Real Micro Crystals - Data Engineering & Exploration

Michael Janus, June 2018

Use the functions on a real (small) data set.

For explanation and how to usage functions, see the notebook imgutils_test_and_explain.ipynb

1. Import the used modules, including the one with test functions:

```
In [1]: import warnings
    warnings.filterwarnings("ignore", category=DeprecationWarning)
    import matplotlib.pyplot as plt
    import pandas as pd
    import imgutils
    import imgutils_test as tst

In [2]: # Re-run this cell if you altered imgutils or imgutils_test
    import importlib
    importlib.reload(imgutils)
    importlib.reload(tst)
```

Out[2]: <module 'imgutils_test' from 'C:\\JADS\\SW\\Grad Proj\\realxtals1\\sources\\imgutils_test.py'>

1. Get image files

2 ..\data\Crystals_Apr_12\Tileset7\Tile_001-003-...
3 ..\data\Crystals_Apr_12\Tileset7\Tile_002-001-...
4 ..\data\Crystals_Apr_12\Tileset7\Tile_002-002-...

5 ..\data\Crystals_Apr_12\Tileset7\Tile_002-003-...

2. Get Image Slice Statistics

This set contains 6 images. Let's slice those up in 4 by 4; this will give total of 6 x 4 x 4 = 96 slices. And also apply the statistics on each slice.

```
In [4]: statfuncs = [imgutils.img_min, imgutils.img_max, imgutils.img_range, imgutils.img_mean, imgutils.img_std, imgutils.img_
median]
    df = imgutils.slicestats(list(df_imgfiles['filename']), 4, 4, statfuncs)
    print("records: ", df.shape[0])
    df.head()
```

records: 96

Out[4]:

: _										Ī	Ī	Ī	
		filename	s_y	s_x	n_y	n_x	alias	img_min	img_max	img_range	img_mean	img_std	img_m
	0	lem:lem:lem:lem:lem:lem:lem:lem:lem:lem:	0	0	4	4	img0_0- 0	5419.0	12927.0	7508.0	8955.557637	489.754848	8960.0
	1	$ \data\Crystals_Apr_12\Tileset7\Tile_001-001$	0	1	4	4	img0_0- 1	5248.0	12854.0	7606.0	8883.137305	501.739963	8893.0
	2	lem:lem:lem:lem:lem:lem:lem:lem:lem:lem:	0	2	4	4	img0_0- 2	6084.0	10737.0	4653.0	8786.996070	327.512136	8786.0
	3	$ \data\Crystals_Apr_12\Tileset7\Tile_001-001$	0	3	4	4	img0_0- 3	7105.0	12208.0	5103.0	8679.430512	273.673569	8679.0
	4	$ \data\Crystals_Apr_12\Tileset7\Tile_001-001$	1	0	4	4	img0_1- 0	4534.0	10926.0	6392.0	8982.867158	380.410977	8980.0

•

•		filename	s_y	s_x	n_y	n_x	alias	img_min	img_max	img_range	img_mean	img_std	img_m
	0	\data\Crystals_Apr_12\Tileset7\Tile_001-001	0	0	4	4	img0_0- 0	5419.0	12927.0	7508.0	8955.557637	489.754848	8960.0
	1	\data\Crystals_Apr_12\Tileset7\Tile_001-001	0	1	4	4	img0_0- 1	5248.0	12854.0	7606.0	8883.137305	501.739963	8893.0
:	2	\data\Crystals_Apr_12\Tileset7\Tile_001-001	0	2	4	4	img0_0- 2	6084.0	10737.0	4653.0	8786.996070	327.512136	8786.0
;	3	\data\Crystals_Apr_12\Tileset7\Tile_001-001	0	3	4	4	img0_0- 3	7105.0	12208.0	5103.0	8679.430512	273.673569	8679.0
	4	\data\Crystals_Apr_12\Tileset7\Tile_001-001	1	0	4	4	img0_1- 0	4534.0	10926.0	6392.0	8982.867158	380.410977	8980.0

```
In [8]: stat_normnames = imgutils.normalized_names(stat_names)
print(stat_normnames)
```

