Assessing Dimensionality (on Tileset7) - July 2017

Created: 5 July 2018
Last update: 10 july 2018

Comparing Manifold Learning Methods / Dimensionality Reduction Techniques

This notebook follows the Dimensionality notebook from Pierluggi

1. Imports

In [1]:
```
# this will remove warnings messages
import warnings
warnings.filterwarnings('ignore')

import numpy as np
import pandas as pd

import matplotlib.pyplot as plt
%matplotlib inline

# import
from time import time
from mpl_toolkits.mplot3d import Axes3D
from matplotlib.ticker import NullFormatter
from matplotlib import offsetbox

from sklearn import manifold, datasets, decomposition, random_projection
from sklearn.preprocessing import LabelEncoder

import imgutils
```

In [17]:
```
# Re-run this cell if you altered imgutils
import importlib
importlib.reload(imgutils)
```

Out[17]:
```
<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 [3]:
```
df = pd.read_csv('../data/Crystals_Apr_12/Tileset7-2.csv', sep=';')
df.head()
```

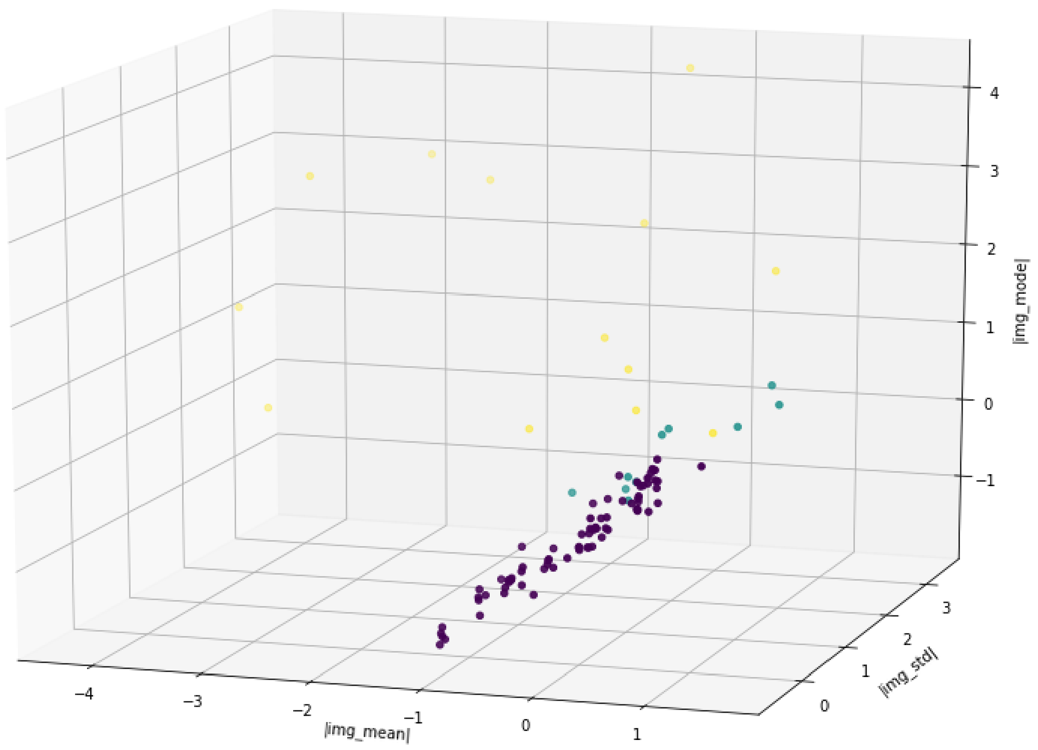
Out[3]:

	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

Quick visual inspection:

In [4]:
```
# trick to convert category labels into color codes
color = pd.DataFrame(df['class'].astype('category'))['class'].cat.codes

