Feature Selection (on Tileset7) - July 2017

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Using random forest (extra forest), existing features can be ranked in order of contribution

(This notebook follows the feature selection notebook from Pierluggi)

Note that this is a different approach then PCA (see notebook 'realxtals1-dimensionality1'). In PCA, the data is transformed onto the 'natural axis' of the data (its eigen vectors) and the top N of these are used, while in feature selection the existing features are being assessed based on their contribution to a classifier.

See e.g.:

- https://www.quora.com/What-is-the-difference-between-principal-component-analysis-PCA-and-feature-selection-in-machine-learning-Is-PCA-a-means-of-feature-selection (https://www.quora.com/What-is-the-difference-between-principal-component-analysis-PCA-and-feature-selection-in-machine-learning-Is-PCA-a-means-of-feature-selection)
- https://stats.stackexchange.com/questions/182711/principal-component-analysis-vs-feature-selection (https://stats.stackexchange.com/questions/182711/principal-component-analysis-vs-feature-selection)

1. Imports

In [84]:
```
# this will remove warnings messages
import warnings
warnings.filterwarnings('ignore')

import numpy as np
import pandas as pd

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

%matplotlib inline

# import
from sklearn.ensemble import ExtraTreesClassifier
from sklearn.preprocessing import LabelEncoder

import imgutils
```

In [85]:
```
# Re-run this cell if you altered imgutils
import importlib
importlib.reload(imgutils)
```

Out[85]:
```
<module 'imgutils' from 'C:\\JADS\\SW\\Grad Proj\\realxtals1\\sources\\imgutils.py'>
```

2. Import Crystal Image Data & Statistics

The data was labeled and exported to csv in the notebook realxtals1_dataeng1.ipynb

About the data:

The CSV contains the image files, slice information (sub-images) and associated statistics, which are the features for which a classifier needs to be found.

The goal is to find the clustering in feature-space and use those to categorize the images. For this particular dataset, a single statistics could be used to label into three classes:

A = subimage contains no crystal,
B = part of subimage contains crystal,
C = (most of) subimage contains crystal

But the labels have been added here for analyses, eventually the data will be unlabelled.

Import data:

In [86]:
```
df = pd.read_csv('../data/Crystals_Apr_12/Tileset7-2.csv', sep=';')
df.head()
```

