DSpectra_2nd_fraction

February 17, 2018

In [1]:
```
# Import modues
# -*- encoding: utf-8 -*-
import numpy as np
import matplotlib as mpl
from matplotlib import rc
import math
import pandas as pd
import os
import itertools
import scipy
from scipy import stats
from scipy import ndimage
import seaborn as sns

import matplotlib as mpl
from matplotlib import cm
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D

from statsmodels.stats.descriptivestats import sign_test
from statsmodels.stats.weightstats import zconfint
from statsmodels.stats.weightstats import *

from skimage import measure
from scipy import ndimage
from scipy import misc

from scipy.stats.stats import pearsonr, spearmanr
from collections import  Counter

# from pandas import ExcelWriter
from sklearn.cross_validation import train_test_split
from sklearn.linear_model import LinearRegression
from sklearn.linear_model import Lasso
from sklearn.linear_model import Ridge
from sklearn.metrics import mean_squared_error
from sklearn.ensemble import RandomForestRegressor
```

```
import statsmodels.stats.api as sm
from sklearn import cross_validation, datasets, linear_model, metrics
from sklearn.naive_bayes import MultinomialNB
from sklearn.ensemble import RandomForestClassifier
from sklearn.preprocessing import OneHotEncoder

from sklearn.cluster import KMeans
from sklearn.neighbors import KNeighborsClassifier
from sklearn.metrics import classification_report, accuracy_score, f1_score, precision_s
from sklearn import cross_validation, datasets, grid_search, linear_model, metrics

from scipy.optimize import curve_fit
from scipy import signal

from sklearn import random_projection
from sklearn.decomposition import RandomizedPCA
from sklearn.decomposition import PCA
from sklearn import manifold
from sklearn.cluster import KMeans
import pickle
sns.set_style("whitegrid")
sns.set_palette('Accent')

rc('font', family='Arial')  # change font for russian

% matplotlib inline
print 'Import Ready'
```

```
Import Ready
```

```
/usr/local/lib/python2.7/dist-packages/sklearn/cross_validation.py:41: DeprecationWarning: This
  "This module will be removed in 0.20.", DeprecationWarning)
/usr/local/lib/python2.7/dist-packages/statsmodels/compat/pandas.py:56: FutureWarning: The panda
  from pandas.core import datetools
/usr/local/lib/python2.7/dist-packages/sklearn/grid_search.py:42: DeprecationWarning: This modul
  DeprecationWarning)
```

In [2]:
```
# Help function
def grain_to_num(x):
    if x == 'grain':
        return 5000
    elif x == 'rawgrain':
        return 7000
    else:
        return int(x)
```

```
        markers = ['o','s','d','v','h','>','<','*','^','+']
        markers_line = ['-o','-s','-d','-v', '-h', '->','-<', '-*']

        cmap = plt.get_cmap('Accent')
        colors = [cmap(i) for i in np.linspace(0, 1, 10)][1:]
```

```
In [38]: # Load datasets
         spe_df_npks_prep = pd.read_pickle('spe_df_cl_type')  # load smooth spectra
```

```
In [39]: # Drop useless data
         spe_df_npks_prep = spe_df_npks_prep.loc[(spe_df_npks_prep.fraction != '100.dry') &
                                                 (spe_df_npks_prep.fraction != '500.dry')]
```

```
In [40]: # Class is disbalansed
         print Counter(spe_df_npks_prep.fraction)
```

```
Counter({'100': 29, '500': 26, 'grain': 24, 'rawgrain': 10})
```

```
In [41]: # Add data to rawgrain class with bootstrap (create 20 false data to rawgrain)
         add_rawgrain_prep = spe_df_npks_prep[spe_df_npks_prep['fraction'] == 'rawgrain']

         add_rawgrain_prep = add_rawgrain_prep.loc[:, [u'base_s',u'Si', u'P',
                                    u'S', u'Cl', u'K',
                                    u'Ca', u'Ti', u'Mn',
                                    u'Fe', u'Sr', u'Mo_Coh', u'Mo']]

         mi = add_rawgrain_prep.min(axis=0)
         ma = add_rawgrain_prep.max(axis=0)
         all_d = []
         for j in xrange(len(mi)):
             all_d.append(np.random.randint(mi[j],ma[j],20))
         c = add_rawgrain_prep.columns.tolist()
         false_rawgrain_prep = pd.DataFrame(np.transpose(np.array(all_d)), columns=c)
         false_rawgrain_prep['fraction'] = 'rawgrain'

         spe_df_npks_prep = pd.concat([spe_df_npks_prep, false_rawgrain_prep])
         print Counter(spe_df_npks_prep.fraction)
```

```
Counter({'rawgrain': 30, '100': 29, '500': 26, 'grain': 24})
```

```
In [42]: # Use normalization
         fraction_labels = spe_df_npks_prep.fraction
         ftype_name = Counter(fraction_labels).keys()
         shifr = dict(zip(ftype_name, xrange(len(ftype_name))))
         print 'Shifr fraction: ', shifr
         fraction_labels = [shifr[x] for x in fraction_labels]
         print 'Fraction: ', Counter(fraction_labels)
```

```
data_smooth = spe_df_npks_prep[[u'base_s',u'Si', u'P',
                                u'S', u'Cl', u'K',
                                u'Ca', u'Ti', u'Mn',
                                u'Fe', u'Sr', u'Mo_Coh', u'Mo']]

data_prep_r = (data_smooth - data_smooth.mean()) / (data_smooth.max() - data_smooth.min

data_prep_z = (data_smooth - data_smooth.mean()) / data_smooth.std()
```

```
Shifr fraction:  {'100': 0, 'rawgrain': 1, 'grain': 2, '500': 3}
Fraction:  Counter({1: 30, 0: 29, 3: 26, 2: 24})
```

In [43]:
```
# Check the shape
print data_smooth.shape, data_prep_r.shape, data_prep_z.shape
```

```
(109, 13) (109, 13) (109, 13)
```

In [48]:
```
def classif_art3(all_data, all_labels, tdata=''):
    # We will evaluate different approaches to classification with the selection of par
    '''
    Function for optimmize classification and calculate main quality metrics.