# plot it in 3 dimensions, choosing some stats
fig0 = plt.figure(figsize=(16, 12))
plt.suptitle("Tileset 7",fontsize=14)
ax = fig0.add_subplot(111, projection='3d')
ax.scatter(df['|img_mean|'], df['|img_std|'], df['|img_mode|'], c=color)
ax.set_xlabel('|img_mean|')
ax.set_ylabel('|img_std|')
ax.set_zlabel('|img_mode|')
ax.view_init(14, -72)
```

Tileset 7



3. Vectorize the data for sklearn manifold methods

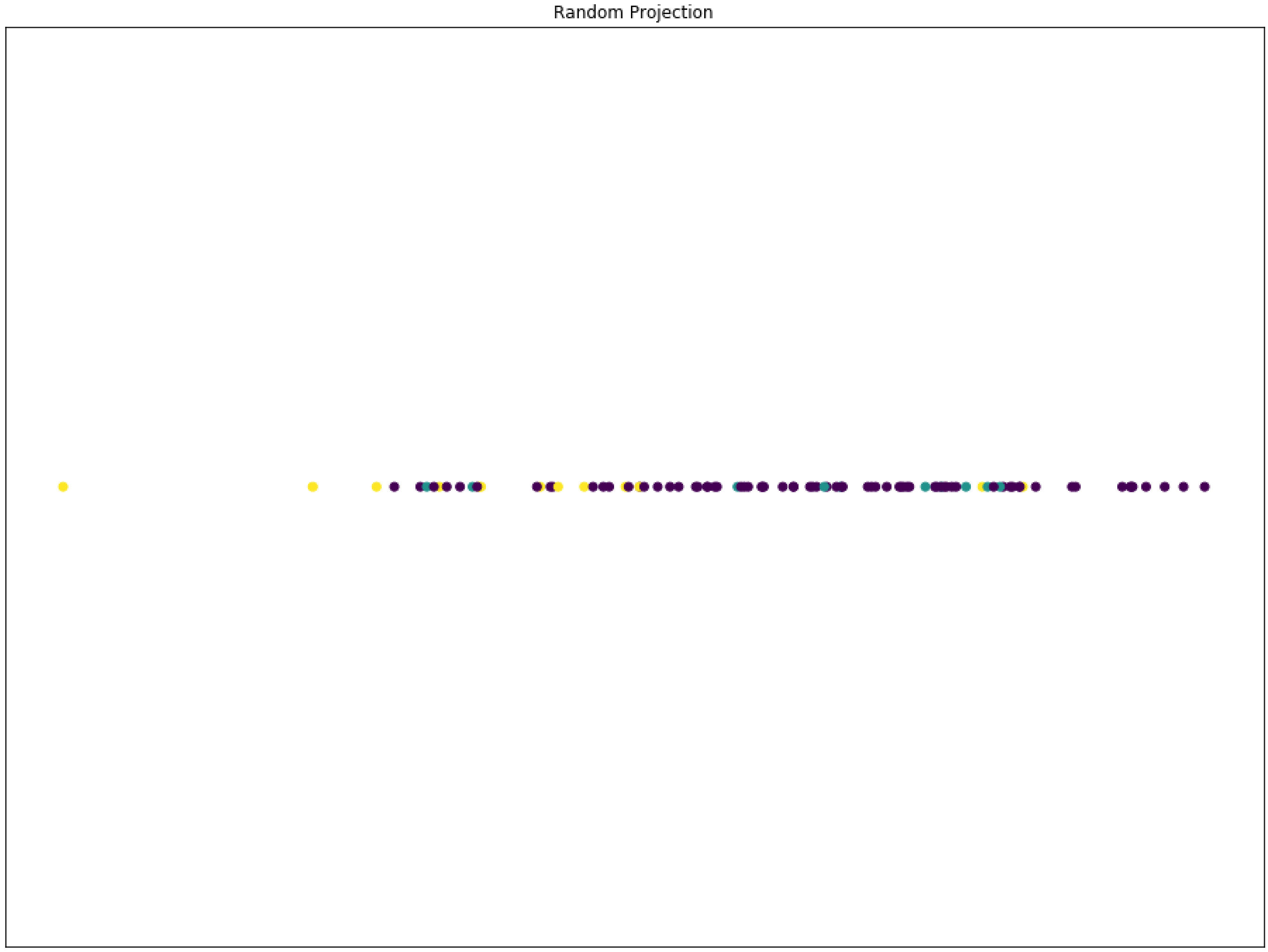
In [5]:
```
# convert labels into values
le = LabelEncoder()
df["|class|"] = le.fit_transform(df["class"])
```

In [6]:
```
# convert into X Y vectors:
feature_cols = ['|img_std|', '|img_mean|','|img_skewness|', '|img_mode|', '|img_kurtosis|']
X = df.loc[:,feature_cols]
Y = df.loc[:,'|class|']
```

4. Try two methods

A. Random Projections

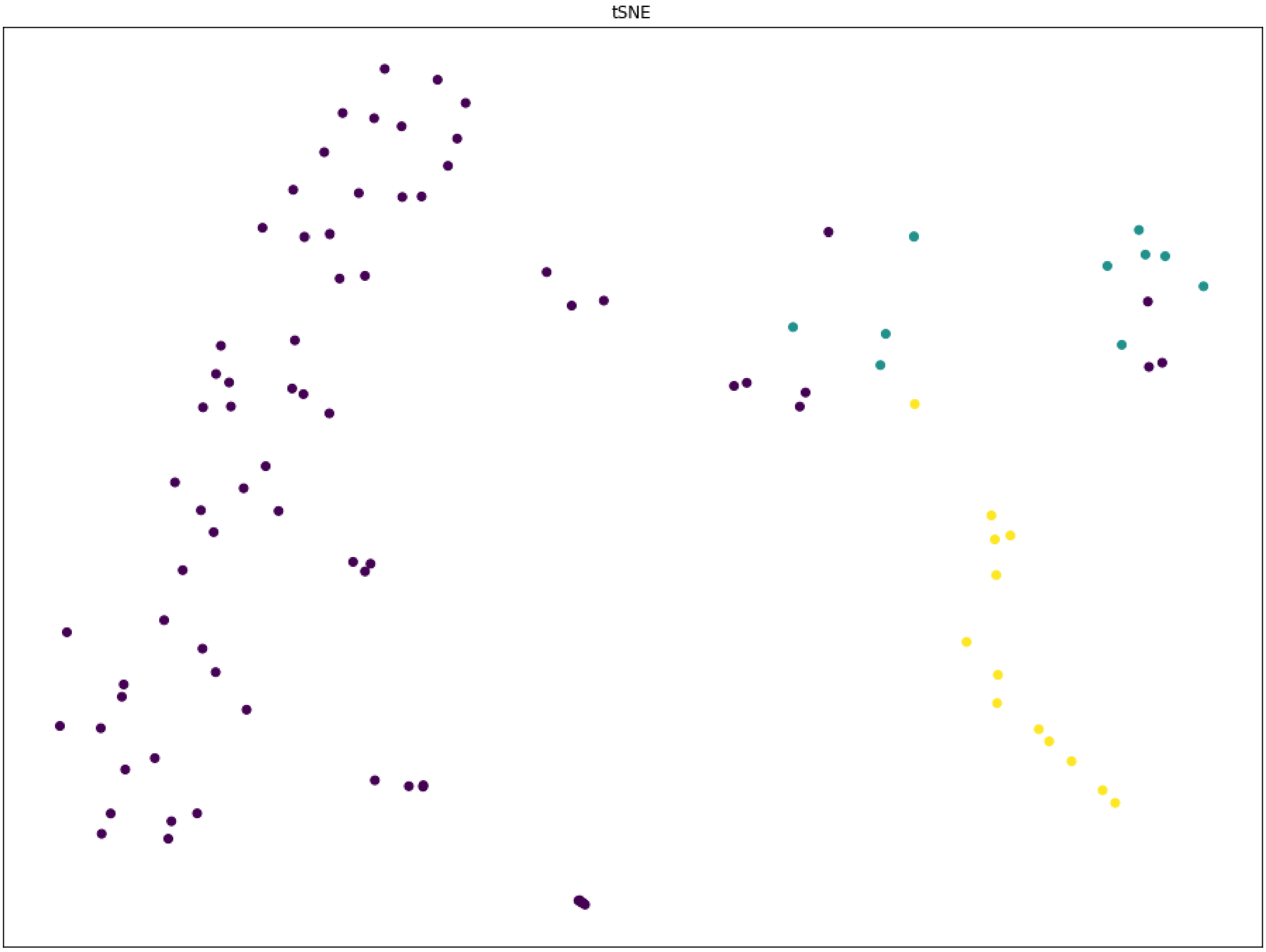
In [7]:
```
rp = random_projection.SparseRandomProjection(n_components=2, random_state=20)