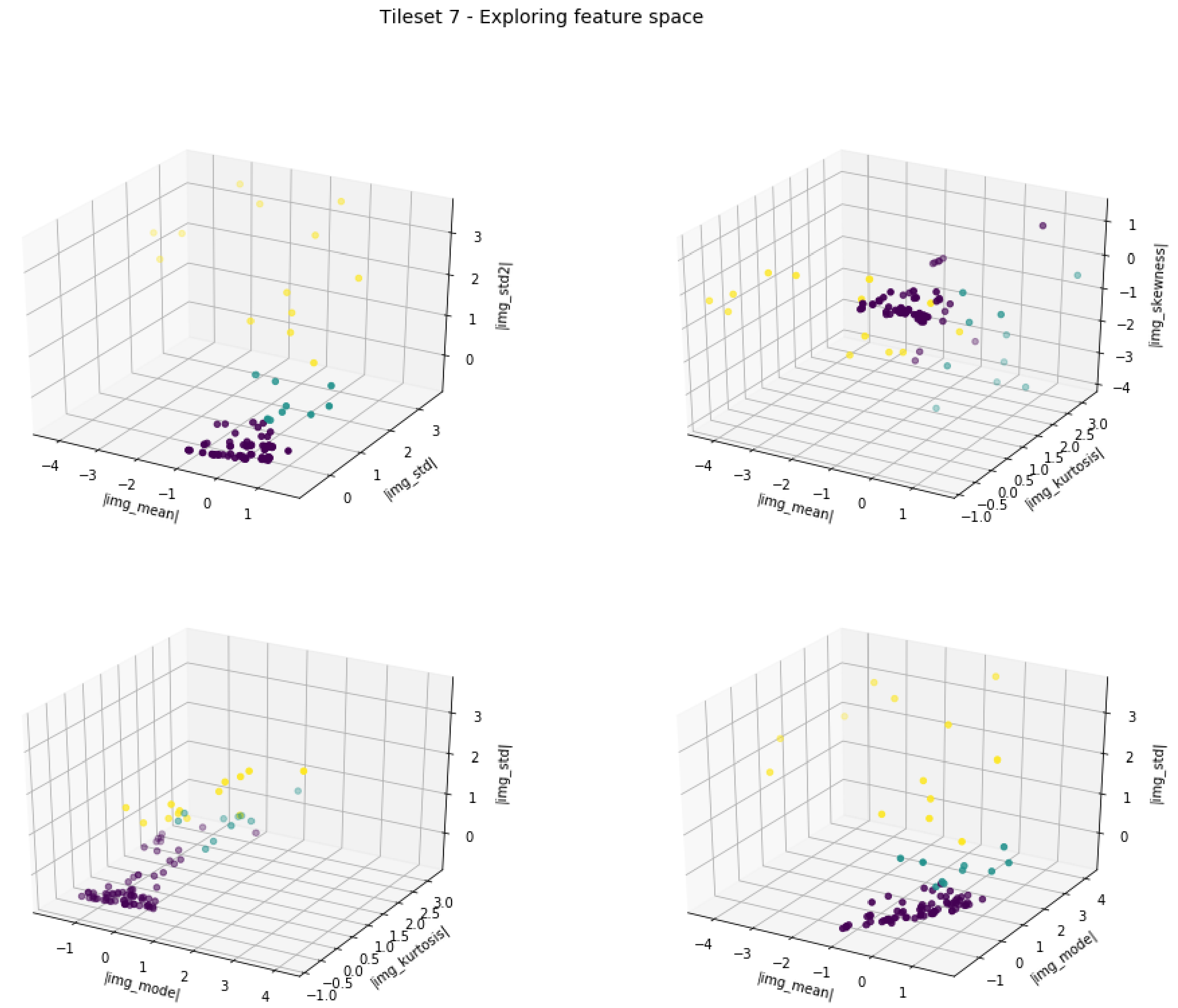
Out[86]:

	Unnamed: 0	filename	s_y	s_x	n_y	n_x	alias	img_mean	img_std	img_kurtosis	img_skewnes
0	0	..\data\Crystals_Apr_12\Tileset7\Tile_001-001-...	0	0	4	4	img0_0-0	8955.557637	489.754848	4.163737	0.107415
1	1	..\data\Crystals_Apr_12\Tileset7\Tile_001-001-...	0	1	4	4	img0_0-1	8883.137305	501.739963	6.528225	-0.146746
2	2	..\data\Crystals_Apr_12\Tileset7\Tile_001-001-...	0	2	4	4	img0_0-2	8786.996070	327.512136	1.323241	-0.110828
3	3	..\data\Crystals_Apr_12\Tileset7\Tile_001-001-...	0	3	4	4	img0_0-3	8679.430512	273.673569	0.112149	0.008591
4	4	..\data\Crystals_Apr_12\Tileset7\Tile_001-001-...	1	0	4	4	img0_1-0	8982.867158	380.410977	0.168520	0.033678

3. Quick visual inspection of the 'feature space'

In [87]:

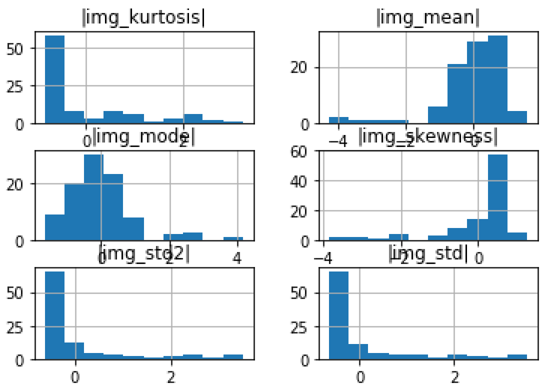
```
# plot it in 3 dimensions, choosing some stat combinations
fig0 = plt.figure(figsize=(16, 12))
plt.suptitle("Tileset 7 - Exploring feature space",fontsize=14)

# trick to convert category labels into color codes
color = pd.DataFrame(df['class'].astype('category'))['class'].cat.codes

def scatter_3d(ax, df, feat1, feat2, feat3, colors):
    ax.scatter(df[feat1], df[feat2], df[feat3], c=colors)
    ax.set_xlabel(feat1)
    ax.set_ylabel(feat2)
    ax.set_zlabel(feat3)


ax = fig0.add_subplot(221, projection='3d')
scatter_3d(ax, df, '|img_mean|', '|img_std|', '|img_std2|', color)

ax = fig0.add_subplot(222, projection='3d')
scatter_3d(ax, df, '|img_mean|', '|img_kurtosis|', '|img_skewness|', color)

ax = fig0.add_subplot(223, projection='3d')
scatter_3d(ax, df, '|img_mode|', '|img_kurtosis|', '|img_std|', color)

ax = fig0.add_subplot(224, projection='3d')
scatter_3d(ax, df, '|img_mean|', '|img_mode|', '|img_std|', color)

plt.show()
```



From visual inspection of these graphs, I would expect the std, std2 and kurtosis to be the most important features (they seem like the most seperating ones, though the mean has quite a big variance). Also look at the histograms (to get idea of the variance):

In [88]:
```
df.hist(['|img_mean|','|img_std|', '|img_std2|', '|img_kurtosis|', '|img_skewness|','|img_mode|'])
```

Out[88]:
```
array([[<matplotlib.axes._subplots.AxesSubplot object at 0x000000000E01BCF8>,
        <matplotlib.axes._subplots.AxesSubplot object at 0x000000000DC2E160>],
       [<matplotlib.axes._subplots.AxesSubplot object at 0x000000000E0CF400>,
        <matplotlib.axes._subplots.AxesSubplot object at 0x000000000C8EF1D0>],
       [<matplotlib.axes._subplots.AxesSubplot object at 0x000000000E272B70>,
        <matplotlib.axes._subplots.AxesSubplot object at 0x000000000E272860>]],
      dtype=object)
```



4. Assess feature imporance (using extra trees classifier)

(sort of random forest, an ensemble method that will create classifiers based on random subsets)

First vectorize the data:

In [89]:
```
# convert labels into values
le = LabelEncoder()
df["|class|"] = le.fit_transform(df["class"])
```

In [90]:
```
# convert into X Y vectors:
feature_cols = ['|img_std|', '|img_mean|','|img_skewness|', '|img_mode|', '|img_kurtosis|', '|img_std2|']
X = df.loc[:,feature_cols]
y = df.loc[:,'|class|']
```

Then generate the classifier 'extra tries' and extract the importances

(a la Pierluggi)

In [91]:
```
# Build a forest and compute the feature importances
forest = ExtraTreesClassifier(n_estimators=500,random_state=0)
forest.fit(X, y)
```

Out[91]:
```
ExtraTreesClassifier(bootstrap=False, class_weight=None, 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=500, n_jobs=1,
           oob_score=False, random_state=0, verbose=0, warm_start=False)
```

In [92]:
```
# Extracting feature importance:
importances = forest.feature_importances_
std = np.std([tree.feature_importances_ for tree in forest.estimators_],
             axis=0)
indices = np.argsort(importances)[::-1]

# Print the feature ranking
print("Feature ranking:")

for f in range(X.shape[1]):
    print("%d. feature %d '%s' (%f)" % (f + 1, indices[f], feature_cols[indices[f]], importances[indices[f]]))
```

```
Feature ranking:
1. feature 5 '|img_std2|' (0.331023)
2. feature 0 '|img_std|' (0.310544)
3. feature 2 '|img_skewness|' (0.111690)
4. feature 3 '|img_mode|' (0.100443)
5. feature 4 '|img_kurtosis|' (0.082564)
6. feature 1 '|img_mean|' (0.063736)
```

