Gridsearch, pipeline, confustion matrix, ROC

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1 Start for Random forest in a grid

[24]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
```

[25]:
```
df = pd.read_csv("glassTrain.csv",  index_col=0)
df_test = pd.read_csv("glassTest.csv",  index_col=0)
```

1.1 Using the best features given by mlxtend feature selection

[4]:
```
mlx_df = df[ ['RI', 'Na', 'Mg', 'Si', 'K', 'Ba', 'Fe', 'type'] ]
mlx_test_df = df_test[['RI', 'Na', 'Mg', 'Si', 'K', 'Ba', 'Fe'] ]

X_test = mlx_test_df.values
X = mlx_df.iloc[:, :-1 ].values
y = mlx_df.iloc[:, -1: ].values.flatten()
```

[5]:
```
from sklearn.pipeline import make_pipeline
from sklearn.model_selection import GridSearchCV
from sklearn.ensemble import RandomForestClassifier
```

[6]:
```
rf_pipe = make_pipeline( RandomForestClassifier( n_estimators=500
                              , max_depth= 100
                             , n_jobs=-1))
```

[7]:
```
rf_pipe.fit(X,y)
```

[7]:
```
Pipeline(memory=None,
         steps=[('randomforestclassifier',
                 RandomForestClassifier(bootstrap=True, class_weight=None,
                                        criterion='gini', max_depth=100,
                                        max_features='auto',
                                        max_leaf_nodes=None,
                                        min_impurity_decrease=0.0,
                                        min_impurity_split=None,
```

```
                                        min_samples_leaf=1, min_samples_split=2,
                                        min_weight_fraction_leaf=0.0,
                                        n_estimators=500, n_jobs=-1,
                                        oob_score=False, random_state=None,
                                        verbose=0, warm_start=False))],
         verbose=False)
```

1.2 Use Random forest pipeline with grid

[26]:
```
depth_range = { 'randomforestclassifier__max_depth' :[5, 10, 15, 25, 50, 100] }

gs = GridSearchCV(estimator=rf_pipe,
                  param_grid=depth_range,
                  scoring='f1_macro',
                  cv=6,
                  n_jobs=-1,
                 iid= True)

gs = gs.fit(X, y)
```

[27]:
```
print(gs.best_score_)
print(gs.best_params_)
```

```
0.6202102286525855
{'randomforestclassifier__max_depth': 15}
```

[28]:
```
y_pred_test =  gs.predict(X_test).astype(int)
output = pd.DataFrame( y_pred_test)
output['Id'] = output.index
output=output.rename(columns={ 0: "label"})
output.to_csv("submission_test_gsrf_f1_macro.csv", index=False)
```

[29]:
```
# import sklearn
# sorted(sklearn.metrics.SCORERS.keys())
```

1.3 Random forest with nested CV

[30]:
```
from sklearn.model_selection import cross_val_score
depth_range = { 'randomforestclassifier__max_depth' :[5, 10, 15, 25, 50, 100] }


gs = GridSearchCV(estimator=rf_pipe,
                  param_grid=depth_range,
                  scoring='accuracy',
                  cv=3,
                  n_jobs=-1,
```

```
                  iid= True)