X_rp = rp.fit_transform(X)

fig = plt.figure(figsize=(16, 12))
fig = plt.scatter(X_rp[:, 0], X_rp[:, 1], c=color)
fig = plt.title("Random Projection")
fig = plt.xticks([]), plt.yticks([])
```



does not go too well, plots it all on one line (if you reduce number of variables, it looks better)

B. The Most Advanced: tSNE

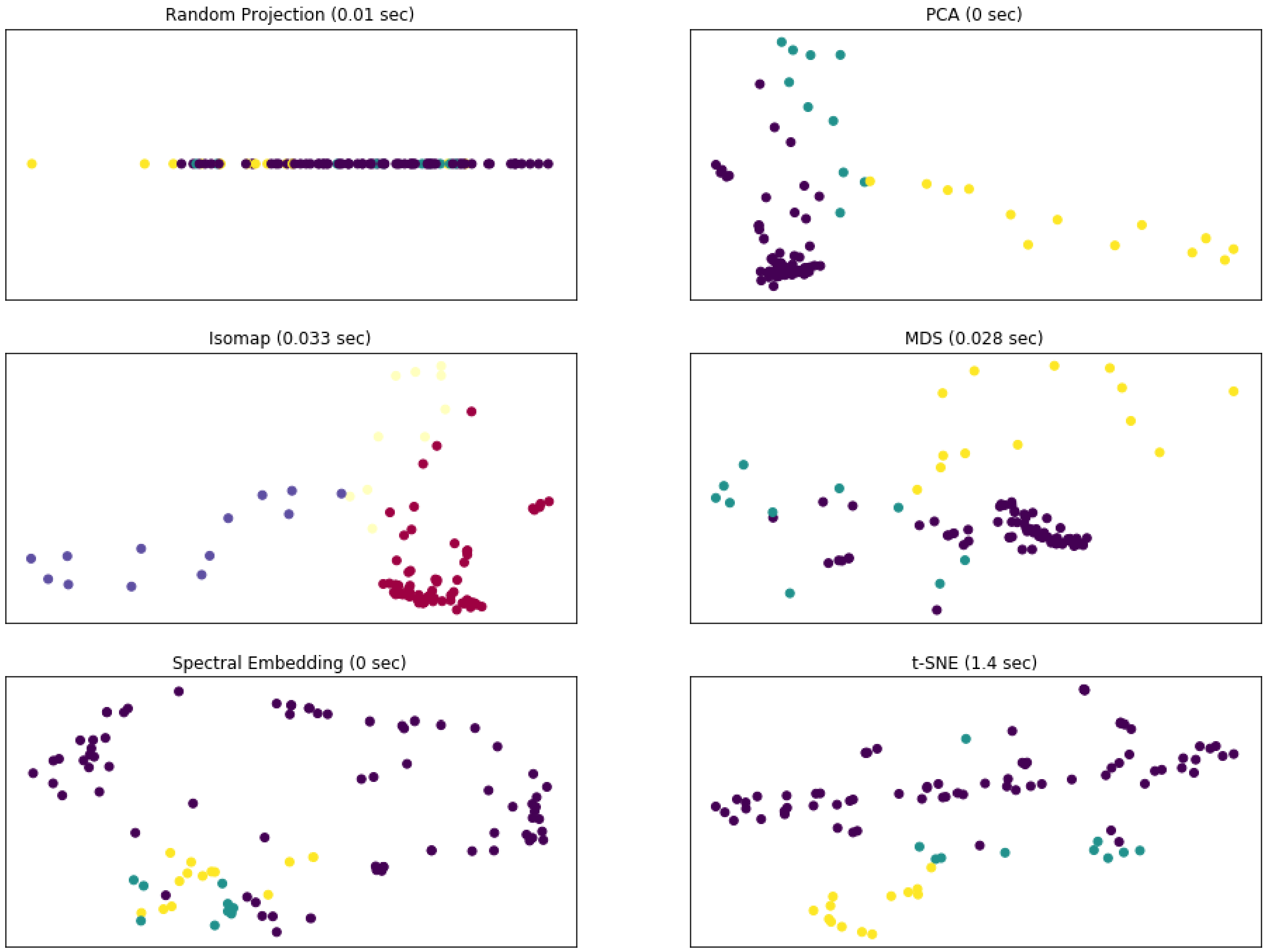
In [8]:
```
tsne = manifold.TSNE(n_components=2, random_state=0)