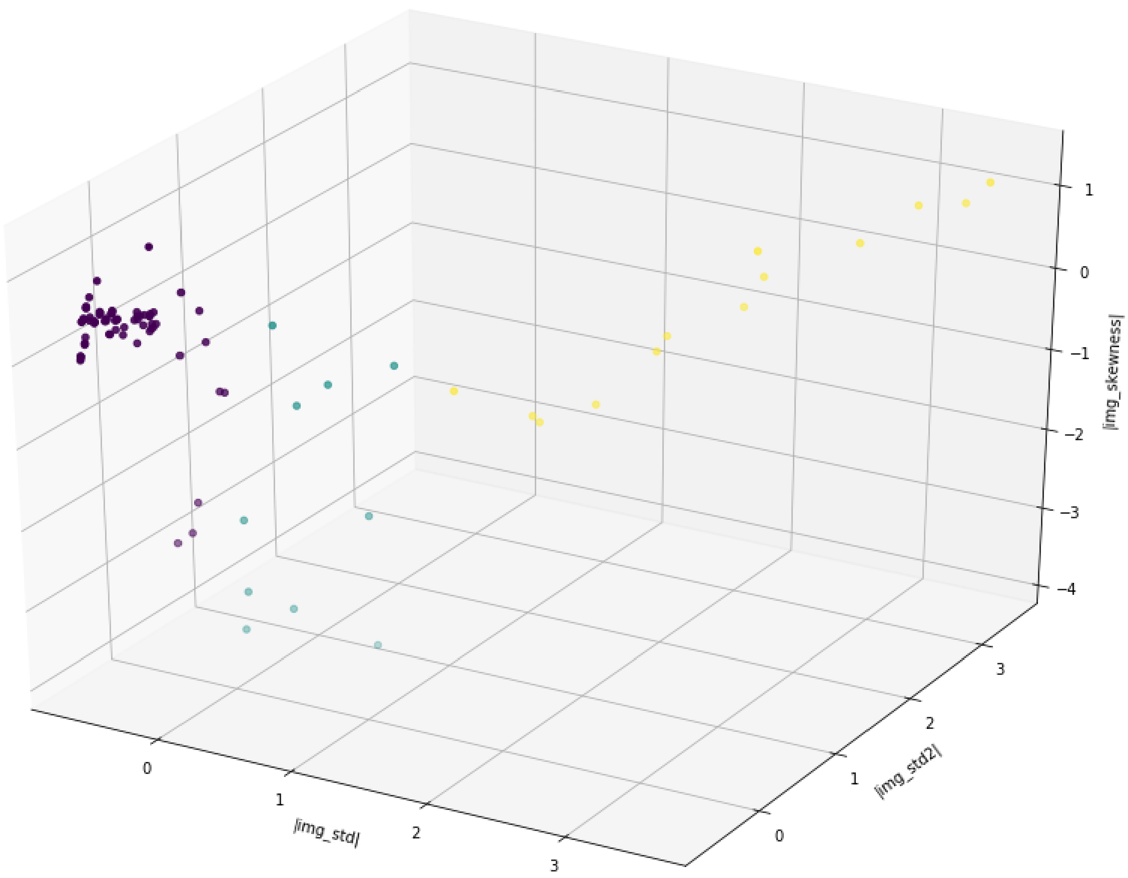
Hmmm, I am surprised that skewness scores higher than kurtosis.

Visually inspect the important features

Let's make some plots based on the first 3 most important ones

In [93]:
```
fig0 = plt.figure(figsize=(16, 12))
plt.suptitle("Tileset 7 - The 3 Most Important Features",fontsize=14)
ax = fig0.add_subplot(111, projection='3d')
scatter_3d(ax, df, '|img_std|', '|img_std2|', '|img_skewness|', color)
```