    Return:
        outputs with data
    Parameters:
        train_data
        train_labels
        test_data - data for test
        test_labels - labels for test
        tdata - type of data, if needed
    '''

    # Split to train and test
    print Counter(all_labels)
    train_data, test_data, train_labels, test_labels = cross_validation.train_test_spli
                                                test_size=0.2,train_size=0.8,stratify=all_l
    print Counter(train_labels)
    print Counter(test_labels)
    # CV startegy and mertics
    #  -   ,    20 %
    cv = cross_validation.StratifiedShuffleSplit(train_labels, n_iter = 10, test_size =
    cv_metricks = cross_validation.StratifiedShuffleSplit(all_labels, n_iter = 10, test
    metrics_all = ['accuracy', 'precision_macro', 'f1_macro', 'recall_macro']
    metriks_names = ['accuracy', 'precision_macro', 'f1_macro', 'recall_macro']

    # 1 - Linear classification with gradient descent
    print '\t\tLinesr classif:'
```

```
log_regressor = linear_model.SGDClassifier(penalty='none', shuffle=True, random_sta
# grid search
parameters_grid = {
    'loss': ['hinge', 'log','squared_loss', 'modified_huber'],
    'fit_intercept': [True, False],
    'max_iter' : np.linspace(1000, 15000, 5, dtype=int),  #
}
grid_cv = grid_search.GridSearchCV(log_regressor, parameters_grid, scoring = 'f1_ma
grid_cv.fit(train_data, train_labels)
print 'Best with grid search: '
print '\testimator: ', grid_cv.best_estimator_
print '\tscore: ', grid_cv.best_score_
print '\tparameters: ', grid_cv.best_params_
print '\tfeatures importamce: '
a = train_data.columns
imp = np.mean(np.abs(grid_cv.best_estimator_.coef_),0)
b = imp / np.sum(imp) * 100.
importances = pd.DataFrame(zip(a, b))
importances.columns = ['feature name', 'importance']
print '\t', importances.sort_values(by='importance', ascending=False)

print "\tDetailed classification report:"
y_true, y_pred = test_labels, grid_cv.best_estimator_.predict(test_data)
print '\t', classification_report(y_true, y_pred)

for i in xrange(len(metrics_all)):
    scor = metrics_all[i]
    scoring = cross_validation.cross_val_score(grid_cv.best_estimator_, all_data, a
                                             scoring = scor, cv = cv_metricks)
    print 'Best SGDLin ' + metriks_names[i] + ' mean:{}, max:{}, min:{}, std:{}'.fo
                                                 scoring.min(), scoring.std())


# 2 - RidgeClassifier
print
ridge_classifier = linear_model.SGDClassifier(penalty='l2', random_state=0)
print '\t\tRidge Classifire:'
# grid search
parameters_grid = {
    'loss': ['hinge', 'log','squared_loss', 'modified_huber'],
    'fit_intercept': [True, False],
    'max_iter': np.linspace(1000,15000, 5, dtype=int),
    'alpha': np.linspace(0.0001, 1., num = 10)  #
}
grid_cv = grid_search.GridSearchCV(ridge_classifier, parameters_grid, scoring = 'f1
grid_cv.fit(train_data, train_labels)
print 'Best with grid search: '
print '\testimator: ', grid_cv.best_estimator_
```

```
print '\tscore: ', grid_cv.best_score_
print '\tparameters: ', grid_cv.best_params_
print '\tfeatures importamce: '
a = train_data.columns
imp = np.mean(np.abs(grid_cv.best_estimator_.coef_),0)
b = imp / np.sum(imp) * 100.