X_tsne = tsne.fit_transform(X)

fig = plt.figure(figsize=(16, 12))
fig = plt.scatter(X_tsne[:, 0], X_tsne[:, 1], c=color)
fig = plt.title("tSNE")
fig = plt.xticks([]), plt.yticks([])
```



5. Try a bunch of dimensionality reduction techniques

In [9]:
```
n_neighbors = 20
n_components = 2

fig = plt.figure(figsize=(16, 12))

#----------------------------------------------------------------------x
print("Computing Random Projection")
rp = random_projection.SparseRandomProjection(n_components=2, random_state=20)
t0 = time()
X_rp = rp.fit_transform(X)
t1 = time()
plt.subplot(3,2,1)
plt.scatter(X_rp[:, 0], X_rp[:, 1], c=color)
plt.title("Random Projection (%.2g sec)" % (t1 - t0))
plt.xticks([]), plt.yticks([])

#----------------------------------------------------------------------
print("Computing PCA")
pca = decomposition.TruncatedSVD(n_components=2)
t0 = time()
X_pca = pca.fit_transform(X)
t1 = time()
plt.subplot(3,2,2)
plt.scatter(X_pca[:, 0], X_pca[:, 1], c=color)
plt.title("PCA (%.2g sec)" % (t1 - t0))
plt.xticks([]), plt.yticks([])

#----------------------------------------------------------------------
print("Computing Isomap")
iso = manifold.Isomap(n_neighbors, n_components)
t0 = time()
X_iso = iso.fit_transform(X)
t1 = time()
plt.subplot(3,2,3)
plt.scatter(X_iso[:, 0], X_iso[:, 1], c=color, cmap=plt.cm.Spectral)
plt.title("Isomap (%.2g sec)" % (t1 - t0))
plt.xticks([]), plt.yticks([])

#----------------------------------------------------------------------
print("Computing MDS")
mds = manifold.MDS(n_components, max_iter=100, n_init=1)
t0 = time()
X_mds = mds.fit_transform(X)
t1 = time()
plt.subplot(3,2,4)
plt.scatter(X_mds[:, 0], X_mds[:, 1], c=color)
plt.title("MDS (%.2g sec)" % (t1 - t0))
plt.xticks([]), plt.yticks([])

#----------------------------------------------------------------------
print("Computing Specral Embedding")
se = manifold.SpectralEmbedding(n_components=n_components,
                                n_neighbors=n_neighbors)
t0 = time()
X_se = se.fit_transform(X)
t1 = time()
plt.subplot(3,2,5)
plt.scatter(X_se[:, 0], X_se[:, 1], c=color)
plt.title("Spectral Embedding (%.2g sec)" % (t1 - t0))
plt.xticks([]), plt.yticks([])

#----------------------------------------------------------------------
print("Computing t-SNE")
tsne = manifold.TSNE(n_components=n_components, init='pca', random_state=0)
t0 = time()
X_tsne = tsne.fit_transform(X)
t1 = time()
plt.subplot(3,2,6)
plt.scatter(X_tsne[:, 0], X_tsne[:, 1], c=color)
plt.title("t-SNE (%.2g sec)" % (t1 - t0))
plt.xticks([]), plt.yticks([]);
```