scores = cross_val_score(gs, X, y, scoring='accuracy', cv=3)
scores
```

[30]:
```
array([0.65306122, 0.625     , 0.60869565])
```

[31]:
```
gs.fit(X,y)
```

[31]:
```
GridSearchCV(cv=3, error_score='raise-deprecating',
             estimator=Pipeline(memory=None,
                                steps=[('randomforestclassifier',
                                        RandomForestClassifier(bootstrap=True,
class_weight=None,
                                                               criterion='gini',
                                                               max_depth=100,
max_features='auto',
max_leaf_nodes=None,
min_impurity_decrease=0.0,
min_impurity_split=None,
min_samples_leaf=1,
min_samples_split=2,
min_weight_fraction_leaf=0.0,
                                                               n_estimators=500,
                                                               n_jobs=-1,
                                                               oob_score=False,
random_state=None,
                                                               verbose=0,
warm_start=False))],
                                verbose=False),
             iid=True, n_jobs=-1,
             param_grid={'randomforestclassifier__max_depth': [5, 10, 15, 25,
                                                               50, 100]},
             pre_dispatch='2*n_jobs', refit=True, return_train_score=False,
             scoring='accuracy', verbose=0)
```

[32]:
```
y_pred = gs.predict(X)
from sklearn.metrics import confusion_matrix
confmat = confusion_matrix(y_true=y, y_pred=y_pred, labels=[1, 2, 3, 5, 6, 7] )
print(confmat)
```

```
[[46  1  0  0  0  0]
 [ 3 48  0  0  0  0]
 [ 4  6  1  0  0  0]
 [ 0  0  0  9  0  0]
```

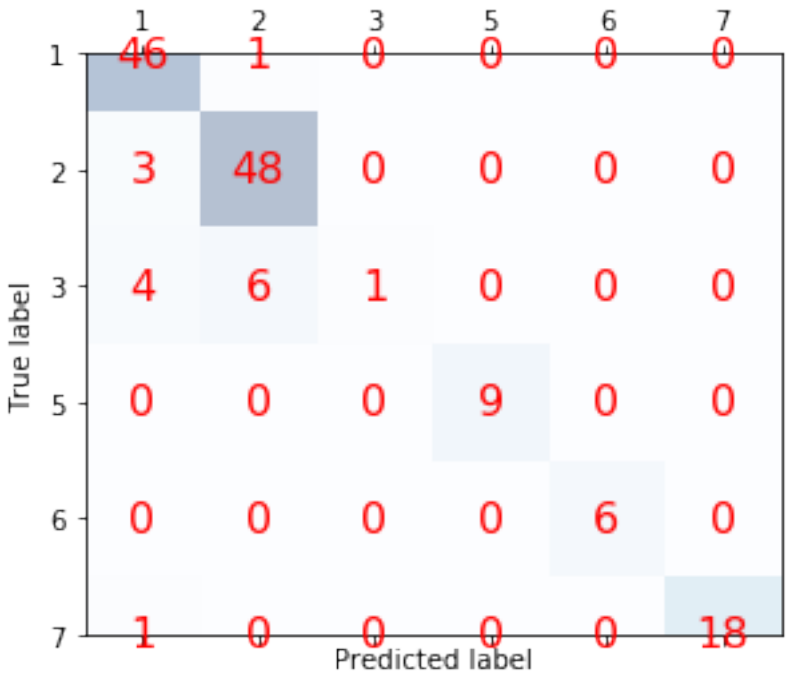
```
[ 0  0  0  0  6  0]
[ 1  0  0  0  0 18]]
```

[33]:
```
df.type.value_counts()
```

[33]:
```
2    51
1    47
7    19
3    11
5     9
6     6
Name: type, dtype: int64
```

1.4 Plot confusion matrix

[35]:
```
fig, ax = plt.subplots()
ax.matshow(confmat, cmap=plt.cm.Blues, alpha=0.3)
labels=[ 1, 2, 3, 5, 6, 7]
for i, ii in enumerate(labels):
    for j, jj in enumerate(labels):
        ax.text(x=j, y=i, s=confmat[i, j], va='center', ha='center',␣
 ↪fontsize=16, color='red')

plt.xlabel('Predicted label')
plt.ylabel('True label')

plt.xticks(ticks=[0,1,2,3,4,5] , labels=labels )
plt.yticks(ticks=[0,1,2,3,4,5] , labels=labels )
plt.show()
```



2 Start of SVC

[36]:
```
from sklearn.model_selection import train_test_split
X_train, X_cross, y_train, y_cross = train_test_split(X, y , test_size=0.3,␣
 ↪stratify=y, random_state=1)
```

[37]:
```
from sklearn.svm import SVC
from sklearn.preprocessing import StandardScaler
from sklearn.pipeline import make_pipeline
from sklearn.model_selection import GridSearchCV
```

[38]:
```
# make pipeline
pipe_svc = make_pipeline(StandardScaler(), SVC(kernel='rbf',random_state=1))