Tileset 7 - The 3 Most Important Features

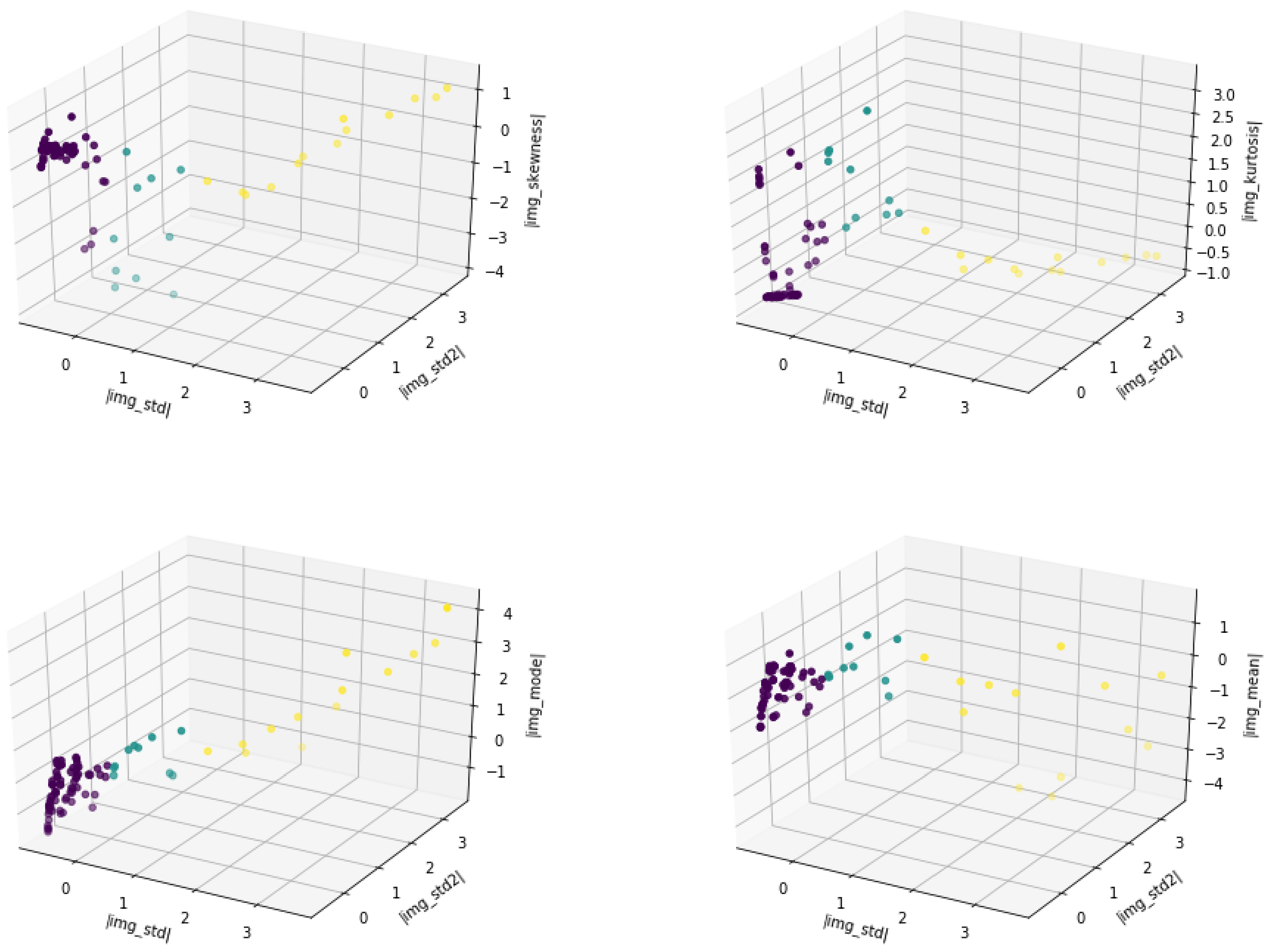


Indeed with these three variables they are clearly separatable.

