hdf5_docs

April 30, 2019

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@date: 04/29/19

```
In [1]:          import numpy as np
         from matplotlib import pyplot as plt
         import h5py
```

0.1 Data Files

1. Data is split up into batches... e.g `batch_*h5`.

2. The file names are labeled according to their data partition... e.g. `batch_train*` belongs to training data.
3. `dev` and `test` are for development and testing, respectively.
4. **The data is not shuffled!**

```
In [2]: f = h5py.File('/data/smc_19/batch_train_0.h5', mode='r', swmr=True)
```

Each particular data sample is stored in a separate `h5group`.
Here are the names of the samples (i.e. groups) in the file.

```
In [3]: keys = list(f.keys())
         keys
```

```
Out[3]: ['sample_0_0',
          'sample_10_0',
          'sample_11_0',
          'sample_12_0',
          'sample_13_0',
          'sample_14_0',
          'sample_15_0',
          'sample_17_0',
          'sample_18_0',
          'sample_1_0',
          'sample_20_0',
          'sample_21_0',
          'sample_22_0',
          'sample_23_0',
```

```
 'sample_25_0',
 'sample_26_0',
 'sample_27_0',
 'sample_28_0',
 'sample_29_0',
 'sample_2_0',
 'sample_30_0',
 'sample_31_0',
 'sample_32_0',
 'sample_33_0',
 'sample_34_0',
 'sample_35_0',
 'sample_37_0',
 'sample_38_0',
 'sample_39_0',
 'sample_3_0',
 'sample_41_0',
 'sample_42_0',
 'sample_43_0',
 'sample_44_0',
 'sample_45_0',
 'sample_46_0',
 'sample_47_0',
 'sample_48_0',
 'sample_49_0',
 'sample_50_0',
 'sample_51_0',
 'sample_52_0',
 'sample_53_0',
 'sample_55_0',
 'sample_56_0',
 'sample_57_0',
 'sample_58_0',
 'sample_59_0',
 'sample_6_0',
 'sample_7_0',
 'sample_8_0']
```

0.2 Data Attributes

With each `sample` is associated different attributes.

```
In [4]: idx = np.random.randint(0, len(list(f.keys())))
        key = keys[idx]
        group = f[key]
        list(group.attrs.items())
```

```
Out[4]: [('space_group', b'2'),
         ('material', b'mp-763064'),
```

```
('energy_keV', 100),
('z_dirs', array([[[ 1,  1,  0],
        [ 1, -1,  1],
        [-1,  1,  3]]])),
('y_dirs', array([[[-1.33333333,  1.        , -1.        ],
        [ 0.66666667,  0.        ,  1.        ],
        [-0.66666667,  0.        , -1.        ]]])),
('semi_angles_rad', array([0.00276776, 0.0028678 , 0.00367309])),
('d_hkls_angstrom', array([3.34336566, 3.22673953, 2.51930512])),
('abc_angstrom', array([4.6456035 , 7.54737513, 7.59231027])),
('angles_degree', array([75.75270737, 91.58467769, 89.08634999])),
('formula', 'Fe8 O14 F2')]
```

1. `material` is the material name (solids) as cataloged in the materials project https://materialsproject.org/
2. `energy_keV` is the electron beam energy (in keV).
3. `z_dir` are the crystallographic (hkl) normal directions of the material from which CBED was acquired.
4. `y_dir` are the crystallographic (hkl) transverse directions of the material from which CBED was acquired.
5. `semi_angles_rad` are the half-angles of convergence of the incident electron beam (in radians).
6. `d_hkls_angstrom` are the d-spacing of the Bragg reflections from which CBED was acquired (in Å).
7. `abc_angstrom` are the lattice constants (a, b, c) of the material (in Å).
8. `angles_degree` are the lattice angles (α, β, γ) of the material (in degrees).
9. `chemical formula` is the chemical formula of the material.

And 0. `space_group` **is the space group number (1 - 230) as specified by the conventions of crystallography**. see https://en.wikipedia.org/wiki/List_of_space_groups

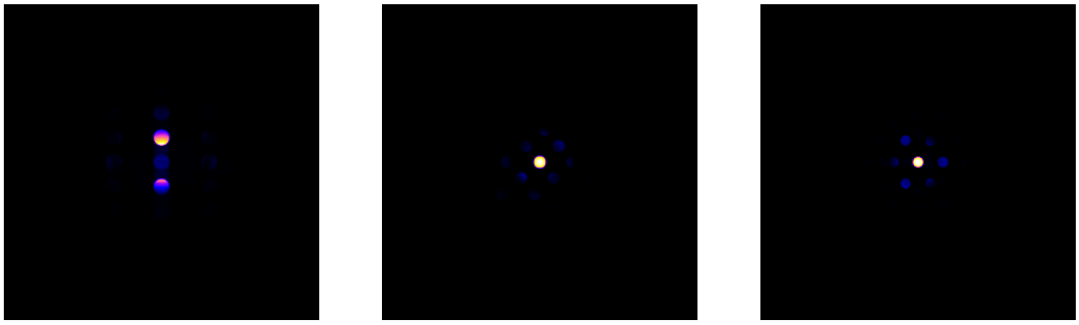
In addition to the classification task of the space group `0`, the following attributes can be used as labels in a multi-task ML algorithm: `2`, `6`, `7`, `8`, and `9`.

0.3 Data

The data for each sample is saved as `h5dataset`, with name `cbed_stack`, with dimensions of (3,512,512).
The first axis contains the 3 different crystallographic directions or material orientations (corresponding to `z_dirs` and `y_dirs`).
The 2nd and 3rd axis are the diffraction intensities (in reciprocal space).

```
In [5]: idx = np.random.randint(0, len(list(f.keys())))
        key = keys[idx]
        group = f[key]
        list(group.items())
        cbed_stack = group['cbed_stack'][()]
        list(group.attrs.items())
        fig, axes = plt.subplots(1,3, figsize=(16,12))
        for ax, cbed in zip(axes.flatten(), cbed_stack):
```

```
        ax.imshow(cbed, cmap='gnuplot2')
        ax.axis('off')
```



0.3.1 Note

CBED data will always have orders of magnitude intensity change from the center of the image. As such **proper scaling** should always be applied. The appropriate scaling function is up to you. Below is $^{1/4}$ scaling.

```
In [6]: fig, axes = plt.subplots(1,3, figsize=(16,12))
        for ax, cbed in zip(axes.flatten(), cbed_stack):
            ax.imshow(cbed**0.25, cmap='gnuplot2')
            ax.axis('off')
        plt.show()
```