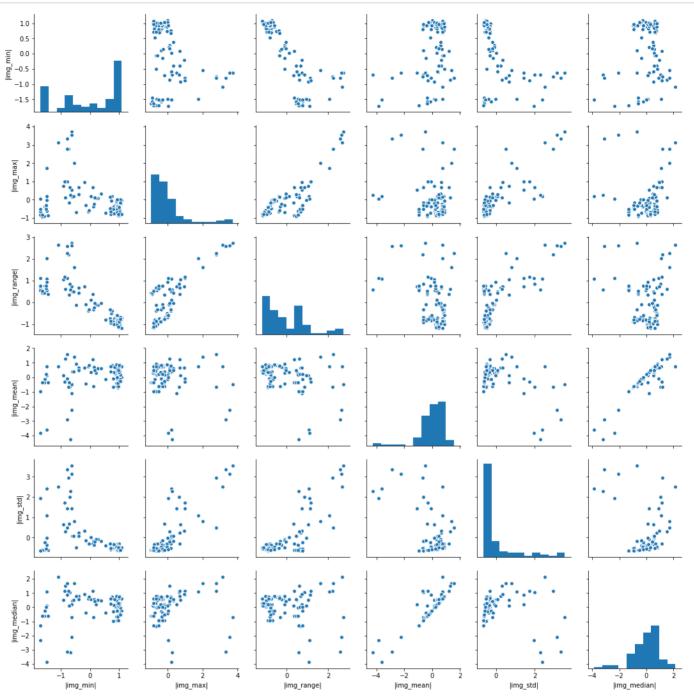
['|img_min|', '|img_max|', '|img_range|', '|img_mean|', '|img_std|', '|img_median|']

3. Check some combinations for patterns

(using the seaborn pairplot)

In [9]: import seaborn as sb



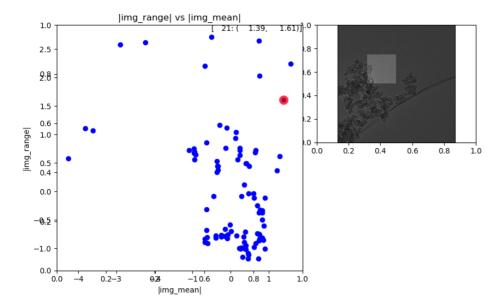


4. Inspect interactively

Let's inspect some combinations that have 'signs of clustering' in the interactive graph

In [11]: %matplotlib notebook

In [22]: | imgutils.plotwithimg(df, '|img_mean|', '|img_range|', imgutils.highlightimgslice)



Looks likt the sort-of cluster in lower right are points without a crystal

```
In [ ]: imgutils.plotwithimg(df, '|img_mean|', '|img_median|', imgutils.highlightimgslice, True)
```

The separation is not representative, the group at top-left contains both with and without micro crystals

```
In [ ]: imgutils.plotwithimg(df, '|img_range|', '|img_std|', imgutils.highlightimgslice, True)
```

This looks better, bottom left are empty regions, top-left have crystals.

5. Heatmaps

Let's do an attempt to create a score for a heatmap. Looks like |img_std| is most infromative

1.07195892 -0.5602243 -0.65242612]]

[3.1514378

```
In [25]: imgname = df_imgfiles.iloc[0]['filename']
        imgs, heats = imgutils.getimgslices_fromdf(df, imgname, '|img_std|')
        imgutils.showheatmap(imgs, heats, opacity=0.7)
        print(heats)
        [[-0.10099756 -0.07945079 -0.39267662 -0.4894673 ]
         [-0.32505447 -0.38569278 0.06486636 1.95016713]]
In [26]: imgname = df_imgfiles.iloc[1]['filename']
        imgs, heats = imgutils.getimgslices_fromdf(df, imgname, '|img_std|')
        imgutils.showheatmap(imgs, heats, opacity=0.7)
        print(heats)
        [[-0.30616301 -0.3702352 -0.44774946 -0.51603165]
         [ 2.50175087  0.80320234  0.65300243  -0.180137  ]
         [ 3.1514378
                     1.07195892 -0.5602243 -0.65242612]]
In [27]: imgname = df_imgfiles.iloc[2]['filename']
        imgs, heats = imgutils.getimgslices_fromdf(df, imgname, '|img_std|')
        imgutils.showheatmap(imgs, heats, opacity=0.7)
        print(heats)
        [[-3.25663596e-01 -3.98403099e-01 -4.54799075e-01 -5.20120403e-01]
         [ 2.32004465e-01 3.33913520e-01 -4.85345650e-04 -1.48112655e-01]
         [-3.12944453e-01 -5.22354114e-01 -5.79775101e-01 -6.29787851e-01]
```