But I think with the kurtosis or some of the others it would also work, as long as std and std2 are in there. So let's compare

```
In [94]: fig0 = plt.figure(figsize=(16, 12))
         plt.suptitle("Tileset 7 - Combinations of important features",fontsize=14)
         ax = fig0.add_subplot(221, projection='3d')
         scatter_3d(ax, df, '|img_std|', '|img_std2|', '|img_skewness|', color)
         ax = fig0.add_subplot(222, projection='3d')
         scatter_3d(ax, df, '|img_std|', '|img_std2|', '|img_kurtosis|', color)
         ax = fig0.add_subplot(224, projection='3d')
         scatter_3d(ax, df, '|img_std|', '|img_std2|', '|img_mean|', color)
         ax = fig0.add_subplot(223, projection='3d')
         scatter_3d(ax, df, '|img_std|', '|img_std2|', '|img_mode|', color)
```

Tileset 7 - Combinations of important features



Indeed the std and std are leading, but you need a 3rd dimension for separation. Looking at the importances this is maybe not so surprising, as skewness, kurtosis, mode and mean are rather close.

5. Comparing result with Dimensionality Reduction Techniques

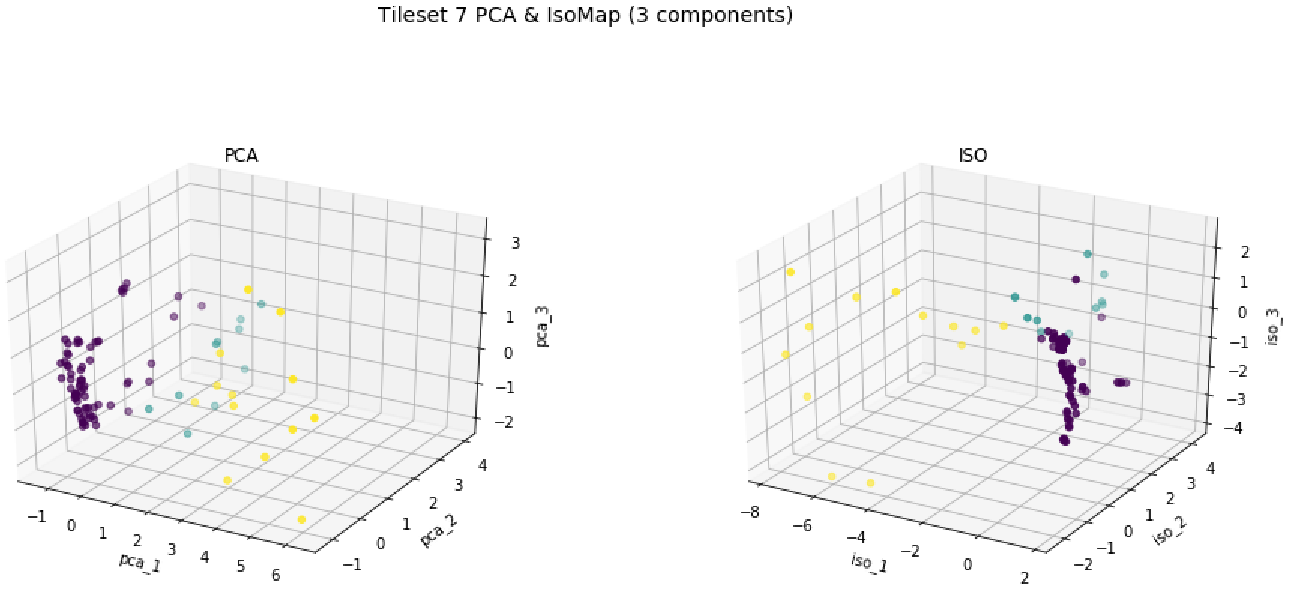
(this has been analyzed in realxtals1-dimensionality1. To keep this notebook self-contained and independend, we do the dimensionality reduction here instead of exporting from the other notebook)

```
In [95]: from sklearn import manifold, decomposition, datasets, random_projection
```

First assess PCA and IsoMap with 3 components

(looked most promising in dimensionality assessment)