# Define ranges of parameter values:
param_range  = [0.0001, 0.001, 0.01, 0.1, 1.0, 10.0, 100.0, 1000.0] # For␣
 ↪regularization parameter C.
param_range2 = [0.0001, 0.001, 0.01, 0.1, 1.0, 10.0, 100.0]         # For␣
 ↪scaling parameter gamma og rbf-kernel.

param_grid   = [ {'svc__C': param_range, 'svc__gamma': param_range2  }  ]

gs = GridSearchCV(estimator=pipe_svc,
```

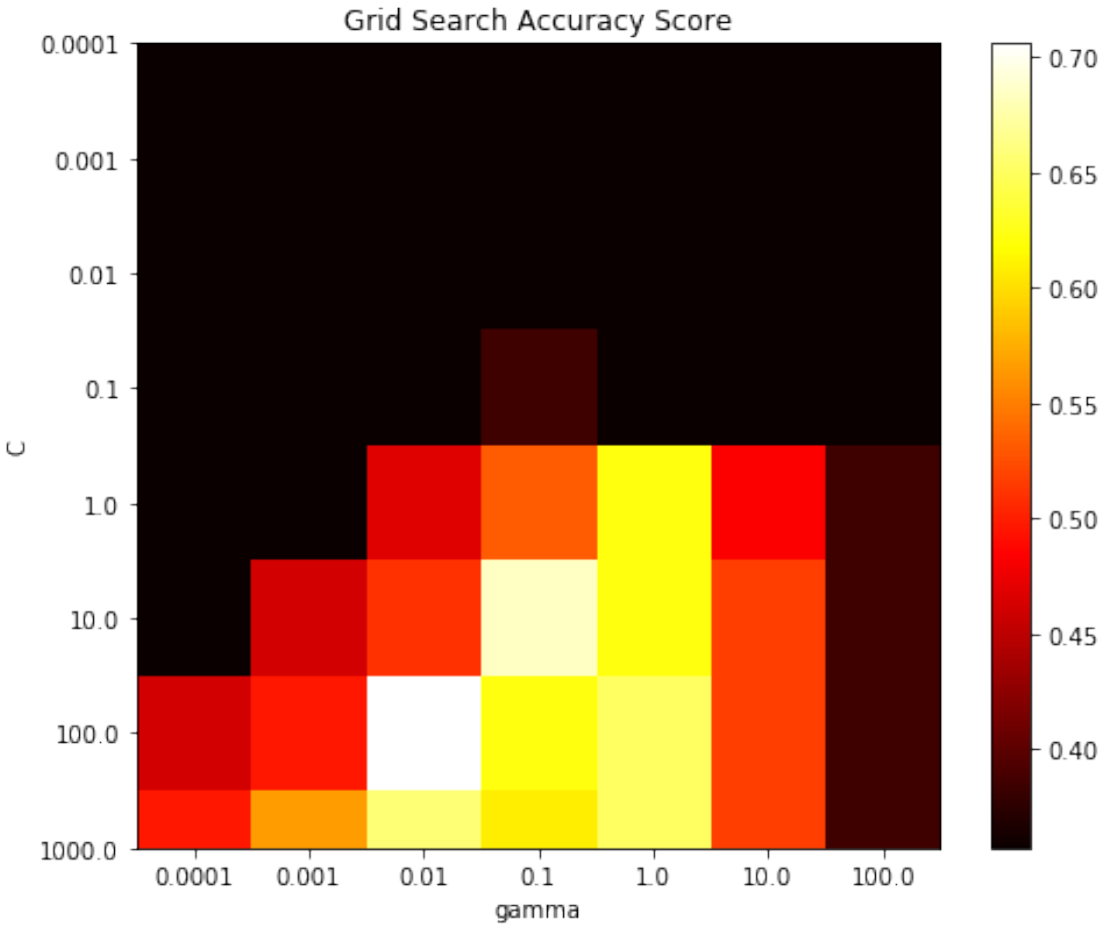
```
                    param_grid=param_grid,
                    scoring='accuracy',
                    cv=6,
                    n_jobs=-1)