```
Computing Random Projection
Computing PCA
Computing Isomap
Computing MDS
Computing Specral Embedding
Computing t-SNE
```



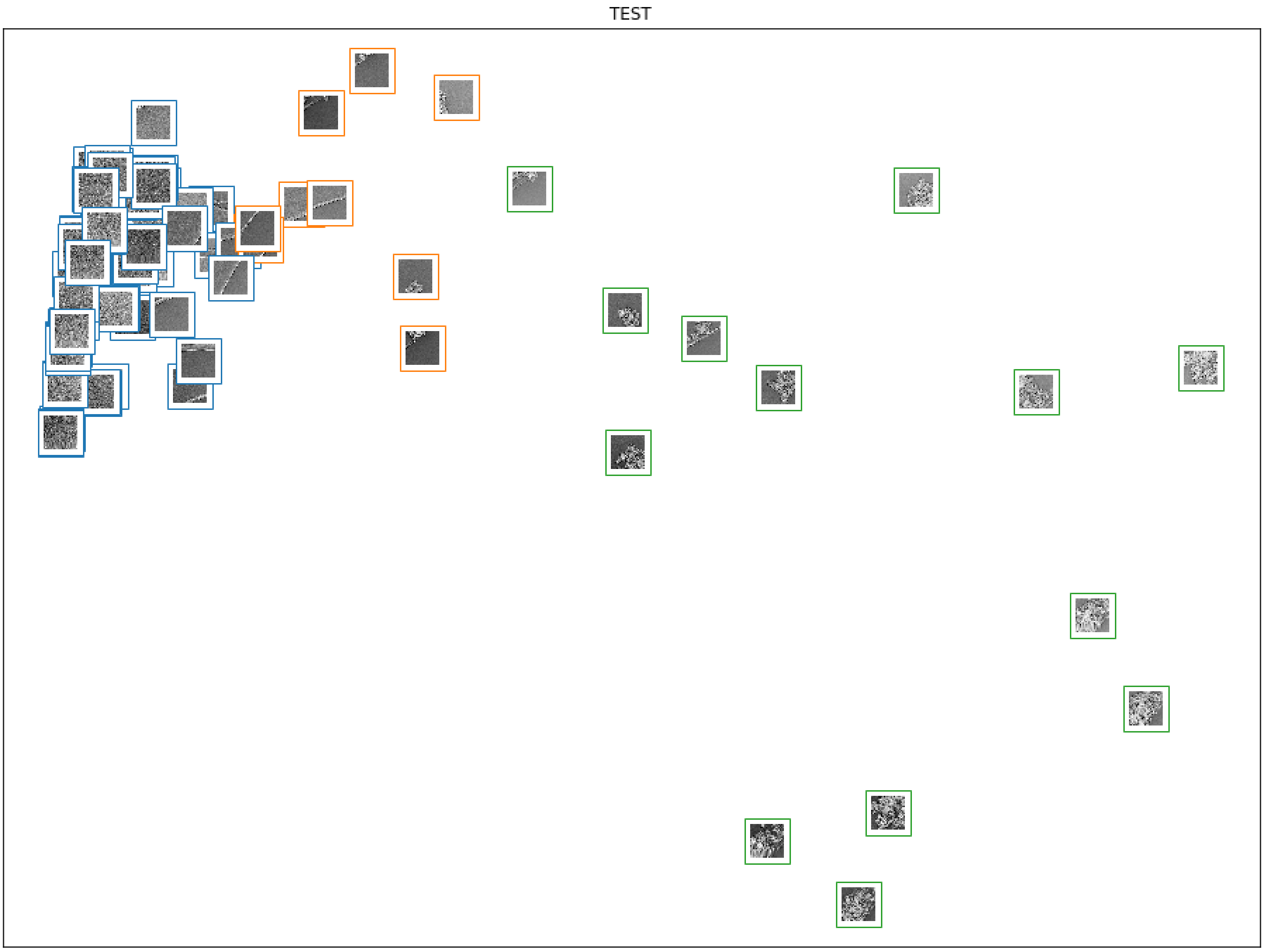
For this dataset, PCA and IsoMap look most promising

6. Improve visualization: plot with images as annotations

First a try-out with own code, snippets from the internet and reading into matplotlib API

In [10]:
```
from skimage.transform import resize
from matplotlib.offsetbox import (OffsetImage, AnnotationBbox)
import imgutils

def plot_with_imgs(X, df_img, class_field, title, ax=None, img_size=(24,24)):
    """Generates a scatter plot with thumbnails of the images corresponding to the data points. """

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

    # with ax, an existing subplot can be filled
    if (ax==None):
        fig = plt.figure(figsize=(16, 12))
        ax = fig.add_subplot(111)

    plt.scatter(X[:, 0], X[:, 1], c=colors)

    cmap = plt.cm.get_cmap('tab10')

    for i in range(X.shape[0]):
        img = imgutils.getimgslice(df_img, i)
        thumbnail = resize(img, img_size)

        imagebox = OffsetImage(thumbnail,cmap=plt.cm.gray_r)
        imagebox.image.axes = ax
        xy = (X[i,0],X[i,1])
        ab = AnnotationBbox(imagebox, xy, bboxprops =dict(edgecolor=cmap(colors[i])))
        #ab.set_zorder(0)
        ax.add_artist(ab)


    plt.title(title)
    plt.xticks([]), plt.yticks([])
```

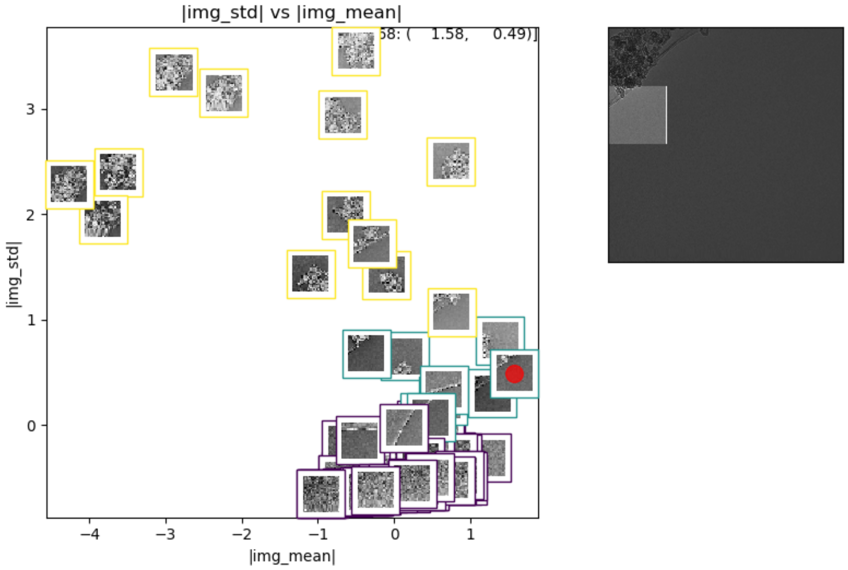
In [11]:
```
plot_with_imgs(X.values, df, 'class', 'TEST' )
```



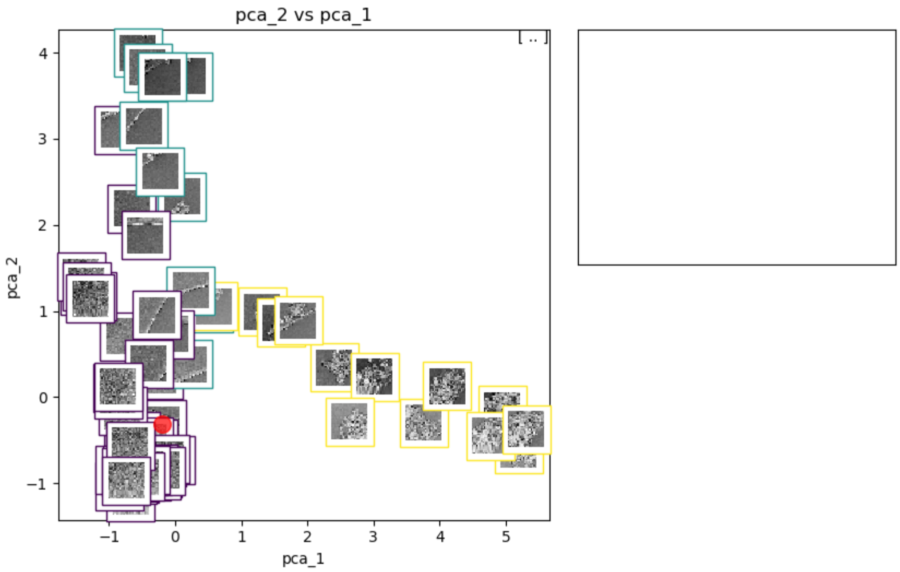
Looks good. Would be even better if I can combine this with the interactive plotting I created in imgutils.

So let's extend those methods with the image annotations... (adjusting imgutils) ... and test the result

In [14]:
```
# now use the updated plotwithimg
%matplotlib notebook
imgutils.plotwithimg(df, '|img_mean|', '|img_std|', imgutils.highlightimgslice, cat_field='class', interactive=True, th
umbnails=True)
```



In [15]:
```
# and now the pca one
df['pca_1'] = X_pca[:,0].tolist()
df['pca_2'] = X_pca[:,1].tolist()