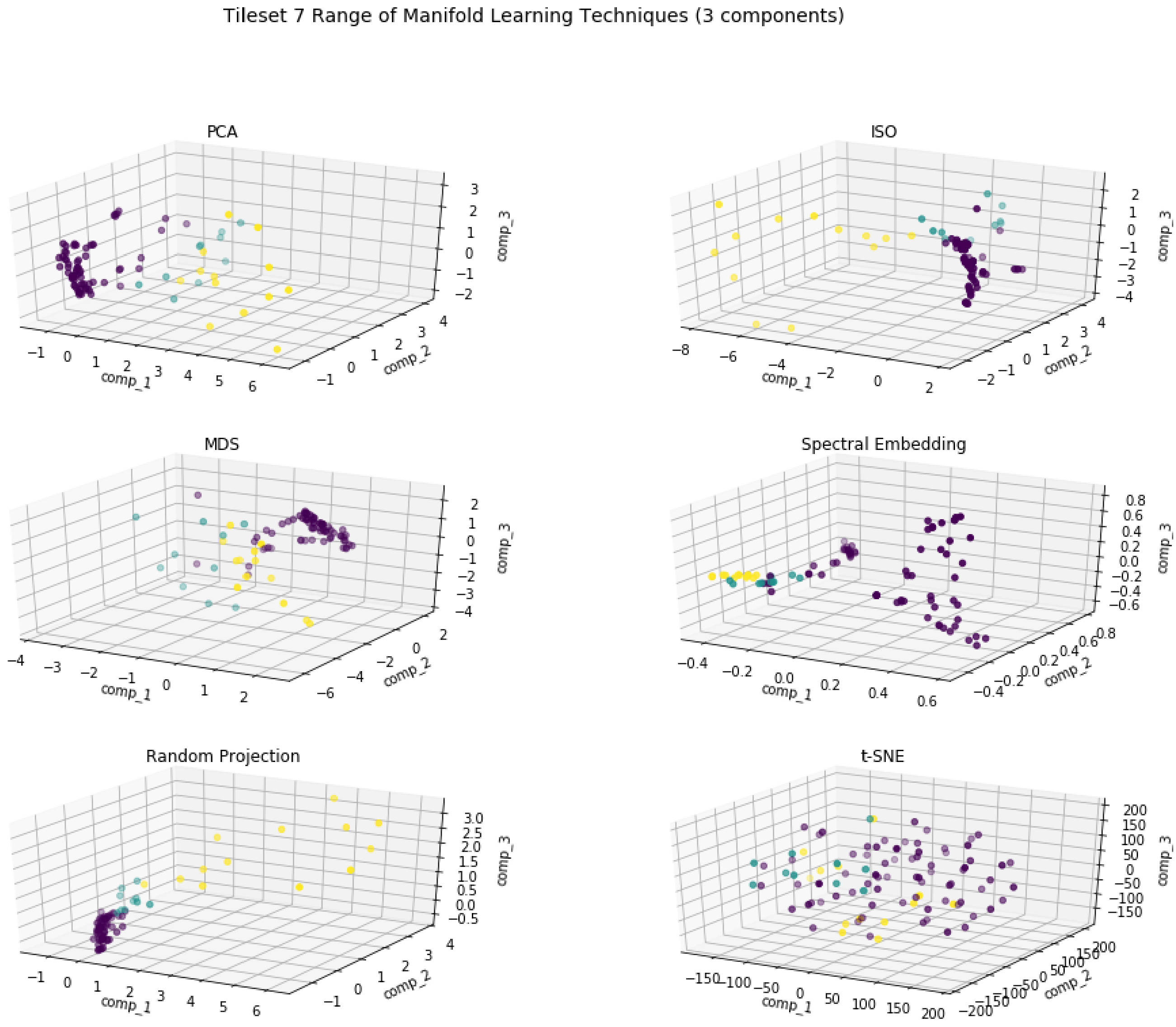
In [96]:
```
# Create graph
fig0 = plt.figure(figsize=(16, 12))
plt.suptitle("Tileset 7 PCA & IsoMap (3 components)",fontsize=14)

# PCA (or SVD, which is almost the same)
title = 'PCA'
fieldnames = ['pca_1','pca_2','pca_3']
pca = decomposition.TruncatedSVD(n_components=3)
X_fit = pca.fit_transform(X)
df_pca = pd.DataFrame(X_fit[:,0:3], columns=fieldnames)
ax = fig0.add_subplot(221, projection='3d', title=title)
scatter_3d(ax, df_pca, fieldnames[0],fieldnames[1],fieldnames[2], color)

# Iso Map
title = 'ISO'
fieldnames = ['iso_1','iso_2','iso_3']
iso = manifold.Isomap(n_neighbors=10, n_components=3)
X_fit = iso.fit_transform(X)
df_pca = pd.DataFrame(X_fit[:,0:3], columns=fieldnames)
ax = fig0.add_subplot(222, projection='3d', title=title)
scatter_3d(ax, df_pca, fieldnames[0],fieldnames[1],fieldnames[2], color)
```