gs = gs.fit(X, y)
print(gs.best_score_)
print(gs.best_params_)
```

```
0.7062937062937062
{'svc__C': 100.0, 'svc__gamma': 0.01}
```

```
C:\ProgramData\Anaconda3\lib\site-
packages\sklearn\model_selection\_search.py:814: DeprecationWarning: The default
of the `iid` parameter will change from True to False in version 0.22 and will
be removed in 0.24. This will change numeric results when test-set sizes are
unequal.
  DeprecationWarning)
```

[39]:
```
scores = gs.cv_results_['mean_test_score'].
 ↪reshape(len(param_range),len(param_range2))
```

[40]:
```
plt.figure(figsize=(8, 6))
plt.subplots_adjust(left=.2, right=0.95, bottom=0.15, top=0.95)
plt.imshow(scores, interpolation='nearest', cmap=plt.cm.hot)
plt.xlabel('gamma') # 1/(softness of decision boundary), i.e. small = soft
plt.ylabel('C')     # 1/(size of support vector margin), i.e. large = tight␣
 ↪margin
plt.colorbar()
plt.xticks(np.arange(len(param_range2)), param_range2)
plt.yticks(np.arange(len(param_range)), param_range)
plt.title('Grid Search Accuracy Score')
plt.show()
```



2.1 Fine Tune gamma and C

[41]:
```
# make pipeline
pipe_svc = make_pipeline(StandardScaler(), SVC(kernel='rbf',random_state=1))

# Define ranges of parameter values:
param_range  = [10.0, 20.0, 30.0, 40.0, 50.0, 60.0, 70.0, 80.0, 90.0, 100.0] #␣
 ↪For regularization parameter C.
param_range2 = [0.01,0.002,0.003, 0.004,0.005,0.006, 0.007,0.008,0.009, 0.1] #␣
 ↪For scaling parameter gamma og rbf-kernel.

param_grid   = [ {'svc__C': param_range, 'svc__gamma': param_range2  }  ]