%matplotlib notebook
imgutils.plotwithimg(df, 'pca_1', 'pca_2', imgutils.highlightimgslice, cat_field='class', interactive=True, thumbnails=
True)
```

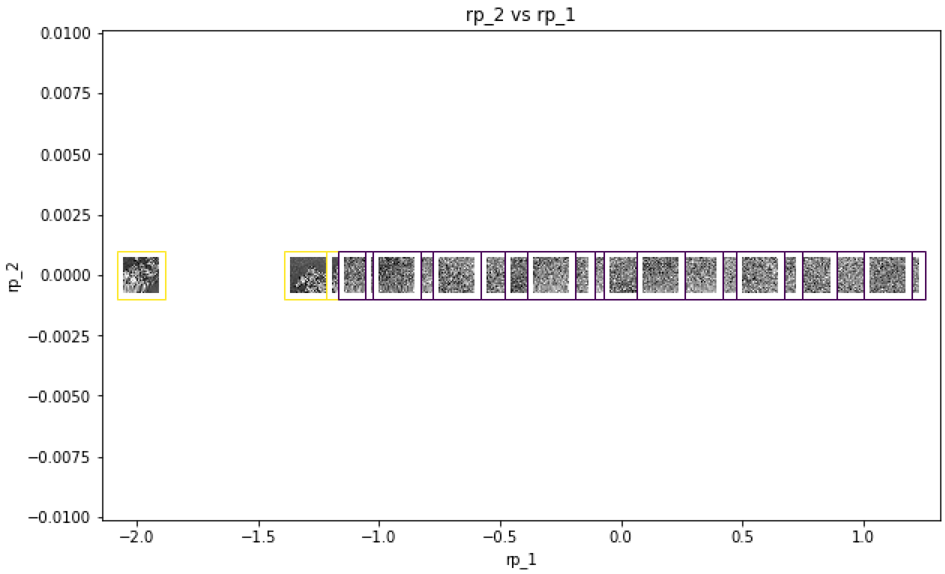


7. Show the different techniques with the new visualization

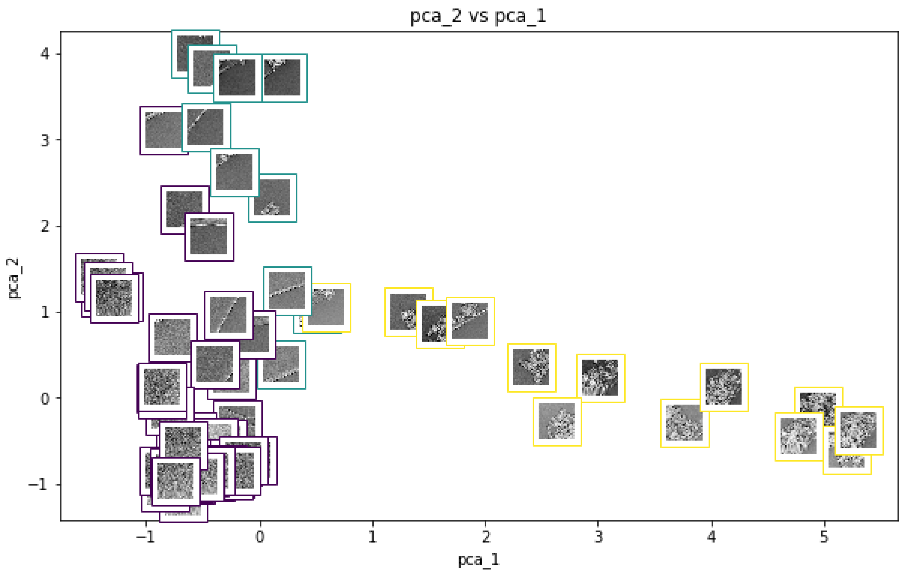
In [18]:
```
# Try now to use on all dimensionality reduction tricks:
n_neighbors = 20
n_components = 2

