28]:
```
plot_grid_search(search, dummy_f1, 'C', param2='gamma', xscale='log')
```





In [29]:
```
evaluate_model(search, 'Sigmoid SVM')
```

```
Training time = 0.0019948482513427734 sec
Accuracy = 0.5232558139534884
Precision = 0.5232558139534884
Recall = 0.5232558139534884
F1 = 0.5232558139534884
Train F1 = 0.609375
```




```
Example of correct classification (y_pred = 1, y_test = 1)
RI     1.5172
Na    13.3800
Mg     3.5000
Al     1.1500
Si    72.8500
K      0.5000
Ca     8.4300
Ba     0.0000
Fe     0.0000
Name: 24, dtype: float64

Example of misclassification (y_pred = 2, y_test = 5)
RI     1.52151
Na    11.03000
Mg     1.71000
Al     1.56000
Si    73.44000
K      0.58000
Ca    11.62000
Ba     0.00000
Fe     0.00000
Name: 166, dtype: float64
```

3.7 Nearest Neighbors

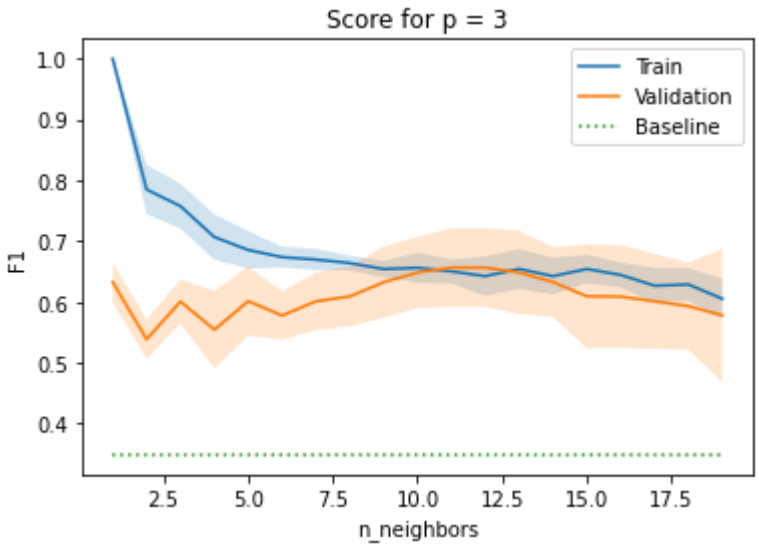
Ακολουθεί βελτιστοποίηση του k-nearest neighbors classifier ως προς τις παραμέτρους n_neighbors και p. Στον πολυδιάστατο χώρο των χαρακτηριστικών οι k πλησιέστεροι γείτονες του κάθε δείγματος ψηφίζουν για να αποφασίσουν την κλάση στην οποία ανήκει. Για να βρεθούν οι πλησιέστεροι γείτονες χρησιμοποιείται η απόσταση minkowski:

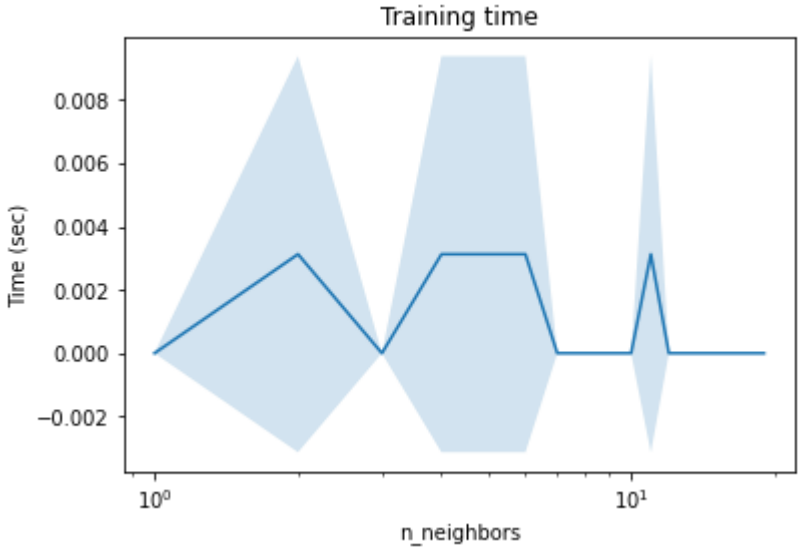
$$d_p(\mathbf{x}, \mathbf{y}) = \sqrt[p]{\sum_i (x_i - y_i)^p}$$