importances = pd.DataFrame(zip(a, b))
importances.columns = ['feature name', 'importance']
print '\t', importances.sort_values(by='importance', ascending=False)

print "\tDetailed classification report:"
y_true, y_pred = test_labels, grid_cv.best_estimator_.predict(test_data)
print '\t', classification_report(y_true, y_pred)

for i in xrange(len(metrics_all)):
    scor = metrics_all[i]
    scoring = cross_validation.cross_val_score(grid_cv.best_estimator_, all_data, a
                                               scoring = scor, cv = cv_metricks)
    print 'Best Ridge ' + metriks_names[i] + ' mean:{}, max:{}, min:{}, std:{}'.for



# 3 - Lasso (L1) linear regression
print
print '\t\tLasso Classifire:'
lasso_classifire = linear_model.SGDClassifier(penalty='l1', random_state=0)
parameters_grid = {
    'loss': ['hinge', 'log','squared_loss', 'modified_huber'],
    'fit_intercept': [True, False],  # center data
    'max_iter': np.linspace(1000,15000, 5, dtype=int),
    'alpha': np.linspace(0.0001, 1., num = 10)  #
}
grid_cv = grid_search.GridSearchCV(lasso_classifire, parameters_grid, scoring = 'f1
grid_cv.fit(train_data, train_labels)
print 'Best with grid search: '
print '\testimator: ', grid_cv.best_estimator_
print '\tscore: ', grid_cv.best_score_
print '\tparameters: ', grid_cv.best_params_
print '\tfeatures importamce: '
a = train_data.columns
imp = np.mean(np.abs(grid_cv.best_estimator_.coef_),0)
b = imp / np.sum(imp) * 100.
importances = pd.DataFrame(zip(a, b))
importances.columns = ['feature name', 'importance']
print '\t', importances.sort_values(by='importance', ascending=False)

print "\tDetailed classification report:"
y_true, y_pred = test_labels, grid_cv.best_estimator_.predict(test_data)
```

```
        print '\t', classification_report(y_true, y_pred)

        for i in xrange(len(metrics_all)):
            scor = metrics_all[i]
            scoring = cross_validation.cross_val_score(grid_cv.best_estimator_, all_data, a
                                                        scoring = scor, cv = cv_metricks)
            print 'Best L1 ' + metriks_names[i] + ' mean:{}, max:{}, min:{}, std:{}'.format
                                                            scoring.min(), scoring.std())

        # nonlinear Random Forest
        print
        rf_classifier = RandomForestClassifier(random_state=0)
        print '\t\tRandom Forest:'
        parameters_grid = {
            'n_estimators' : range(2, 100, 20),
            'max_features' : ['auto', 'sqrt', 'log2', None],
            'max_depth': [None] + range(2,13,5),
            'bootstrap' : [False, True],
            'class_weight': ['balanced', None]
        }
        grid_cv = grid_search.GridSearchCV(rf_classifier, parameters_grid, scoring = 'f1_ma
        grid_cv.fit(train_data, train_labels)
        print 'Best with grid search: '
        print '\testimator: ', grid_cv.best_estimator_
        print '\tscore: ', grid_cv.best_score_
        print '\tparameters: ', grid_cv.best_params_
        print '\tfeatures importamce: '
        importances = pd.DataFrame(zip(train_data.columns, grid_cv.best_estimator_.feature_
        importances.columns = ['feature name', 'importance']
        print '\t', importances.sort_values(by='importance', ascending=False)
        print "\tDetailed classification report:"
        y_true, y_pred = test_labels, grid_cv.best_estimator_.predict(test_data)
        print '\t', classification_report(y_true, y_pred)

        for i in xrange(len(metrics_all)):
            scor = metrics_all[i]
            scoring = cross_validation.cross_val_score(grid_cv.best_estimator_, all_data, a
                                                        scoring = scor, cv = cv_metricks)
            print 'Best RF ' + metriks_names[i] + ' mean:{}, max:{}, min:{}, std:{}'.format
                                                            scoring.min(), scoring.std())
```

In [49]:
```
# Calculate classification for fraction with data
#
list_df = [data_smooth, data_prep_r, data_prep_z]
list_names=['spe_df_npks_prep', 'data_prep_r', 'data_prep_z']
for i in xrange(len(list_df)):
    name = list_names[i]
    all_df_class = list_df[i]
```

```
            print
            print '\t Start new data classification ' + name
            print
            all_df_class.dropna(inplace=True)

            all_df_class = all_df_class.astype(float, inplace=True)
            classif_art3(all_data=all_df_class, all_labels=fraction_labels, tdata='fraction '+n
            print
```

```
         Start new data classification spe_df_npks_prep

Counter({1: 30, 0: 29, 3: 26, 2: 24})
Counter({1: 24, 0: 23, 3: 21, 2: 19})
Counter({0: 6, 1: 6, 2: 5, 3: 5})
                Linesr classif:
```

```
/usr/local/lib/python2.7/dist-packages/ipykernel_launcher.py:10: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame

See the caveats in the documentation: http://pandas.pydata.org/pandas-docs/stable/indexing.html#