# as this needs to plot multiple in a single sell, disable interactivity
%matplotlib inline

#------------------------------------------------------------------------x
print("Computing Random Projection")
rp = random_projection.SparseRandomProjection(n_components=2, random_state=20)
t0 = time()
X_rp = rp.fit_transform(X)
t1 = time()
title ="Random Projection (%.2g sec)" % (t1 - t0)
fieldname1 = 'rp_1'
fieldname2 = 'rp_2'
df[fieldname1] = X_rp[:,0].tolist()
df[fieldname2] = X_rp[:,1].tolist()
imgutils.plotwithimg(df, fieldname1, fieldname2, imgutils.getimgslice, cat_field='class', thumbnails=True, interactive=
False)

#------------------------------------------------------------------------
print("Computing PCA")
pca = decomposition.TruncatedSVD(n_components=2)
t0 = time()
X_pca = pca.fit_transform(X)
t1 = time()
title = "PCA (%.2g sec)" % (t1 - t0)
fieldname1 = 'pca_1'
fieldname2 = 'pca_2'
df[fieldname1] = X_pca[:,0].tolist()
df[fieldname2] = X_pca[:,1].tolist()
imgutils.plotwithimg(df, fieldname1, fieldname2, imgutils.getimgslice, cat_field='class', thumbnails=True, interactive=
False)

#------------------------------------------------------------------------
print("Computing Isomap")
iso = manifold.Isomap(n_neighbors, n_components)
t0 = time()
X_iso = iso.fit_transform(X)
t1 = time()
title = "Isomap (%.2g sec)" % (t1 - t0)
fieldname1 = 'iso_1'
fieldname2 = 'iso_2'
df[fieldname1] = X_iso[:,0].tolist()
df[fieldname2] = X_iso[:,1].tolist()
imgutils.plotwithimg(df, fieldname1, fieldname2, imgutils.getimgslice, cat_field='class', thumbnails=True, interactive=
False)

#------------------------------------------------------------------------
print("Computing MDS")
mds = manifold.MDS(n_components, max_iter=100, n_init=1)
t0 = time()
X_mds = mds.fit_transform(X)
t1 = time()
title ="MDS (%.2g sec)" % (t1 - t0)
fieldname1 = 'mds_1'
fieldname2 = 'mds_2'
df[fieldname1] = X_mds[:,0].tolist()
df[fieldname2] = X_mds[:,1].tolist()
imgutils.plotwithimg(df, fieldname1, fieldname2, imgutils.getimgslice, cat_field='class', thumbnails=True, interactive=
False)

#------------------------------------------------------------------------
print("Computing Specral Embedding")
se = manifold.SpectralEmbedding(n_components=n_components,
                                n_neighbors=n_neighbors)
t0 = time()
X_se = se.fit_transform(X)
t1 = time()
title = "Spectral Embedding (%.2g sec)" % (t1 - t0)
fieldname1 = 'se_1'
fieldname2 = 'se_2'
df[fieldname1] = X_se[:,0].tolist()
df[fieldname2] = X_se[:,1].tolist()
imgutils.plotwithimg(df, fieldname1, fieldname2, imgutils.getimgslice, cat_field='class', thumbnails=True, interactive=
False)


#------------------------------------------------------------------------
print("Computing t-SNE")
tsne = manifold.TSNE(n_components=n_components, init='pca', random_state=0)
t0 = time()
X_tsne = tsne.fit_transform(X)
```