In [30]:
```
from sklearn import neighbors

model = neighbors.KNeighborsClassifier()
pipe = pipeline.Pipeline([('scaler', scaler), ('pca', pca), ('model', model)])

param_grid = {
    'model__n_neighbors': np.arange(1, 20),
    'model__p': np.arange(1, 5)
}

search = model_selection.GridSearchCV(pipe, param_grid, n_jobs=-1, scoring='f1_mi
search.fit(x_train, y_train)

print('Best F1 =', search.best_score_)
print('Best params =', search.best_params_)
```

```
Best F1 = 0.6566153846153846
Best params = {'model__n_neighbors': 11, 'model__p': 3}
```

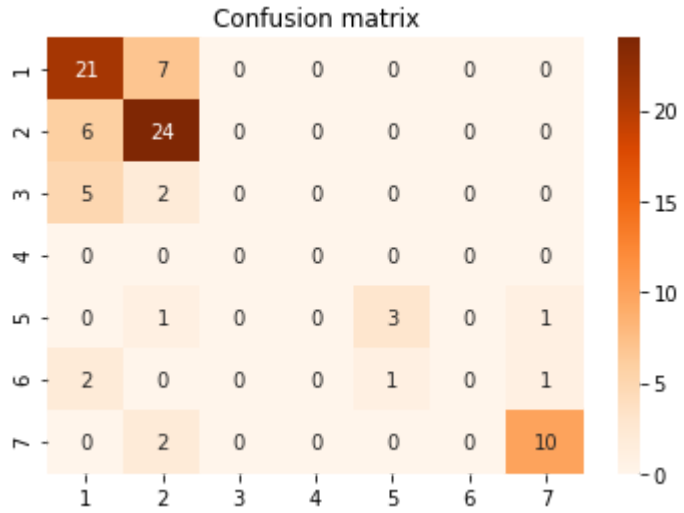
In [31]:
```
plot_grid_search(search, dummy_f1, 'n_neighbors', param2='p')
```





In [32]:
```
evaluate_model(search, 'Nearest Neighbors')
```

```
Training time = 0.015621423721313477 sec
Accuracy = 0.6744186046511628
Precision = 0.6744186046511628
Recall = 0.6744186046511628
F1 = 0.6744186046511628
Train F1 = 0.640625
```




```
Example of correct classification (y_pred = 1, y_test = 1)
RI     1.5172
Na    13.3800
Mg     3.5000
Al     1.1500
Si    72.8500
K      0.5000
Ca     8.4300
Ba     0.0000
Fe     0.0000
Name: 24, dtype: float64

Example of misclassification (y_pred = 2, y_test = 5)
RI     1.52151
Na    11.03000
Mg     1.71000
Al     1.56000
Si    73.44000
K      0.58000
Ca    11.62000
Ba     0.00000
Fe     0.00000
Name: 166, dtype: float64
```