gs = GridSearchCV(estimator=pipe_svc,
                  param_grid=param_grid,
                  scoring='accuracy',
```

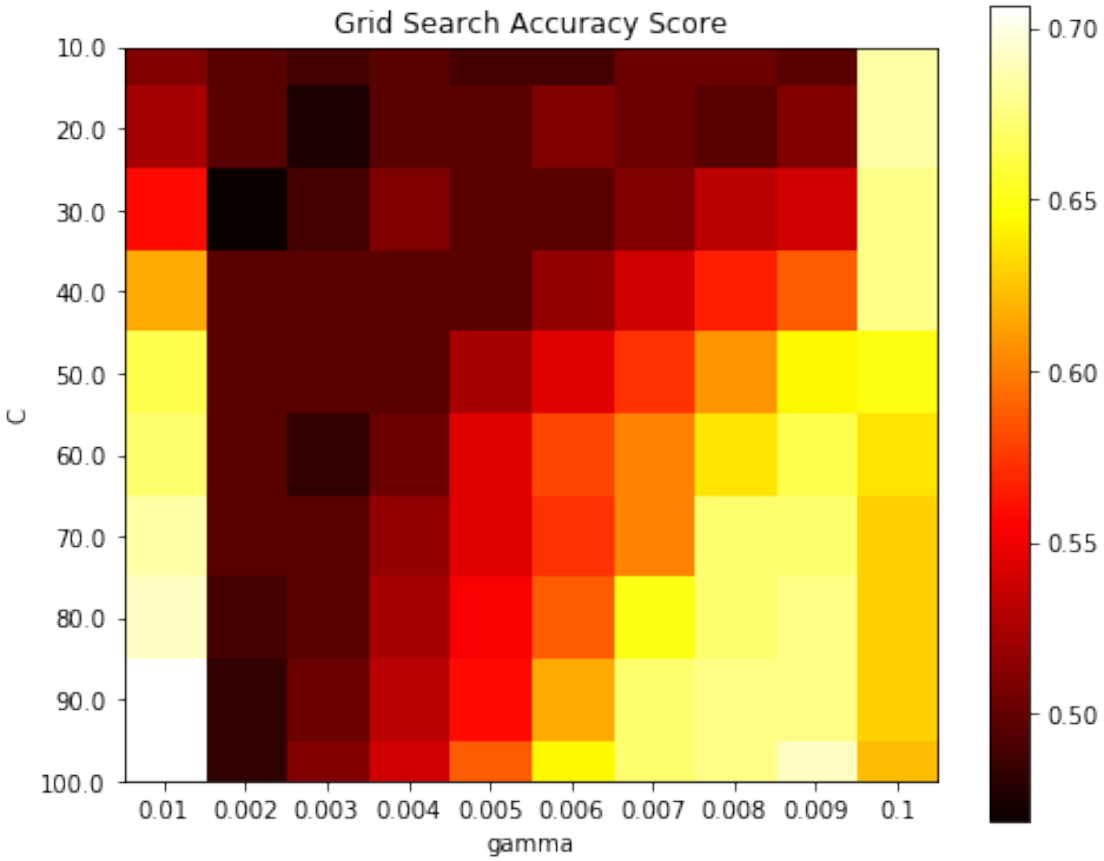
```
                  cv=6,
                  n_jobs=-1)

gs = gs.fit(X, y)
print(gs.best_score_)
print(gs.best_params_)
```

```
0.7062937062937062
{'svc__C': 90.0, 'svc__gamma': 0.01}
```

```
C:\ProgramData\Anaconda3\lib\site-
packages\sklearn\model_selection\_search.py:814: DeprecationWarning: The default
of the `iid` parameter will change from True to False in version 0.22 and will
be removed in 0.24. This will change numeric results when test-set sizes are
unequal.
  DeprecationWarning)
```

[42]:
```
scores = gs.cv_results_['mean_test_score'].
 ↪reshape(len(param_range),len(param_range2))
```

[43]:
```
plt.figure(figsize=(8, 6))
plt.subplots_adjust(left=.2, right=0.95, bottom=0.15, top=0.95)
plt.imshow(scores, interpolation='nearest', cmap=plt.cm.hot)
plt.xlabel('gamma') # 1/(softness of decision boundary), i.e. small = soft
plt.ylabel('C')     # 1/(size of support vector margin), i.e. large = tight␣
 ↪margin
plt.colorbar()
plt.xticks(np.arange(len(param_range2)), param_range2)
plt.yticks(np.arange(len(param_range)), param_range)
plt.title('Grid Search Accuracy Score')
plt.show()
```



2.2 Nested Cross Validation

[44]:
```
from sklearn.model_selection import cross_val_score

pipe_svc = make_pipeline(StandardScaler(), SVC(kernel='rbf',random_state=1))
param_range  = [10.0, 20.0, 30.0, 40.0, 50.0, 60.0, 70.0, 80.0, 90.0, 100.0] #␣
 ↪For regularization parameter C.
param_range2 = [0.01,0.002,0.003, 0.004,0.005,0.006, 0.007,0.008,0.009, 0.1] #␣
 ↪For scaling parameter gamma og rbf-kernel.

