Examples of using PyXAS GUI

Inside *example* folder, there are 3 files:

1. "NMC-LLZO.h5": 2D XANES image. This image stack derives from one slice of 3D xanes-tomography taken across the Ni absorption edge.
   The .h5 file has the following structure:
      /img_xanes: flat-field normalized image stack
      /X_eng: an energy list of energy associated with XANES image stack
2. ref_NiO.txt: reference spectrum of Ni^{2+} collected from NiO particles
3. ref_LiNiO2.txt: reference spectrum of Ni^{3+} collected from $LiNiO_2$ particles

Step-by-step of 2D XANES fitting

- **Data loading (Tab: Prep.):**
  In the "Load image" section, select "hdf" as the file type.
  In "Dataset for XANES", input "img_xanes", which is attribute name of 2D XANES image stack.
  In "Dataset for Energy", input "X_eng", which is attribute name of XANES energy list.
  Then click "Load image" button to load the example image file "NMC_LLZO.h5".
  Note:
  i. It supports image binning to reduce the image size, simply by clicking the "XANES Binning" button.
  ii. Example of manual input of an energy list: self.xanes_eng = numpy.arange(8.2, 8.5, 0.001),

- **Image alignment (Tab: Prep.)**
  1. Draw ROI: click "Draw ROI", and then use mouse to drag an area in the image display window to define the ROI. Multiple ROIs will be listed in the "ROI list", with names of "roi_0", "roi_1", etc.
  2. To align image using ROI, in the "ROI index" field, input the index of ROI that will be used to align with, e.g., if using roi_0, input digit "0" in that field.
  3. Select the reference image. Generally, the reference image should have good contrast. E.g., input "100" in the "Ref. Image" field, for which it will use the 101th image as reference. (Note: image index starts with 0, so "100" refers to the 101th image)
  4. Choose the alignment algorithm, e.g., "StackReg"
  5. Click the "Align Img (ROI)"

  Note: most of the processed image data will be named as "Image updated" in the image display window.

- **Edge normalization (Tab. Prep. & Norm.)**
  1. Take -log of image if necessary. For the current example, we don't need to take negative natural log. For regular TXM XANES image, negative natural log is required, by clicking "Norm. TXM (-log)" button.
  2. Check energy range of pre-edge and post-edge

Select the one of the ROI listed in the "ROI list", click "Plot Spec.". For this example (see ROI spectrum below), pre-edge can be defined with energies below 8.33 keV, and post-edge can be defined for all energies above 8.4 keV.

3. Under the "**Norm**." tab, input the pre and post-edge energy range in the relevant fields: "Pre-edge start/end" and "post-edge start/end"
4. To check how does the edge normalization work, click "Norm Spec (ROI)". It will plot the raw spectrum and edge-normalized spectrum averaged from the ROI region as selected.
   Note: if this is material that will be used as a reference material, click the "Save Spec" button to save the normalized spectrum for use as the reference spectrum required for the subsequent XANES fitting.
5. Once we are satisfied with the defined energy range of pre/post edge, we can perform the edge normalization for the whole image, simply by clicking "Norm Image"
   Note: we provide two methods for edge normalization.
   i. If image is noisy, use method 1. It will calculate slope of the absorption curve of pre/post range by averaging all the pixel values from areas that contains materials, and keep the slope unchanged and then fit the offset of the absorption curve for individual pixel.
   ii. If image has good signals, use method 2. It will calculate the linear slope and offset of absorption curve individually for each pixel.

- **2D XANES fitting (Tab: Fit Spec.)**
1. Load reference spectra: click "Load Ref." to load "ref_NiO.txt" and "ref_LiNiO2.txt"
   We can assign labels for these two ref. spectra. E.g, input "Ni2, Ni3" in the "Elem." filed.
2. Click "Fit 2D"
   Note 1: The fitting will use the image data which is currently displayed in the image display window. Make sure we selected the proper dataset. Mostly, we should use "Image updated".
   Note 2: for fitting using iterative method (e.g, Conj. Grad), give the relevant parameters, and then click "Fit 2D (iter)"
3. After fitting, additional image datasets will be added in the image display window: "**XANES Fit thickness**", "**XANES Fit (ratio, summed to 1)**", "**XANES Fit (Elem, concentration)**" and "**XANES Fit error**".
   Note: XANES Fit (Elem, concentration) = XANES Fit (ratio, summed to 1) x XANES Fit thickness.
4. Fitting evaluation
   We can view the "XANES Fit error" to check the fitting quality.
   We can also check the fitting results from specific ROI region. E.g., if we would like to check ROI 1, put "1" in the "ROI #" field. Then click "Plot ROI fit". It will plot both the experimental data and fitted curve. A good match indicates a good fitting.
5. The fitting results can be saved in a .h5 file by clicking "Save 2D Fit".

- **Segmentation/Mask (Tab: Img. Tools)**
1. Threshold mask:
   E.g., generate mask from "XANES Fit error": display the "XANES Fit error" and select a threshold value. E.g., we would like to remove regions with fitting error larger than 0.3. Then

we can write ">0.3" in the field of "Gen. Mask1(2) Thresh:", then click "Gen. Mask1(2)" button.
Note: the mask will be applied to all the images in the package.
To remove the mask, simply by clicking "Rmv, Mask1(2)"

2. Clustering mask:
   i. Choose the "Raw image" in the image display window.
   ii. Under "Clustering Mask", check the checkbox "Use stack". If we would like to use part of image stack, e.g., from image #20 to #40, put "20" in "start:" and "40" in "end:".
   iii. Put the desired number of components, e.g., "4" in the field of "comp #"
   iv. Click "Gen. Mask"
   v. A new image dataset "Smart Mask" will be added to the image display window for visualization.
   vi. For the 4 masks generated (because we set comp# to be 4), if we would like to apply the second mask to the image, in the image display window, navigate the slider-bar to the second mask, then click "Apply mask". It will propagate the mask to all images. We can remove it by click "Rmv. mask".

- **Miscellaneous**
  1. Colormix (**Tab Img. Tools**):
     After XANES fitting, we can use colormix to generate a colored image to represent the distribution of element with different oxidation states, e.g., Ni^{2+} and Ni^{3+}.
     i. In image display window, select the fitted results, e.g., "**XANES Fit (Elem, concentration)**"
     ii. Under section of "Other Tools", click "Color Mix". The colored image will be added to image display window. We can save the color image by clicking "Save current image" to save it.
  2. Basic image processing:
     We provide basic image processing tools, such as image dilation, erosion, fill-hole, median filters to remove noises.

- **Call functions from python environment**
  All functions inside the package can be called in a python environment. Users can look though the functions in the sub-folder /pyxas.