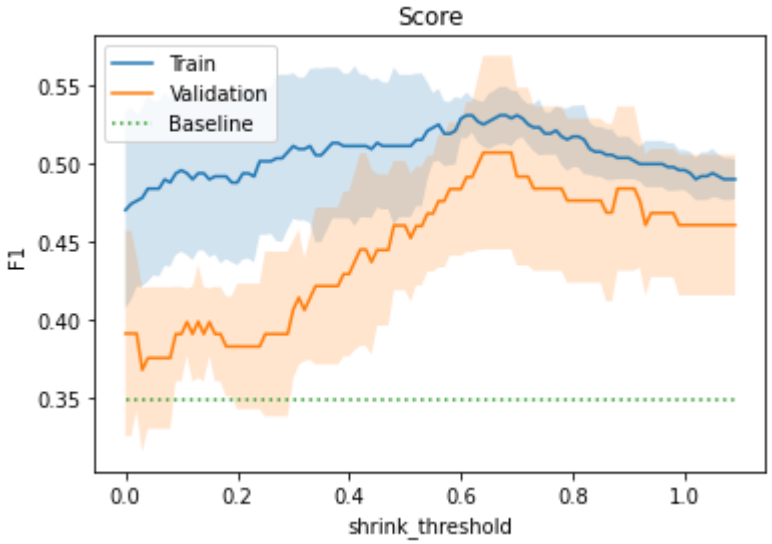
3.8 Nearest Class Centroid

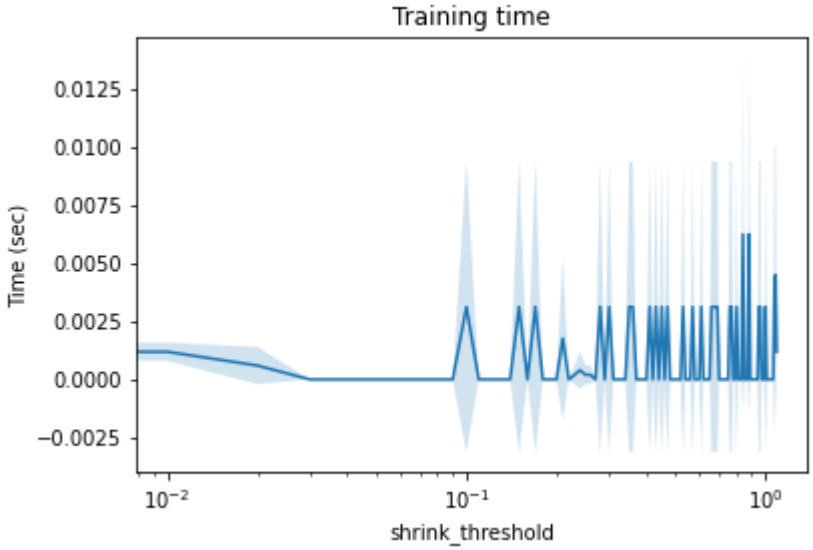
Κάθε κλάση στον Nearest Class Centroid classifier αντιπροσωπεύεται απο το centroid των μελών της.

In [33]:
```
model = neighbors.NearestCentroid()
pipe = pipeline.Pipeline([('scaler', scaler), ('pca', pca), ('model', model)])

param_grid = {
    'model__shrink_threshold': np.arange(0, 1.1, 0.01)
}

search = model_selection.GridSearchCV(pipe, param_grid, n_jobs=-1, scoring='f1_mi
search.fit(x_train, y_train)

print('Best F1 =', search.best_score_)
print('Best params =', search.best_params_)
```

```
Best F1 = 0.5073846153846154
Best params = {'model__shrink_threshold': 0.64}
```

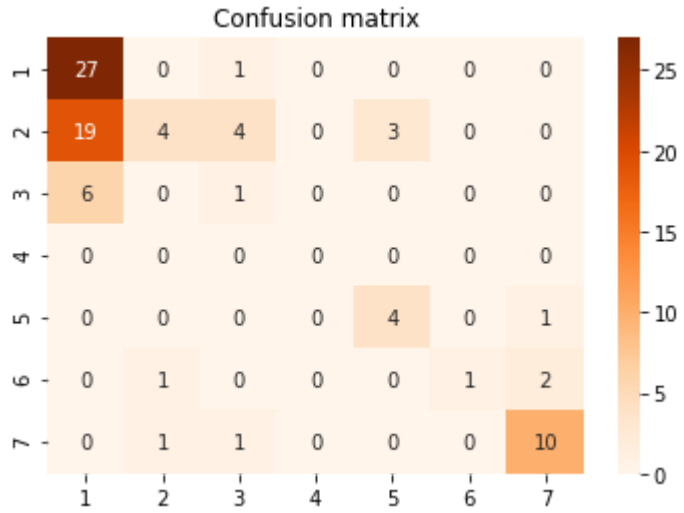
In [34]:
```
plot_grid_search(search, dummy_f1, 'shrink_threshold')
```





In [35]:
```
evaluate_model(search, 'Nearest Class Centroid')
```

```
Training time = 0.0 sec
Accuracy = 0.5465116279069767
Precision = 0.5465116279069767
Recall = 0.5465116279069767
F1 = 0.5465116279069767
Train F1 = 0.5390625
```




```
Example of correct classification (y_pred = 5, y_test = 5)
RI     1.52151
Na    11.03000
Mg     1.71000
Al     1.56000
Si    73.44000
K      0.58000
Ca    11.62000
Ba     0.00000
Fe     0.00000
Name: 166, dtype: float64

Example of misclassification (y_pred = 1, y_test = 2)
RI     1.51574
Na    14.86000
Mg     3.67000
Al     1.74000
Si    71.87000
K      0.16000
Ca     7.36000
Ba     0.00000
Fe     0.12000
Name: 70, dtype: float64
```

3.9 Σύνοψη αποτελεσμάτων

In [36]:
```
final_results_df = pd.DataFrame(final_results)
final_results_df = final_results_df.style.set_table_styles([dict(selector='th', p
final_results_df.set_properties(**{'text-align': 'left'}).hide_index()
```

Out[36]:

Classifier	Parameters	Train F1	Test F1	Training Time (sec)
Dummy Classifier	strategy = 'most_frequent'	0.3594	0.3488	0.0020
Linear SVM	C = 3.5565	0.6094	0.5233	0.0010
Polynomial SVM	C = 33.9322, degree = 2	0.7656	0.5930	0.0000
RBF SVM	C = 2.0236, gamma = 10.9854	0.8047	0.6977	0.0020
Sigmoid SVM	C = 8.2864, gamma = 0.4942	0.6094	0.5233	0.0020
Nearest Neighbors	n_neighbors = 11, p = 3	0.6406	0.6744	0.0156
Nearest Class Centroid	shrink_threshold = 0.6400	0.5391	0.5465	0.0000