inner_segments = 3
outer_segments = 5
n_models = inner_segments*outer_segments*len(param_grid)
gs = GridSearchCV(estimator  = pipe_svc,
                  param_grid = param_grid,
                  scoring    = 'accuracy',
                  iid        = 'True', # Parameter to be removed (weight score␣
 ↪by size of segment)
                  cv         = inner_segments)
```

```
scores = cross_val_score(gs, X, y,
                         scoring='accuracy', cv=outer_segments)

print('CV accuracy: %.3f +/- %.3f' % (np.mean(scores),
                                      np.std(scores)))
```

```
CV accuracy: 0.651 +/- 0.089
```

[45]:
```
gs.fit(X,y)
```

[45]:
```
GridSearchCV(cv=3, error_score='raise-deprecating',
             estimator=Pipeline(memory=None,
                                steps=[('standardscaler',
                                        StandardScaler(copy=True,
                                                       with_mean=True,
                                                       with_std=True)),
                                       ('svc',
                                        SVC(C=1.0, cache_size=200,
                                            class_weight=None, coef0=0.0,
                                            decision_function_shape='ovr',
                                            degree=3, gamma='auto_deprecated',
                                            kernel='rbf', max_iter=-1,
                                            probability=False, random_state=1,
                                            shrinking=True, tol=0.001,
                                            verbose=False))],
                                verbose=False),
             iid='True', n_jobs=None,
             param_grid=[{'svc__C': [10.0, 20.0, 30.0, 40.0, 50.0, 60.0, 70.0,
                                     80.0, 90.0, 100.0],
                          'svc__gamma': [0.01, 0.002, 0.003, 0.004, 0.005,
                                         0.006, 0.007, 0.008, 0.009, 0.1]}],
             pre_dispatch='2*n_jobs', refit=True, return_train_score=False,
             scoring='accuracy', verbose=0)
```

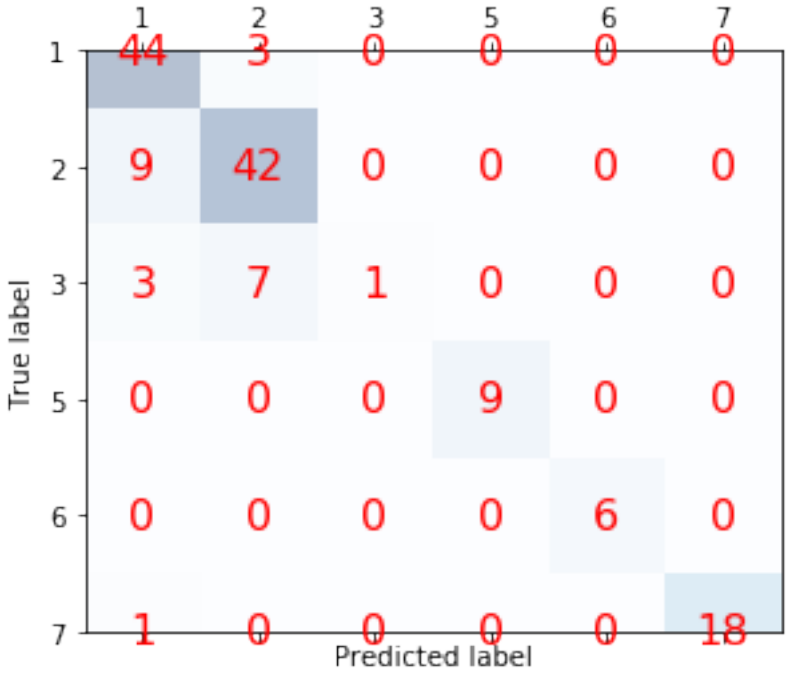
[46]:
```
y_pred_test =  gs.predict(X_test).astype(int)

output = pd.DataFrame( y_pred_test)
output.to_csv("submission_test_gs.csv")
```

2.3 Confusion Matrix

[48]:
```
y_pred = gs.predict(X)
from sklearn.metrics import confusion_matrix
confmat = confusion_matrix(y_true=y, y_pred=y_pred, labels=[1, 2, 3, 5, 6, 7] )
print(confmat)
```