 $[-4.94901820e-01 \ -5.52180410e-01 \ -6.15687209e-01 \ -6.54574240e-01]]$

```
[[-0.5007574 -0.55362623 -0.60028822 -0.64122158]

[-0.48290759 -0.53099997 -0.57905287 -0.63107007]

[-0.47531551 -0.52509339 -0.58101869 -0.63091528]

[-0.49651996 -0.55462781 -0.61553092 -0.6530468 ]]
```

6. Conclusions & Remarks

- The visualization and heatmap concept looks nice.
- Did not use real clustering, but from data exploration just used normalized standard deviation as indicator
- · For larger or different sets (with outliers), I guess a combination of statistics is needed (which was the idea in the first place and let ML figure out what)

7. Next steps

- Export this data set and label it based on std-dev (e.g. 3 cats: none, some, full)
- Export this data set for unsupervised learning
- · Repeat on bigger and more versatile set

Michael Janus, 15 June 2018

Update 5 July 2018

8. Assign labels

inspecting the heats, define 3 cats:

- |img_std|<0 = A (no particle);
- 0<|img_std|<1 = B (partly)
- |img_std|>1 = C (fully)

```
In [30]: def assign_label(score):
    if score<0: return 'A'
    if score>=1: return 'C'
    return 'B'

df['class'] = df.apply(lambda r: assign_label(r['|img_std|']), axis=1)
```

In [31]: df.head()

Out[31]:

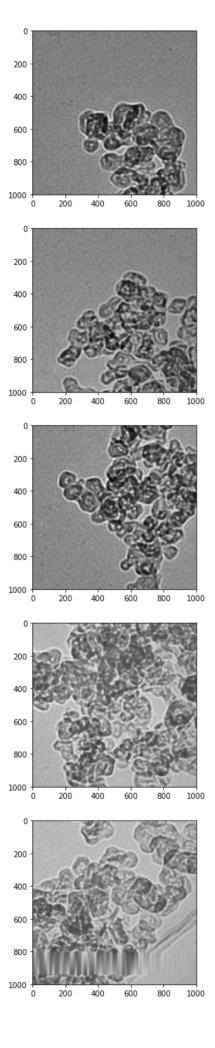
	filename	s_y	s_x	n_y	n_x	alias	img_min	img_max	img_range	img_mean	img_std	img_m
0	\data\Crystals_Apr_12\Tileset7\Tile_001- 001	0	0	4	4	img0_0- 0	5419.0	12927.0	7508.0	8955.557637	489.754848	8960.0
1	\data\Crystals_Apr_12\Tileset7\Tile_001- 001	0	1	4	4	img0_0- 1	5248.0	12854.0	7606.0	8883.137305	501.739963	8893.0
2	\data\Crystals_Apr_12\Tileset7\Tile_001- 001	0	2	4	4	img0_0- 2	6084.0	10737.0	4653.0	8786.996070	327.512136	8786.0
3	\data\Crystals_Apr_12\Tileset7\Tile_001- 001	0	3	4	4	img0_0- 3	7105.0	12208.0	5103.0	8679.430512	273.673569	8679.0
4	\data\Crystals_Apr_12\Tileset7\Tile_001- 001	1	0	4	4	img0_1- 0	4534.0	10926.0	6392.0	8982.867158	380.410977	8980.0

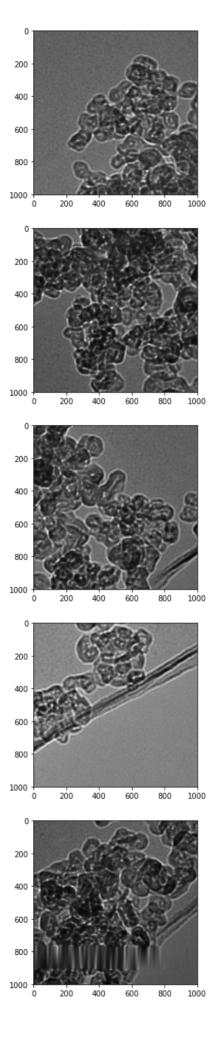
```
In [32]: df2 = df[df['class']=='C']
```