  # Remove the CWD from sys.path while we load stuff.
```

```
Best with grid search:
        estimator:  SGDClassifier(alpha=0.0001, average=False, class_weight=None, epsilon=0.1,
       eta0=0.0, fit_intercept=True, l1_ratio=0.15,
       learning_rate='optimal', loss='log', max_iter=15000, n_iter=None,
       n_jobs=1, penalty='none', power_t=0.5, random_state=0, shuffle=True,
       tol=None, verbose=0, warm_start=False)
        score:  0.707906436529
        parameters:  {'loss': 'log', 'max_iter': 15000, 'fit_intercept': True}
        features importamce:
           feature name  importance
5             K   28.187664
2             P   20.938611
6            Ca   20.753671
4            Cl   11.098228
3             S    9.066928
10           Sr    2.968945
0        base_s    2.167351
9            Fe    1.272086
1            Si    1.262065
7            Ti    0.987836
12           Mo    0.669217
8            Mn    0.369684
11       Mo_Coh    0.257713
```

```
        Detailed classification report:
                     precision    recall  f1-score   support

          0       0.44      0.67      0.53         6
          1       1.00      1.00      1.00         6
          2       0.71      1.00      0.83         5
          3       0.00      0.00      0.00         5

avg / total       0.56      0.68      0.61        22

Best SGDLin accuracy mean:0.757575757576, max:0.969696969697, min:0.636363636364, std:0.10670798
Best SGDLin precision_macro mean:0.691620220058, max:0.975, min:0.516666666667, std:0.1750584610
Best SGDLin f1_macro mean:0.708349065905, max:0.970175438596, min:0.562834224599, std:0.13970372
Best SGDLin recall_macro mean:0.762698412698, max:0.96875, min:0.651785714286, std:0.10502345109

                Ridge Classifire:
Best with grid search:
        estimator:  SGDClassifier(alpha=0.11120000000000001, average=False, class_weight=None,
       epsilon=0.1, eta0=0.0, fit_intercept=False, l1_ratio=0.15,
       learning_rate='optimal', loss='log', max_iter=15000, n_iter=None,
       n_jobs=1, penalty='l2', power_t=0.5, random_state=0, shuffle=True,
       tol=None, verbose=0, warm_start=False)
        score:  0.573010887225
        parameters:  {'alpha': 0.11120000000000001, 'loss': 'log', 'max_iter': 15000, 'fit_inter
        features importamce:
           feature name  importance
5             K   25.535646
6            Ca   19.940428
4            Cl   19.938945
2             P   19.704375
10           Sr    4.384987
3             S    4.170666
7            Ti    1.689760
0        base_s    1.242397
9            Fe    1.209169
1            Si    0.948868
12           Mo    0.511172
8            Mn    0.483565
11       Mo_Coh    0.240022
        Detailed classification report:
                     precision    recall  f1-score   support

          0       0.55      1.00      0.71         6
          1       1.00      1.00      1.00         6
          2       1.00      1.00      1.00         5
          3       0.00      0.00      0.00         5

avg / total       0.65      0.77      0.69        22
```

```
Best Ridge accuracy mean:0.666666666667, max:0.757575757576, min:0.515151515152, std:0.081311562
Best Ridge precision_macro mean:0.542567744004, max:0.632352941176, min:0.333333333333, std:0.08
Best Ridge f1_macro mean:0.580577887926, max:0.673076923077, min:0.375, std:0.0973193668857
Best Ridge recall_macro mean:0.672767857143, max:0.75, min:0.5, std:0.0829041201143

                Lasso Classifire:
Best with grid search:
        estimator:  SGDClassifier(alpha=0.0001, average=False, class_weight=None, epsilon=0.1,
       eta0=0.0, fit_intercept=True, l1_ratio=0.15,
       learning_rate='optimal', loss='modified_huber', max_iter=15000,
       n_iter=None, n_jobs=1, penalty='l1', power_t=0.5, random_state=0,
       shuffle=True, tol=None, verbose=0, warm_start=False)
        score:  0.717817270878
        parameters:  {'alpha': 0.0001, 'loss': 'modified_huber', 'max_iter': 15000, 'fit_interce
        features importamce:
           feature name  importance
5             K   28.182291
2             P   20.966581
6            Ca   20.746615
4            Cl   11.079199
3             S    9.069135
10           Sr    2.972935
0        base_s    2.165077
9            Fe    1.272165
1            Si    1.260527
7            Ti    0.988951
12           Mo    0.669804
8            Mn    0.369702
11       Mo_Coh    0.257017
        Detailed classification report:
                     precision    recall  f1-score   support

          0       0.44      0.67      0.53         6
          1       1.00      1.00      1.00         6
          2       0.71      1.00      0.83         5
          3       0.00      0.00      0.00         5

avg / total       0.56      0.68      0.61        22