```
[[44  3  0  0  0  0]
 [ 9 42  0  0  0  0]
 [ 3  7  1  0  0  0]
 [ 0  0  0  9  0  0]
 [ 0  0  0  0  6  0]
 [ 1  0  0  0  0 18]]
```

[49]:
```
fig, ax = plt.subplots()
ax.matshow(confmat, cmap=plt.cm.Blues, alpha=0.3)
labels=[ 1, 2, 3, 5, 6, 7]
for i, ii in enumerate(labels):
    for j, jj in enumerate(labels):
        ax.text(x=j, y=i, s=confmat[i, j], va='center', ha='center',␣
 ↪fontsize=16, color='red')

plt.xlabel('Predicted label')
plt.ylabel('True label')

plt.xticks(ticks=[0,1,2,3,4,5] , labels=labels )
plt.yticks(ticks=[0,1,2,3,4,5] , labels=labels )
plt.show()
```



3 Start of KPCA pipe

[50]:
```
df = pd.read_csv("glassTrain.csv",  index_col=0)
df_test = pd.read_csv("glassTest.csv",  index_col=0)
```

[51]:
```
X_test = df_test.values
X = df.iloc[:, :-1 ].values
y = df.iloc[:, -1: ].values.flatten()
```

[52]:
```
from sklearn.decomposition import PCA
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
from sklearn.linear_model import LogisticRegression
from sklearn.decomposition import KernelPCA
from sklearn.ensemble import RandomForestClassifier
from sklearn.pipeline import make_pipeline
from sklearn.model_selection import GridSearchCV
```

[53]:
```
X_train, X_cross, y_train, y_cross = train_test_split( X, y , test_size=0.3,␣
 ↪stratify=y, random_state=0)

# make pipeline
pipe_kpca = make_pipeline(StandardScaler(),  KernelPCA(degree=5),␣
 ↪LogisticRegression(solver='lbfgs',multi_class='auto') )
```

[54]:
```
pipe_kpca.fit(X,y)
```

[54]:
```
Pipeline(memory=None,
         steps=[('standardscaler',
                 StandardScaler(copy=True, with_mean=True, with_std=True)),
                ('kernelpca',
                 KernelPCA(alpha=1.0, coef0=1, copy_X=True, degree=5,
                           eigen_solver='auto', fit_inverse_transform=False,
                           gamma=None, kernel='linear', kernel_params=None,
                           max_iter=None, n_components=None, n_jobs=None,
                           random_state=None, remove_zero_eig=False, tol=0)),
                ('logisticregression',
                 LogisticRegression(C=1.0, class_weight=None, dual=False,
                                    fit_intercept=True, intercept_scaling=1,
                                    l1_ratio=None, max_iter=100,
                                    multi_class='auto', n_jobs=None,
                                    penalty='l2', random_state=None,
                                    solver='lbfgs', tol=0.0001, verbose=0,
                                    warm_start=False))],
         verbose=False)
```

[55]:
```
# Define ranges of parameter values:
# gamma_range = [0.0001, 0.001, 0.01, 0.1, 1.0, 10.0, 100.0]  # For scaling␣
 ↪parameter gamma og rbf-kernel.
C_range = [0.0001, 0.001, 0.01, 0.1, 1.0, 10.0, 100.0]
solver_range = ['liblinear', 'newton-cg', 'lbfgs', 'sag', 'saga']

param_grid   = [ {'logisticregression__C': C_range, 'logisticregression__solver':
 ↪ solver_range  }  ]

gs = GridSearchCV(estimator=pipe_kpca,
                  param_grid=param_grid,
                  scoring='accuracy',
                  cv=6,
                  n_jobs=-1)
```

[56]:
```
gs = gs.fit(X, y)
print(gs.best_score_)
print(gs.best_params_)
```