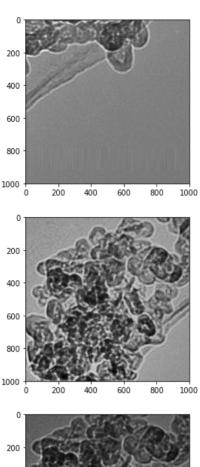
In [33]: print(len(df2))

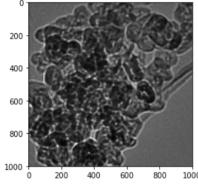
13

```
In [34]: %matplotlib inline
    # check class C images
    for i in range(0,len(df2)):
        img = imgutils.getimgslice(df2, i)
        imgutils.showimg(img)
```

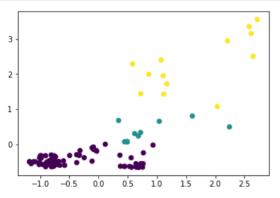






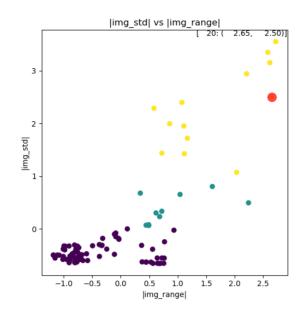


In [35]: # also plot them the img_std vs img_range with the labels
labels = df['class'].tolist()
colors = [(0 if (l=='A') else (1 if (l=='B') else 2)) for 1 in labels]
plt.scatter(df['|img_range|'], df['|img_std|'], c=colors)
plt.show()



ideally we should have this interactive with the images, so extend the infrastructure (done, had to change to interactive scatter plot instead of line plot)

In [37]: %matplotlib notebook
 imgutils.plotwithimg(df, '|img_range|', '|img_std|', imgutils.highlightimgslice, 'class')



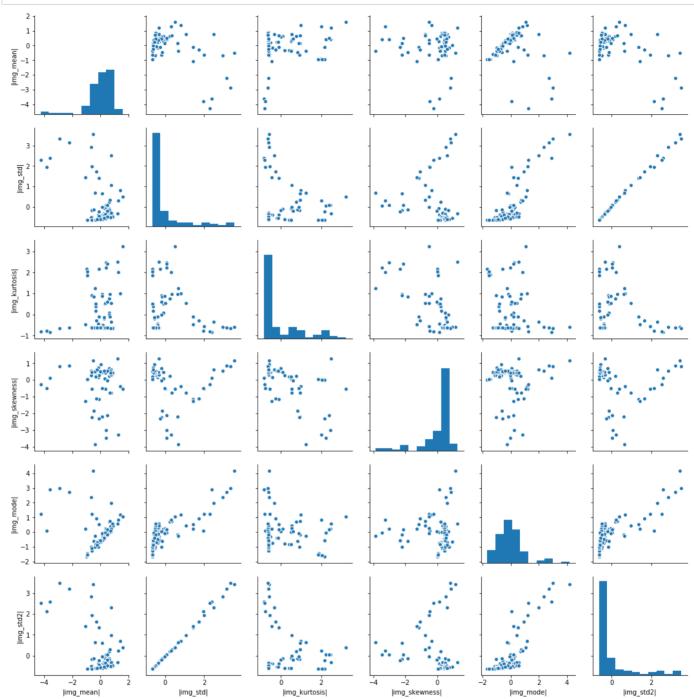


9. Export as csv

In [38]: df.to_csv('../data/Crystals_Apr_12/Tileset7.csv', sep=';')

10. Also other stats

In [41]: stat_names = imgutils.stat_names(statfuncs) + ['img_std2']
 imgutils.normalize(df2, stat_names)



In [43]: #label them based on std (first experiment)
df2['class'] = df.apply(lambda r: assign_label(r['|img_std|']), axis=1)

In [44]: df2.to_csv('../data/Crystals_Apr_12/Tileset7-2.csv', sep=';')