Comparing with range of dimensionality reduction techniques

Let's assess more methods just as in the 'dimensionality notebook', but using three components

In [97]:
```
# Create graph
fig0 = plt.figure(figsize=(16, 12))
plt.suptitle("Tileset 7 Range of Manifold Learning Techniques (3 components)",fontsize=14)

fieldnames = ['comp_1','comp_2','comp_3']

# PCA (or SVD, which is almost the same)
title = 'PCA'
pca = decomposition.TruncatedSVD(n_components=3)
X_fit = pca.fit_transform(X)
df_fit = pd.DataFrame(X_fit[:,0:3], columns=fieldnames)
ax = fig0.add_subplot(321, projection='3d', title=title)
scatter_3d(ax, df_fit, fieldnames[0],fieldnames[1],fieldnames[2], color)

# Iso Map
title = 'ISO'
iso = manifold.Isomap(n_neighbors=10, n_components=3)
X_fit = iso.fit_transform(X)
df_fit = pd.DataFrame(X_fit[:,0:3], columns=fieldnames)
ax = fig0.add_subplot(322, projection='3d', title=title)
scatter_3d(ax, df_fit, fieldnames[0],fieldnames[1],fieldnames[2], color)

# MDS
title = 'MDS'
mds = manifold.MDS(n_components=3, max_iter=100, n_init=1)
X_fit = mds.fit_transform(X)
df_fit = pd.DataFrame(X_fit[:,0:3], columns=fieldnames)
ax = fig0.add_subplot(323, projection='3d', title=title)
scatter_3d(ax, df_fit, fieldnames[0],fieldnames[1],fieldnames[2], color)

# Spectral embedding
title = 'Spectral Embedding'
se = manifold.SpectralEmbedding(n_components=3, n_neighbors=10)
X_fit = se.fit_transform(X)
df_fit = pd.DataFrame(X_fit[:,0:3], columns=fieldnames)
ax = fig0.add_subplot(324, projection='3d', title=title)
scatter_3d(ax, df_fit, fieldnames[0],fieldnames[1],fieldnames[2], color)

# Random Projection
title = 'Random Projection'
rp = random_projection.SparseRandomProjection(n_components=3, random_state=42)
X_fit = rp.fit_transform(X)
df_fit = pd.DataFrame(X_fit[:,0:3], columns=fieldnames)
ax = fig0.add_subplot(325, projection='3d', title=title)
scatter_3d(ax, df_fit, fieldnames[0],fieldnames[1],fieldnames[2], color)

# t-SNE
title = 't-SNE'
tsne = manifold.TSNE(n_components=3, init='pca', random_state=42)
X_fit = tsne.fit_transform(X)
df_fit = pd.DataFrame(X_fit[:,0:3], columns=fieldnames)
ax = fig0.add_subplot(326, projection='3d', title=title)
scatter_3d(ax, df_fit, fieldnames[0],fieldnames[1],fieldnames[2], color)
```



6. More analysis?

7. Conclusions

- From visually inspecting these graphs and comparing those to the 'feature selection method', the 'feature selection' looks more separatable.
- However, the feature selection method requires labeled data in order to train the classifier, while the manifest learning methods does not require labelling

8. Next Steps:

- Try unsupervised learning on this data set (maybe first apply a manifold learning technique to optimize the data?)
- Repeat this notebook on harder dataset

Michael Janus, 17 July 2018