Best L1 accuracy mean:0.730303030303, max:0.878787878788, min:0.636363636364, std:0.075999613357
Best L1 precision_macro mean:0.678022763593, max:0.894444444444, min:0.515384615385, std:0.14100
Best L1 f1_macro mean:0.674434217442, max:0.869543650794, min:0.562834224599, std:0.098688282165
Best L1 recall_macro mean:0.734573412698, max:0.888888888889, min:0.630952380952, std:0.07706247

                Random Forest:
Best with grid search:
        estimator:  RandomForestClassifier(bootstrap=False, class_weight=None, criterion='gini',
```

```
            max_depth=2, 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=42, n_jobs=1,
            oob_score=False, random_state=0, verbose=0, warm_start=False)
        score:  0.950300532801
        parameters:  {'max_features': 'auto', 'n_estimators': 42, 'bootstrap': False, 'max_depth
        features importamce:
           feature name  importance
4            Cl   19.027399
5             K   16.991116
8            Mn   12.770117
6            Ca   12.321435
3             S   11.292295
9            Fe    9.280553
0        base_s    7.815014
2             P    7.778332
10           Sr    2.364107
7            Ti    0.359633
1            Si    0.000000
11       Mo_Coh    0.000000
12           Mo    0.000000
        Detailed classification report:
                     precision    recall  f1-score   support

          0       1.00      0.67      0.80         6
          1       1.00      1.00      1.00         6
          2       0.71      1.00      0.83         5
          3       1.00      1.00      1.00         5

avg / total       0.94      0.91      0.91        22

Best RF accuracy mean:0.890909090909, max:0.969696969697, min:0.787878787879, std:0.043281384415
Best RF precision_macro mean:0.897053571429, max:0.96875, min:0.790674603175, std:0.043341755288
Best RF f1_macro mean:0.886767533937, max:0.96862745098, min:0.78125, std:0.0445423958824
Best RF recall_macro mean:0.890873015873, max:0.972222222222, min:0.782738095238, std:0.04544311


         Start new data classification data_prep_r

Counter({1: 30, 0: 29, 3: 26, 2: 24})
Counter({1: 24, 0: 23, 3: 21, 2: 19})
Counter({0: 6, 1: 6, 2: 5, 3: 5})
                Linesr classif:
Best with grid search:
        estimator:  SGDClassifier(alpha=0.0001, average=False, class_weight=None, epsilon=0.1,
       eta0=0.0, fit_intercept=True, l1_ratio=0.15,
       learning_rate='optimal', loss='log', max_iter=8000, n_iter=None,
```

```
       n_jobs=1, penalty='none', power_t=0.5, random_state=0, shuffle=True,
       tol=None, verbose=0, warm_start=False)
        score:  0.95336996337
        parameters:  {'loss': 'log', 'max_iter': 8000, 'fit_intercept': True}
        features importamce:
           feature name  importance
4            Cl   24.193219
2             P   17.898992
5             K   13.975855
0        base_s    9.818958
3             S    7.837842
6            Ca    7.697182
9            Fe    6.522698
10           Sr    2.964303
8            Mn    2.616000
1            Si    2.390478
12           Mo    1.980904
7            Ti    1.493302
11       Mo_Coh    0.610266
        Detailed classification report:
                     precision    recall  f1-score   support

          0       1.00      1.00      1.00         6
          1       1.00      1.00      1.00         6
          2       1.00      0.80      0.89         5
          3       0.83      1.00      0.91         5

avg / total       0.96      0.95      0.95        22

Best SGDLin accuracy mean:0.930303030303, max:1.0, min:0.787878787879, std:0.0650633653139
Best SGDLin precision_macro mean:0.935109126984, max:1.0, min:0.805555555556, std:0.059994164289
Best SGDLin f1_macro mean:0.928986131902, max:1.0, min:0.794494720965, std:0.0632562679772
Best SGDLin recall_macro mean:0.927529761905, max:1.0, min:0.787202380952, std:0.0656220004953

                Ridge Classifire:
Best with grid search:
        estimator:  SGDClassifier(alpha=0.0001, average=False, class_weight=None, epsilon=0.1,
       eta0=0.0, fit_intercept=True, l1_ratio=0.15,
       learning_rate='optimal', loss='hinge', max_iter=4500, n_iter=None,
       n_jobs=1, penalty='l2', power_t=0.5, random_state=0, shuffle=True,
       tol=None, verbose=0, warm_start=False)
        score:  0.970787545788
        parameters:  {'alpha': 0.0001, 'loss': 'hinge', 'max_iter': 4500, 'fit_intercept': True}
        features importamce:
           feature name  importance
4            Cl   30.799125
2             P   15.640904
5             K   14.732524
```

```
3             S   11.442922
0        base_s    9.579114
6            Ca    6.110882
9            Fe    4.892876
10           Sr    2.471119
7            Ti    1.361369
12           Mo    1.335452
8            Mn    0.718889
1            Si    0.623147
11       Mo_Coh    0.291678
        Detailed classification report:
                     precision    recall  f1-score   support

          0       1.00      1.00      1.00         6
          1       1.00      1.00      1.00         6
          2       1.00      0.80      0.89         5
          3       0.83      1.00      0.91         5

avg / total       0.96      0.95      0.95        22

Best Ridge accuracy mean:0.957575757576, max:1.0, min:0.848484848485, std:0.04535342287
Best Ridge precision_macro mean:0.96152507215, max:1.0, min:0.86038961039, std:0.0419399296346
Best Ridge f1_macro mean:0.956514861343, max:1.0, min:0.847435897436, std:0.0456097543457
Best Ridge recall_macro mean:0.954712301587, max:1.0, min:0.842757936508, std:0.0470953605148

                Lasso Classifire:
Best with grid search:
        estimator:  SGDClassifier(alpha=0.0001, average=False, class_weight=None, epsilon=0.1,
       eta0=0.0, fit_intercept=True, l1_ratio=0.15,
       learning_rate='optimal', loss='log', max_iter=4500, n_iter=None,
       n_jobs=1, penalty='l1', power_t=0.5, random_state=0, shuffle=True,
       tol=None, verbose=0, warm_start=False)
        score:  0.95336996337
        parameters:  {'alpha': 0.0001, 'loss': 'log', 'max_iter': 4500, 'fit_intercept': True}
        features importamce:
           feature name  importance
4            Cl   27.022628
2             P   19.875226
5             K   14.946657
0        base_s    9.369100
3             S    7.628318
6            Ca    7.172481
9            Fe    5.733864
10           Sr    2.791364
8            Mn    1.619879
1            Si    1.527793
12           Mo    1.045450
7            Ti    0.866189
```

```
11       Mo_Coh    0.401050
        Detailed classification report:
                     precision    recall  f1-score   support

          0       1.00      1.00      1.00         6
          1       1.00      1.00      1.00         6
          2       1.00      0.80      0.89         5
          3       0.83      1.00      0.91         5

avg / total       0.96      0.95      0.95        22

Best L1 accuracy mean:0.930303030303, max:1.0, min:0.787878787879, std:0.0636363636364
Best L1 precision_macro mean:0.934722222222, max:1.0, min:0.805555555556, std:0.0595855995425
Best L1 f1_macro mean:0.928212693309, max:1.0, min:0.794494720965, std:0.0627845193021
Best L1 recall_macro mean:0.926736111111, max:1.0, min:0.787202380952, std:0.0649441959432

                Random Forest:
Best with grid search:
        estimator:  RandomForestClassifier(bootstrap=False, class_weight='balanced',
            criterion='gini', max_depth=None, 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=42, n_jobs=1, oob_score=False, random_state=0,
            verbose=0, warm_start=False)
        score:  0.95211996337
        parameters:  {'max_features': 'auto', 'n_estimators': 42, 'bootstrap': False, 'max_depth
        features importamce:
           feature name  importance
4            Cl   23.566913
5             K   14.752712
6            Ca   11.759159
2             P   10.341194
3             S    9.156011
0        base_s    8.704540
8            Mn    7.871371
9            Fe    6.780839
10           Sr    3.234122
7            Ti    1.361330
12           Mo    1.224135
1            Si    0.688572
11       Mo_Coh    0.559100
        Detailed classification report:
                     precision    recall  f1-score   support

          0       1.00      1.00      1.00         6
          1       1.00      1.00      1.00         6
          2       1.00      0.80      0.89         5
```

```
          3       0.83      1.00      0.91         5

avg / total       0.96      0.95      0.95        22

Best RF accuracy mean:0.933333333333, max:1.0, min:0.818181818182, std:0.0465523984719
Best RF precision_macro mean:0.937261904762, max:1.0, min:0.819444444444, std:0.0465252647644
Best RF f1_macro mean:0.930867532236, max:1.0, min:0.813222724987, std:0.048209202012
Best RF recall_macro mean:0.931696428571, max:1.0, min:0.810515873016, std:0.0485437711825


         Start new data classification data_prep_z

Counter({1: 30, 0: 29, 3: 26, 2: 24})
Counter({1: 24, 0: 23, 3: 21, 2: 19})
Counter({0: 6, 1: 6, 2: 5, 3: 5})
                Linesr classif:
Best with grid search:
        estimator:  SGDClassifier(alpha=0.0001, average=False, class_weight=None, epsilon=0.1,
       eta0=0.0, fit_intercept=False, l1_ratio=0.15,
       learning_rate='optimal', loss='squared_loss', max_iter=8000,
       n_iter=None, n_jobs=1, penalty='none', power_t=0.5, random_state=0,
       shuffle=True, tol=None, verbose=0, warm_start=False)
        score:  0.941540824372
        parameters:  {'loss': 'squared_loss', 'max_iter': 8000, 'fit_intercept': False}
        features importamce:
           feature name  importance
3             S   24.579816
5             K   18.726601
4            Cl   18.470774
6            Ca   12.462850
2             P    8.865348
9            Fe    5.778613
0        base_s    4.378655
8            Mn    2.349314
10           Sr    1.642147
1            Si    1.633784
7            Ti    0.621826
12           Mo    0.271309
11       Mo_Coh    0.218964
        Detailed classification report:
                     precision    recall  f1-score   support

          0       0.86      1.00      0.92         6
          1       1.00      1.00      1.00         6
          2       1.00      1.00      1.00         5
          3       1.00      0.80      0.89         5

avg / total       0.96      0.95      0.95        22
```

```
Best SGDLin accuracy mean:0.890909090909, max:1.0, min:0.363636363636, std:0.178864903798
Best SGDLin precision_macro mean:0.924605533356, max:1.0, min:0.632211538462, std:0.101892500714
Best SGDLin f1_macro mean:0.892065701971, max:1.0, min:0.372474747475, std:0.176170682972
Best SGDLin recall_macro mean:0.890079365079, max:1.0, min:0.37003968254, std:0.176496041605

                Ridge Classifire:
Best with grid search:
        estimator:  SGDClassifier(alpha=0.0001, average=False, class_weight=None, epsilon=0.1,
       eta0=0.0, fit_intercept=False, l1_ratio=0.15,
       learning_rate='optimal', loss='squared_loss', max_iter=8000,
       n_iter=None, n_jobs=1, penalty='l2', power_t=0.5, random_state=0,
       shuffle=True, tol=None, verbose=0, warm_start=False)
        score:  0.941540824372
        parameters:  {'alpha': 0.0001, 'loss': 'squared_loss', 'max_iter': 8000, 'fit_intercept'
        features importamce:
           feature name  importance
3            S   24.318503
5            K   18.580339
4           Cl   18.405020
6           Ca   12.362111
2            P    9.218107
9           Fe    5.841083
0       base_s    4.410929
8           Mn    2.405032
10          Sr    1.709629
1           Si    1.665610
7           Ti    0.641261
12          Mo    0.252027
11      Mo_Coh    0.190350
        Detailed classification report:
                     precision    recall  f1-score   support

          0       0.86      1.00      0.92         6
          1       1.00      1.00      1.00         6
          2       1.00      1.00      1.00         5
          3       1.00      0.80      0.89         5

avg / total       0.96      0.95      0.95        22

Best Ridge accuracy mean:0.945454545455, max:1.0, min:0.848484848485, std:0.0402015126104
Best Ridge precision_macro mean:0.953023989899, max:1.0, min:0.8625, std:0.0373364633136
Best Ridge f1_macro mean:0.945767957318, max:1.0, min:0.852479757085, std:0.0388289406955
Best Ridge recall_macro mean:0.943601190476, max:1.0, min:0.84623015873, std:0.0399137917093

                Lasso Classifire:
Best with grid search:
        estimator:  SGDClassifier(alpha=0.0001, average=False, class_weight=None, epsilon=0.1,
```

```
       eta0=0.0, fit_intercept=False, l1_ratio=0.15,
       learning_rate='optimal', loss='squared_loss', max_iter=8000,
       n_iter=None, n_jobs=1, penalty='l1', power_t=0.5, random_state=0,
       shuffle=True, tol=None, verbose=0, warm_start=False)
        score:  0.941540824372
        parameters:  {'alpha': 0.0001, 'loss': 'squared_loss', 'max_iter': 8000, 'fit_intercept'
        features importamce:
           feature name  importance
3             S   24.596737
5             K   18.645693
4            Cl   18.485669
6            Ca   12.421566
2             P    9.017770
9            Fe    5.832272
0        base_s    4.371286
8            Mn    2.386926
1            Si    1.675599
10           Sr    1.666248
7            Ti    0.588801
12           Mo    0.199693
11       Mo_Coh    0.111738
        Detailed classification report:
                    precision    recall  f1-score   support

          0       0.86      1.00      0.92         6
          1       1.00      1.00      1.00         6
          2       1.00      1.00      1.00         5
          3       1.00      0.80      0.89         5

avg / total       0.96      0.95      0.95        22

Best L1 accuracy mean:0.921212121212, max:1.0, min:0.69696969697, std:0.0848484848485
Best L1 precision_macro mean:0.936527777778, max:1.0, min:0.797222222222, std:0.0598506371347
Best L1 f1_macro mean:0.920741887878, max:1.0, min:0.691062801932, std:0.0859173742316
Best L1 recall_macro mean:0.918998015873, max:1.0, min:0.687003968254, std:0.0869531200393

                Random Forest:
Best with grid search:
        estimator:  RandomForestClassifier(bootstrap=True, class_weight='balanced',
            criterion='gini', max_depth=None, 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=62, n_jobs=1, oob_score=False, random_state=0,
            verbose=0, warm_start=False)
        score:  0.943838734795
        parameters:  {'max_features': 'auto', 'n_estimators': 62, 'bootstrap': True, 'max_depth'
        features importamce:
```

```
            feature name  importance
4             Cl   19.941646
5              K   12.788595
6             Ca   12.696793
8             Mn    9.940975
2              P    9.382735
0         base_s    8.888559
3              S    8.119889
9             Fe    5.999332
1             Si    4.078361
7             Ti    3.086870
10            Sr    2.953553
12            Mo    1.300135
11        Mo_Coh    0.822559
        Detailed classification report:
                    precision    recall  f1-score   support

          0       1.00      1.00      1.00         6
          1       1.00      1.00      1.00         6
          2       1.00      1.00      1.00         5
          3       1.00      1.00      1.00         5

avg / total       1.00      1.00      1.00        22

Best RF accuracy mean:0.906060606061, max:1.0, min:0.787878787879, std:0.0566107324008
Best RF precision_macro mean:0.908043831169, max:1.0, min:0.782738095238, std:0.059356867135
Best RF f1_macro mean:0.901421613517, max:1.0, min:0.781512605042, std:0.0593924198908
Best RF recall_macro mean:0.903521825397, max:1.0, min:0.782738095238, std:0.0598294278852
```

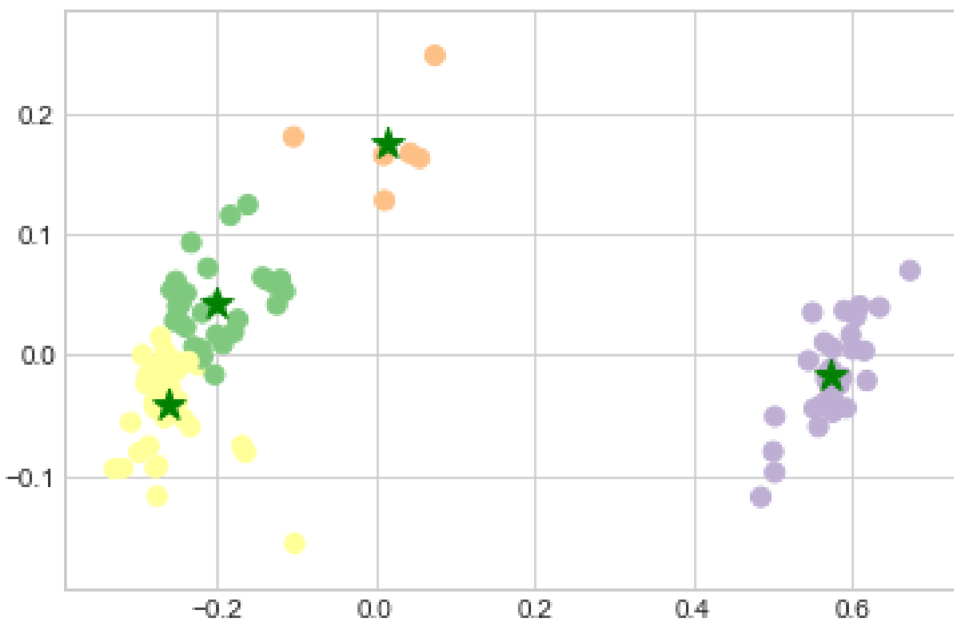
```
In [52]: # PCA
         names = ['data_norm_r', 'data_norm_z']
         datas = [data_prep_r, data_prep_z]
         for ind in xrange(len(datas)):
             print 'Process data: ', names[ind]
             X_raw = datas[ind]
             labels = spe_df_npks_prep.fraction

             print 'Labels counter: ', Counter(labels)
             x_data = X_raw.loc[:, X_raw.columns!='fraction']
             print 'Index len: ', len(x_data.index)
             feature_names = Counter(labels).keys()

             transformer = RandomizedPCA(n_components=2)
             X_2d = transformer.fit_transform(x_data)
             X_2d_norm = (X_2d - X_2d.mean()) / (X_2d.max() - X_2d.min())
             if ind == 1:
```

```
    X_2d_norm = (X_2d - X_2d.mean()) / X_2d.std()
print 'After len: ', X_2d_norm.shape
# over 99.9% variance captured by 2d data
print transformer.explained_variance_ratio_

# do clustering
print 'n_cluster = ', len(Counter(labels))
estimator = KMeans(n_clusters=len(Counter(labels)), init='k-means++', n_init=10)
estimator.fit(X_2d_norm)

labels_t = estimator.labels_
print 'estimator labels: ', Counter(labels_t)

label_color = [colors[l] for l in labels_t]

title_font = {'fontname':'Arial', 'size':'16', 'color':'black', 'weight':'normal',
          'verticalalignment':'bottom'} # Bottom vertical alignment for more space

fig, ax = plt.subplots()
ax.scatter(X_2d_norm[:,0], X_2d_norm[:,1], c=label_color, s=50)
ax.scatter(estimator.cluster_centers_[:,0], estimator.cluster_centers_[:,1], marker

# Calculate all mean for labels
shifr2 = {
    '100': u'pressed powder 100 mkm',
    '500': 'pressed powder 500 mkm',
    'rawgrain': 'granules',
    'grain': 'pressed granules'
}

all_means = []
for f in feature_names:
    x_m = X_2d_norm[labels==f,0].mean()
    y_m = X_2d_norm[labels==f,1].mean()
    all_means.append([round(x_m,3), round(y_m, 3), shifr2[f]])

print all_means

for k in Counter(labels_t).keys():
    x = X_2d_norm[:,0]
    y = X_2d_norm[:,1]
    text_now = ''

    plt.text(
        x[labels_t==k].mean(),
        y[labels_t==k].mean(),
        text_now,
        horizontalalignment='center',
```

```
                bbox=dict(alpha=.5, edgecolor='w', facecolor='w'),
            **title_font
            )

        plt.draw()
        plt.savefig(names[ind] + '_RandomizePCA_article3_2.png', dpi=300)
        plt.show()
```

```
Process data:  data_norm_r
Labels counter:  Counter({'rawgrain': 30, '100': 29, '500': 26, 'grain': 24})
Index len:  109
After len:  (109, 2)
[0.90861113 0.02974156]
n_cluster =  4
estimator labels:  Counter({3: 44, 1: 30, 0: 29, 2: 6})
[[-0.249, -0.029, u'pressed powder 100 mkm'], [0.573, -0.016, 'granules'], [-0.147, 0.057, 'pres
```

```
/usr/local/lib/python2.7/dist-packages/sklearn/utils/deprecation.py:58: DeprecationWarning: Clas
  warnings.warn(msg, category=DeprecationWarning)
```




```
Process data:  data_norm_z
Labels counter:  Counter({'rawgrain': 30, '100': 29, '500': 26, 'grain': 24})
Index len:  109
After len:  (109, 2)
[0.86329941 0.05999724]
```

```
n_cluster =  4
estimator labels:  Counter({3: 40, 1: 33, 0: 30, 2: 6})
[[-0.963, -0.113, u'pressed powder 100 mkm'], [2.147, -0.116, 'granules'], [-0.505, 0.278, 'pres
```

```
/usr/local/lib/python2.7/dist-packages/sklearn/utils/deprecation.py:58: DeprecationWarning: Clas
  warnings.warn(msg, category=DeprecationWarning)
```