```
t1 = time()
title = "t-SNE (%.2g sec)" % (t1 - t0)
fieldname1 = 'tsne_1'
fieldname2 = 'tsne_2'
df[fieldname1] = X_tsne[:,0].tolist()
df[fieldname2] = X_tsne[:,1].tolist()
imgutils.plotwithimg(df, fieldname1, fieldname2, imgutils.getimgslice, cat_field='class', thumbnails=True, interactive=
False)
```

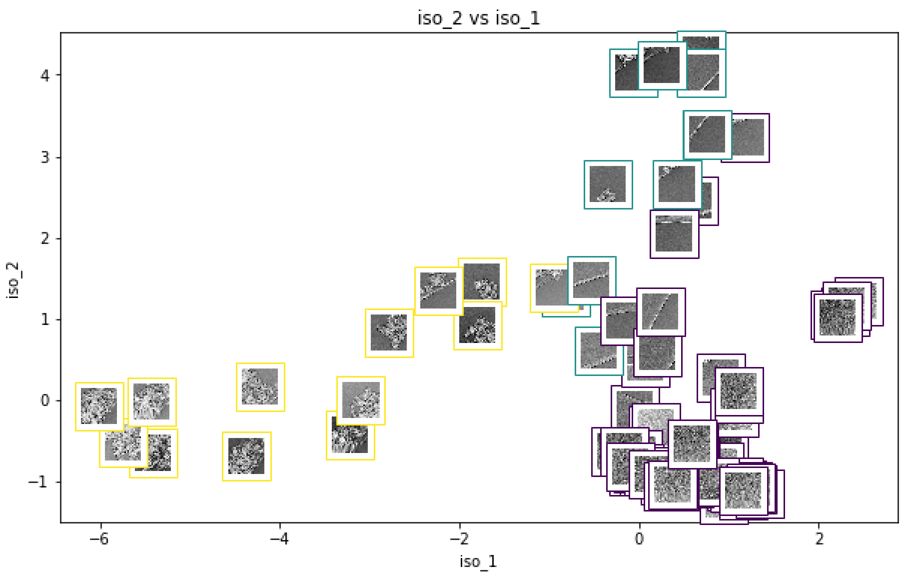
Computing Random Projection



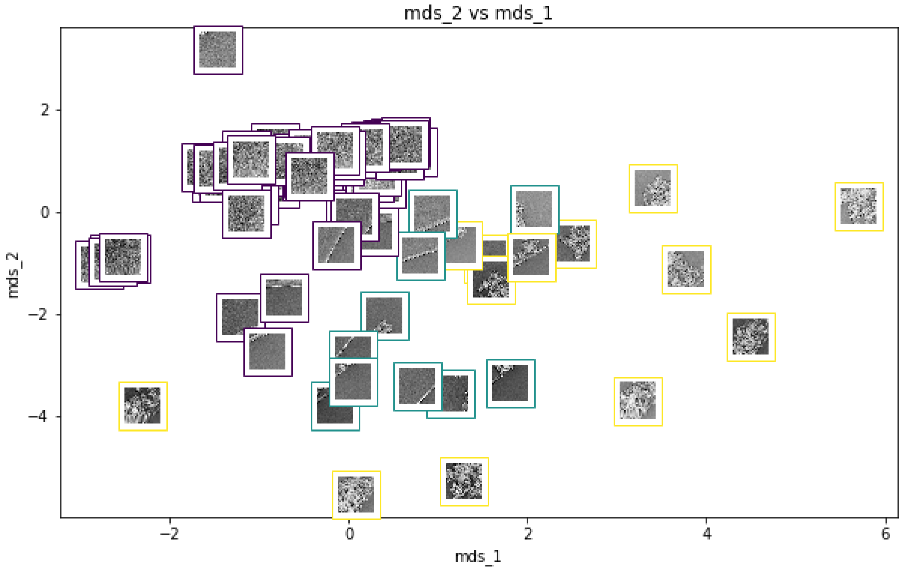
Computing PCA



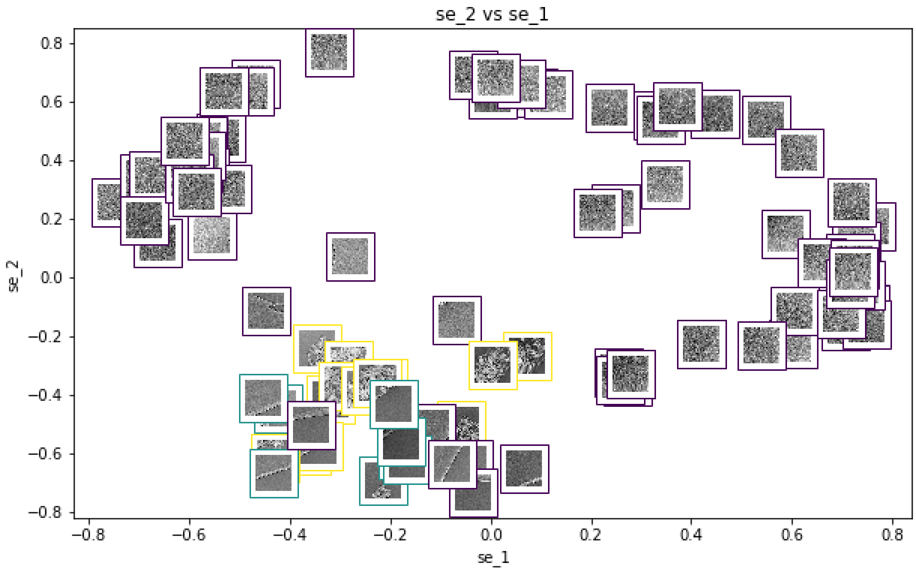
Computing Isomap



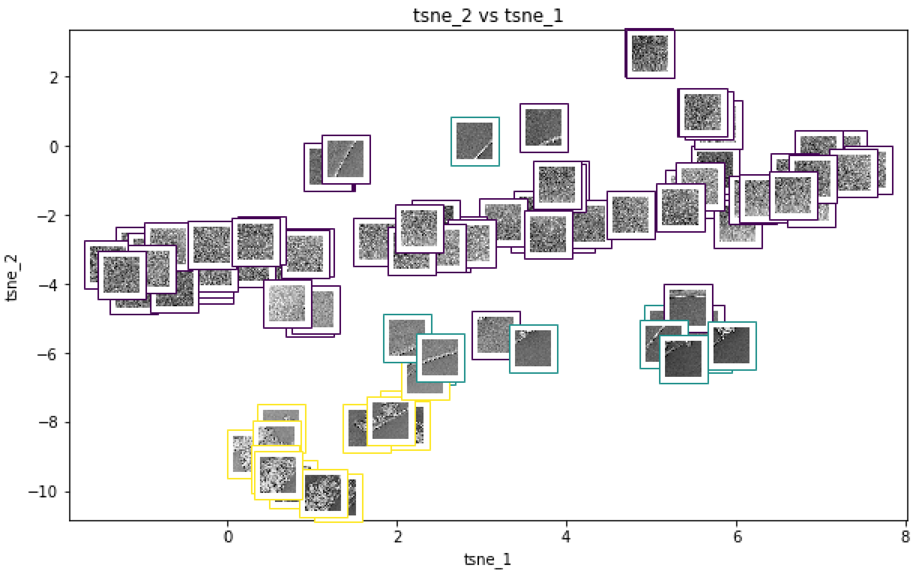
Computing MDS



Computing Specral Embedding



Computing t-SNE



Nice, these type of plots are going to help with the harder data sets.

8. Next Steps:

- Try the 'feature selection' notebook approach on this data set
- Try unsupervised learning on this data set (maybe first apply PCA or IsoMap)
- Repeat this notebook on harder dataset

Michael Janus, 5 July 2018