```
0.5944055944055944
{'logisticregression__C': 100.0, 'logisticregression__solver': 'newton-cg'}
```

```
C:\ProgramData\Anaconda3\lib\site-
packages\sklearn\model_selection\_search.py:814: DeprecationWarning: The default
of the `iid` parameter will change from True to False in version 0.22 and will
be removed in 0.24. This will change numeric results when test-set sizes are
unequal.
  DeprecationWarning)
```

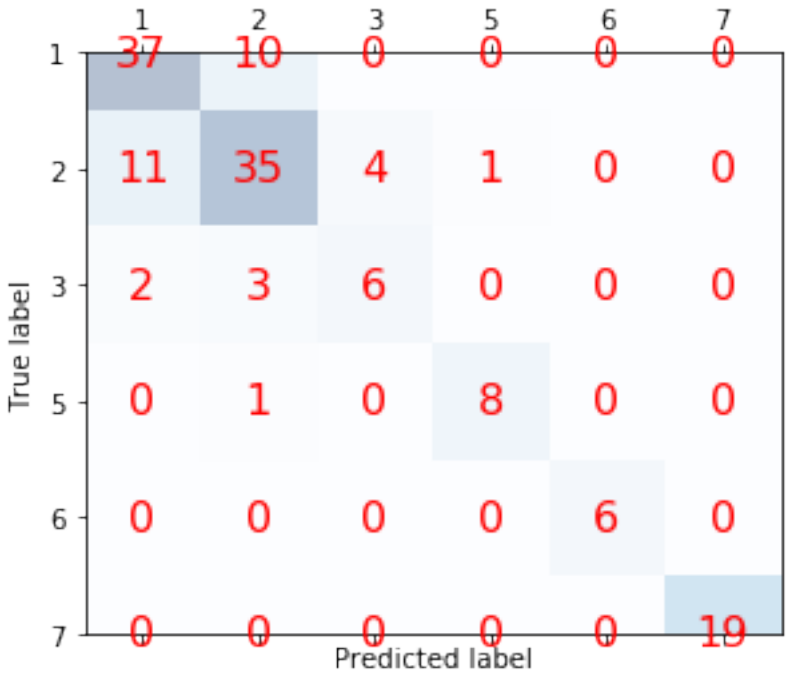
[57]:
```
y_test =  gs.predict(X_test).astype(int)
output = pd.DataFrame( y_test)
output.to_csv("submission_test_gs_lr.csv")
```

3.1 Confusion matrix

[58]:
```
y_pred = gs.predict(X)
from sklearn.metrics import confusion_matrix
confmat = confusion_matrix(y_true=y, y_pred=y_pred, labels=[1, 2, 3, 5, 6, 7] )
print(confmat)
```

```
[[37 10  0  0  0  0]
 [11 35  4  1  0  0]
 [ 2  3  6  0  0  0]
 [ 0  1  0  8  0  0]
 [ 0  0  0  0  6  0]
 [ 0  0  0  0  0 19]]
```

[59]:
```
fig, ax = plt.subplots()
ax.matshow(confmat, cmap=plt.cm.Blues, alpha=0.3)
labels=[ 1, 2, 3, 5, 6, 7]
for i, ii in enumerate(labels):
    for j, jj in enumerate(labels):
        ax.text(x=j, y=i, s=confmat[i, j], va='center', ha='center',␣
 ↪fontsize=16, color='red')

plt.xlabel('Predicted label')
plt.ylabel('True label')

plt.xticks(ticks=[0,1,2,3,4,5] , labels=labels )
plt.yticks(ticks=[0,1,2,3,4,5] , labels=labels )
plt.show()
```



[ ]: