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Machine Learning-based Spectra Classification

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Background

❑ Background (Big data):

- Experiments in photon sciences at synchrotrons or XFELs (e.g. SCS, FXE and HED experiments) always generate a large volume of data.

❑ ML algorithms and its requirements:

- A great amount of data which are clearly annotated and complete for covering the requirements of scientific reuse.

❑ ML, Big Data requirements on Ontologies, and Application Definition:

- The research outputs should align with the '**FAIR**' principles, meaning that data, software, models, and other outputs should be *Findable, Accessible, Interoperable,* and *Reusable*;
- For data re-use, the metadata shall follow a scientific experiment data model; Appropriate NeXus application definitions shall be defined.

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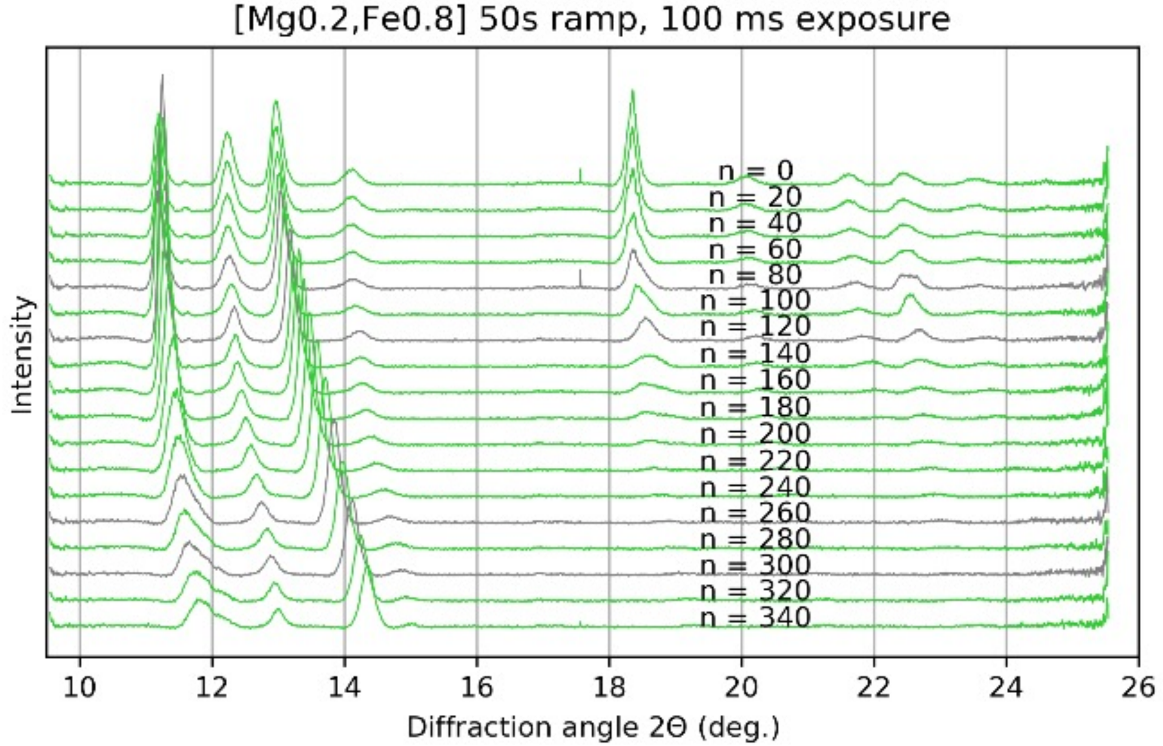
Example of Data Reuse

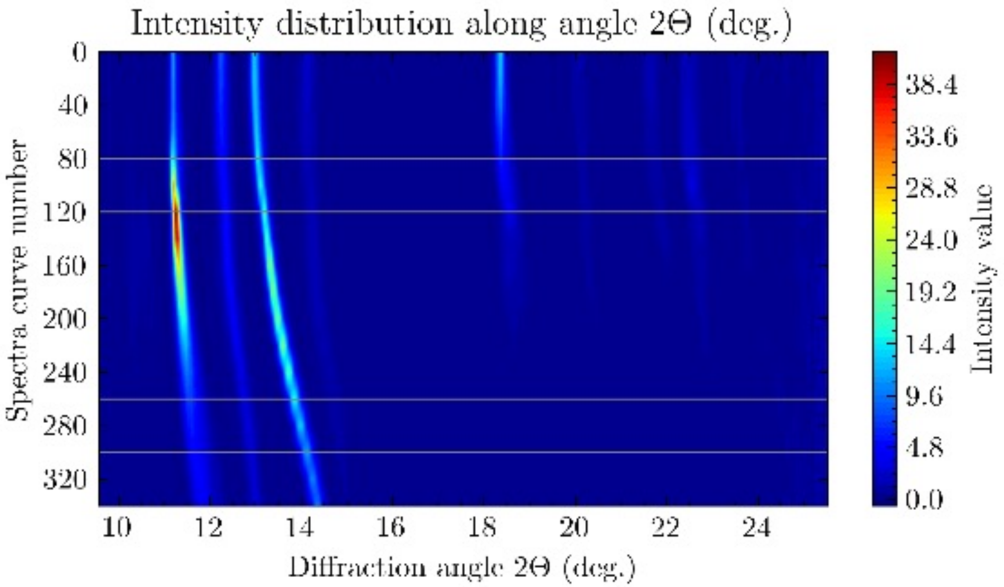
HED Diffraction Spectra data



Data set: 349 samples with each of 4023 features

Two phases: Low and High pressure

Training data: 4 (original)+40 (simulated) = 44

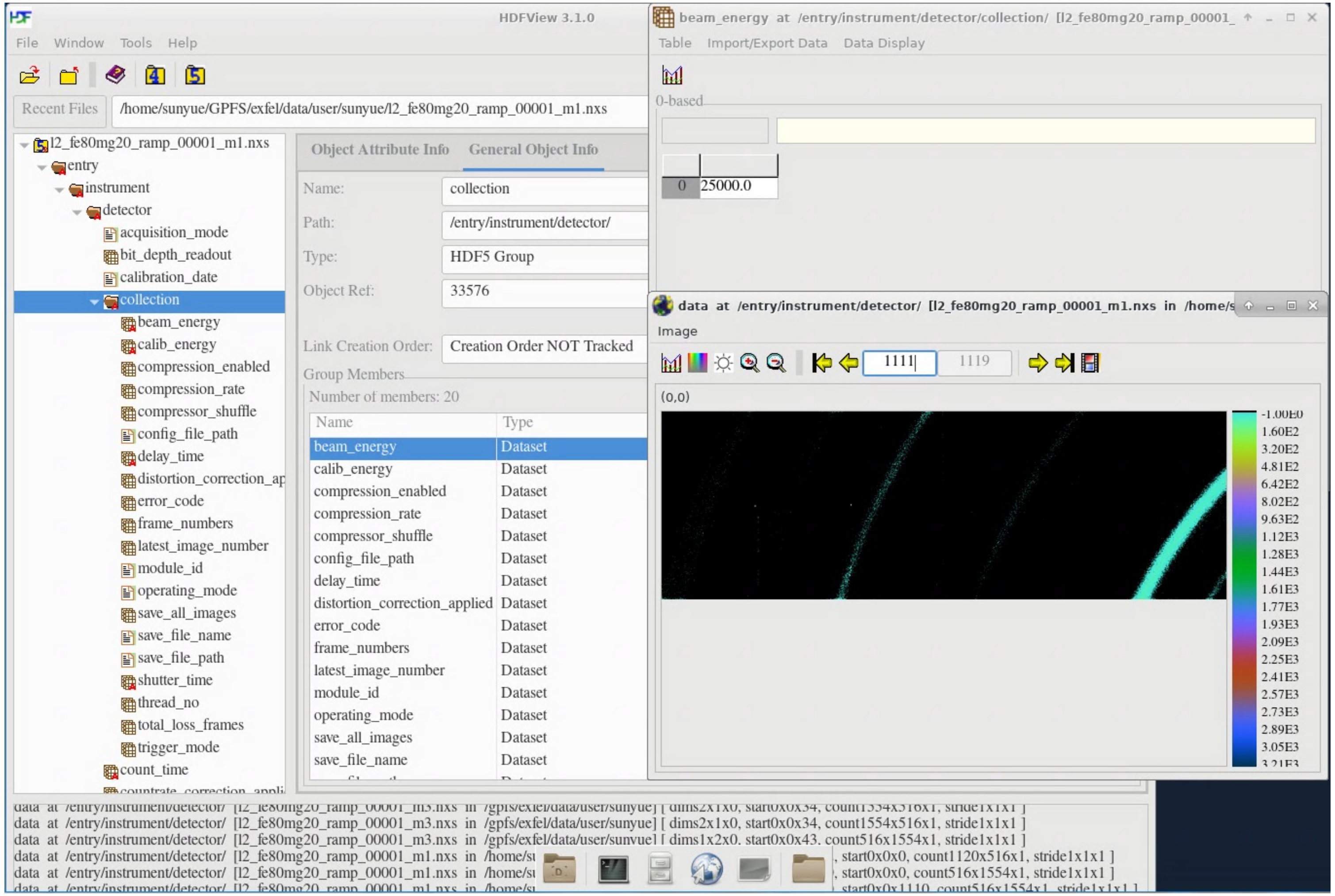


Measured at PETRA III beamline P02.2 using a 25.6 keV beam.

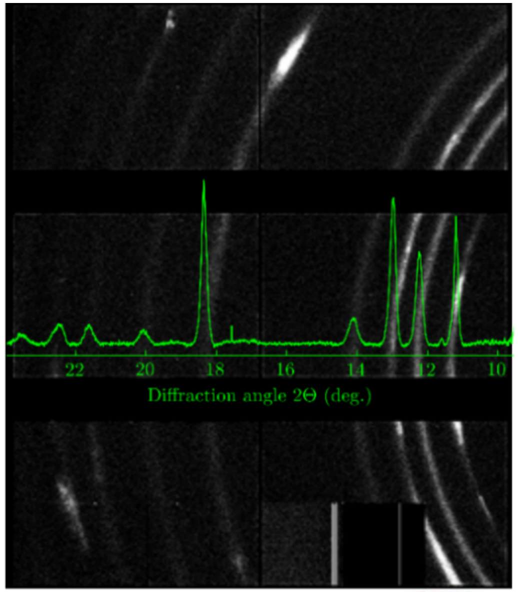
The **major spectral changes** we aim to capture are

- the change of intensity distribution (e.g. drop or appearance) of peaks at certain locations, or
- the shift of those in the spectrum.

NeXus Raw data file example



- NeXus base classes are used, but no application definitions (only free key-values under **NXcollection**).
- No real experimental data was registered (e.g. **beam_energy**).

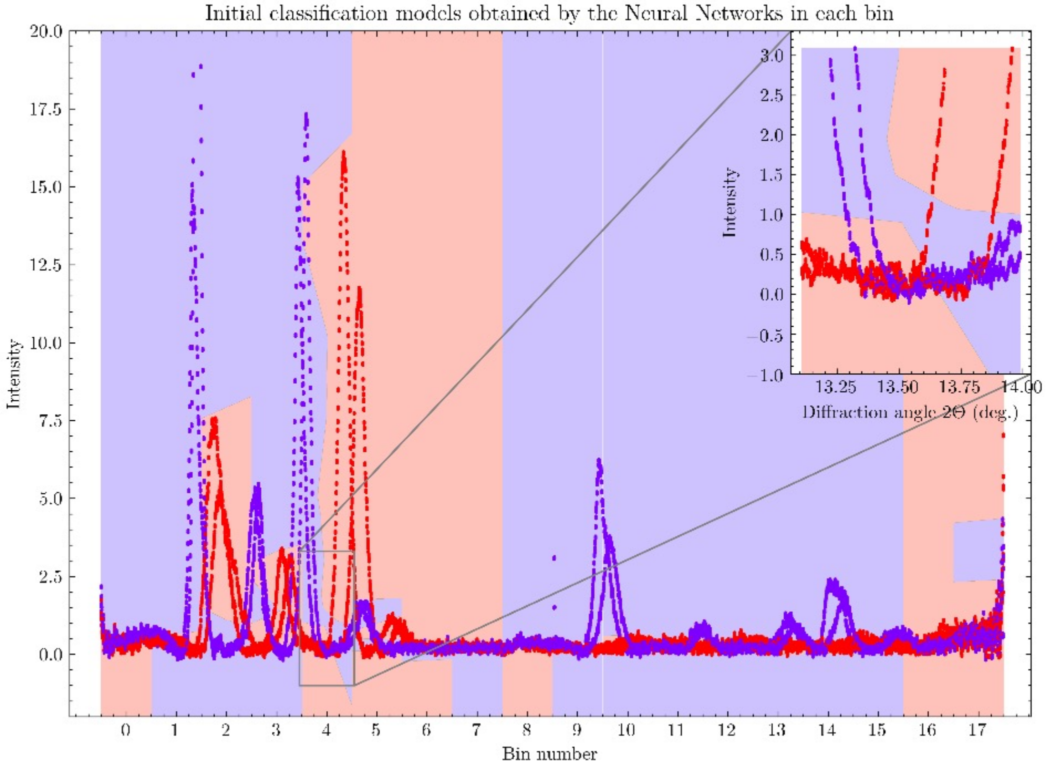


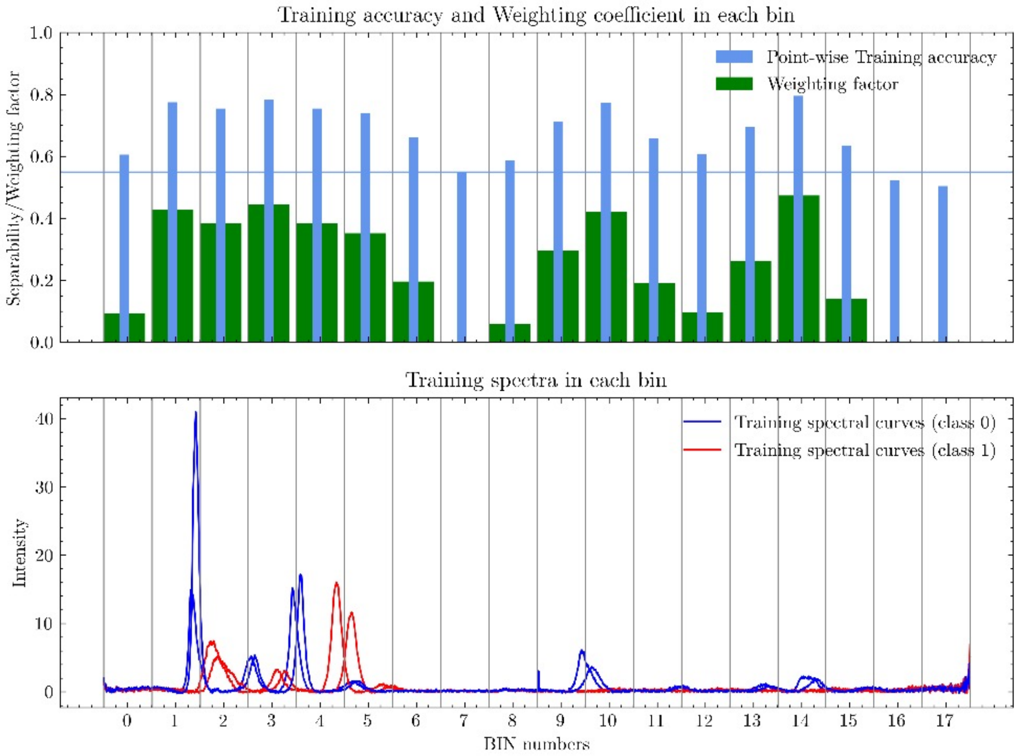
2D diffraction pattern

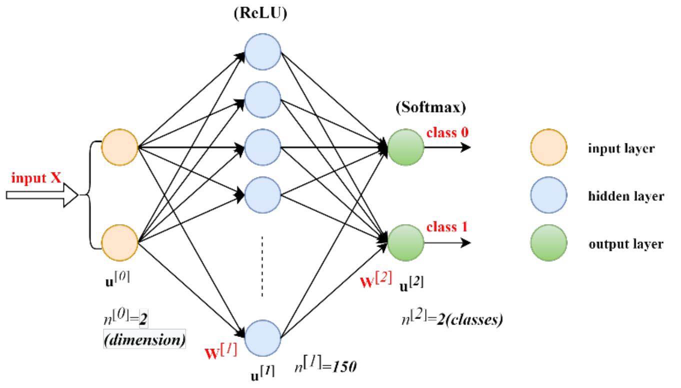
One of the NeXus Raw data file displayed in HDFview software

Two-layer NN with Weighting technique for spectra classification

In this work, the spectra classification task is regarded as a general two-dimensional (2D) space segmentation problem.



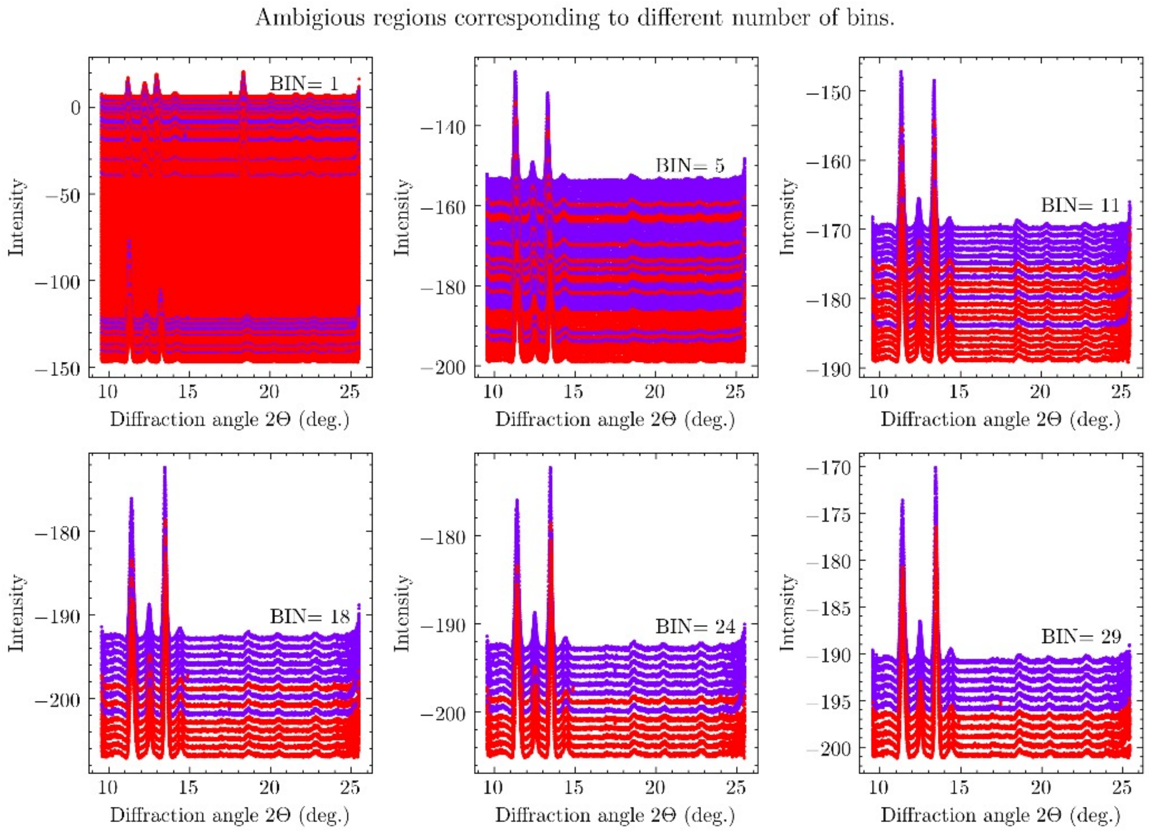


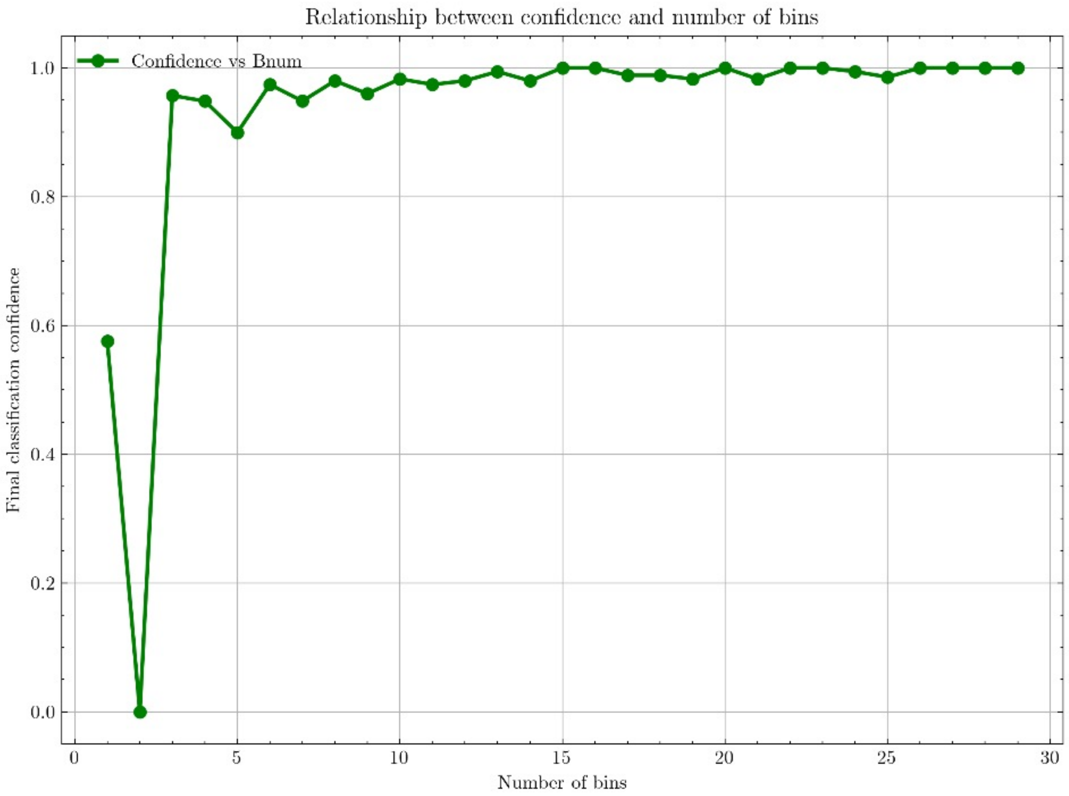


The distribution of point-wise training accuracy (separability), and the believability weighting factor for each bin.

Believability weighting factor:

$$w_b = \max\left(0, 1.4337{A_b}^2 - 0.4337\right)$$





$$L_{curve} = \underset{k \in \{0,\cdots,C-1\}}{\operatorname{argmax}} \sum_{b=1}^{B} w_b \sum_{i=1}^{N_B} \hat{C}_k^{(i)}$$

Performance metrics: $P_{conf} = 1 - \frac{N_f}{N_t}$

- Submitted a paper ‘Machine Learning Applied for Spectra Classification in XFEL Sciences’ to Data Science Journal;
- https://github.com/European-XFEL-examples/panosc-ml-spectra-classification.

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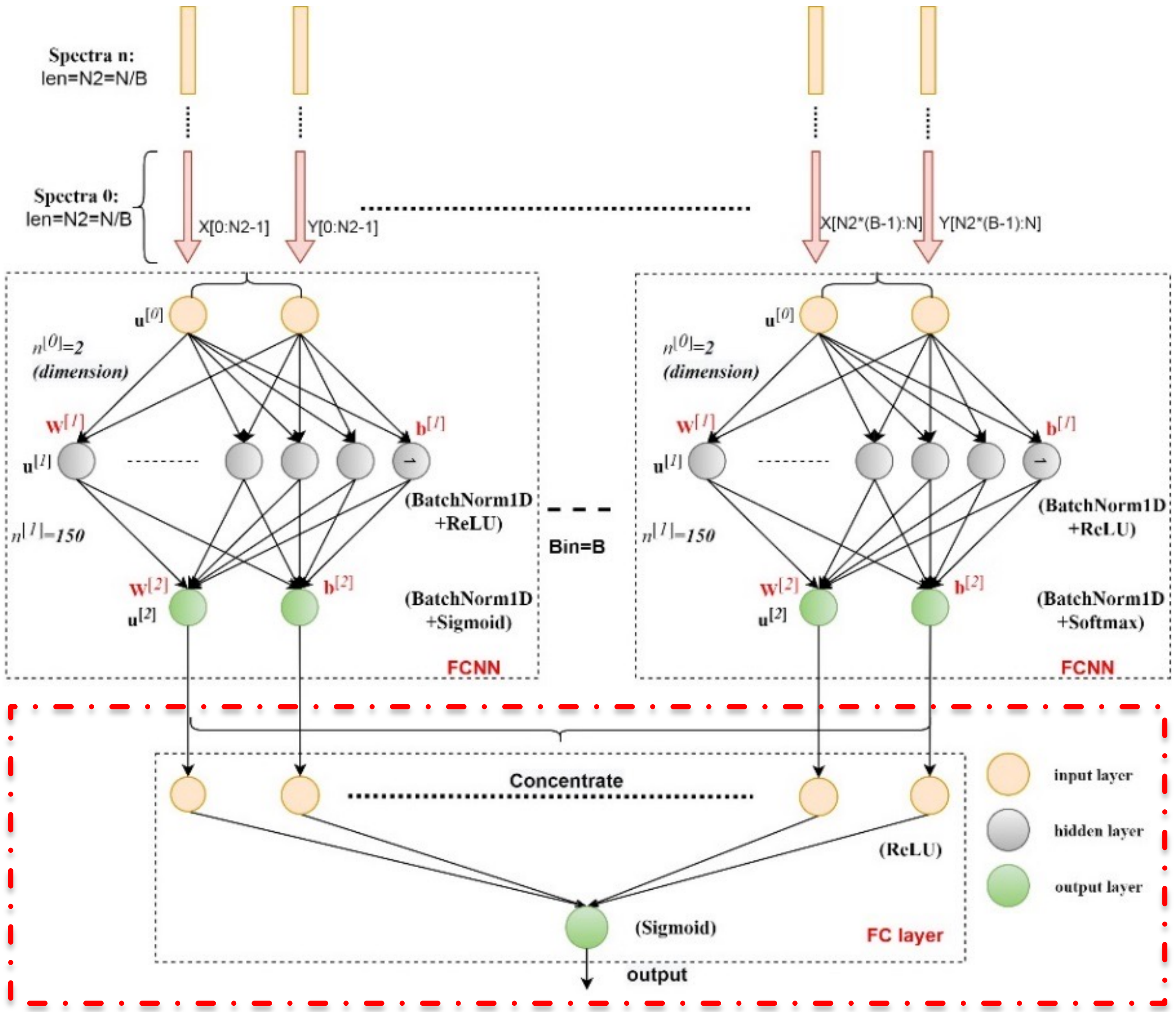
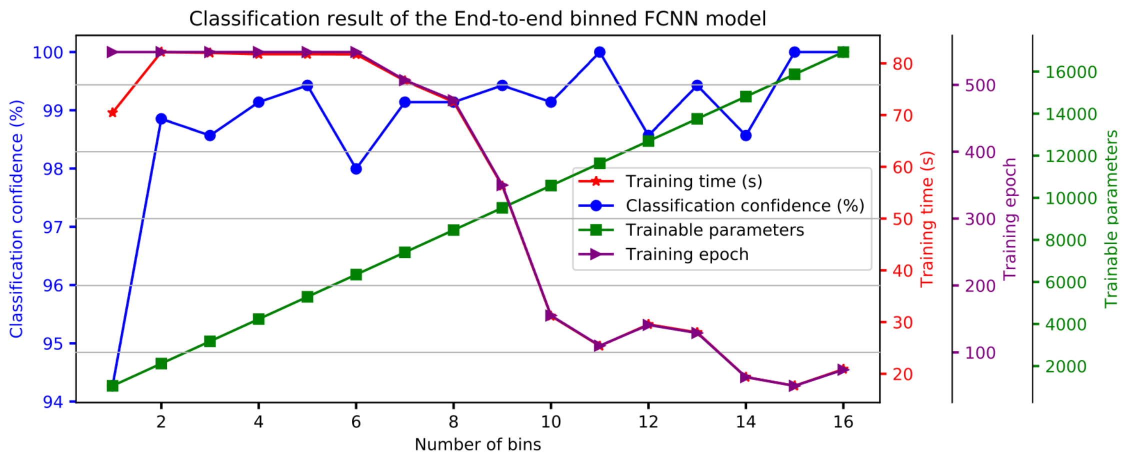
End-to-End FCNN with automatically capturing weighting factors model



End-to-end FCNN with automatically capturing weighting factors model

Classification results under different number of bins:



As the number of bins increases:

Classification confidence increases;

Trainable parameters increase linearly;

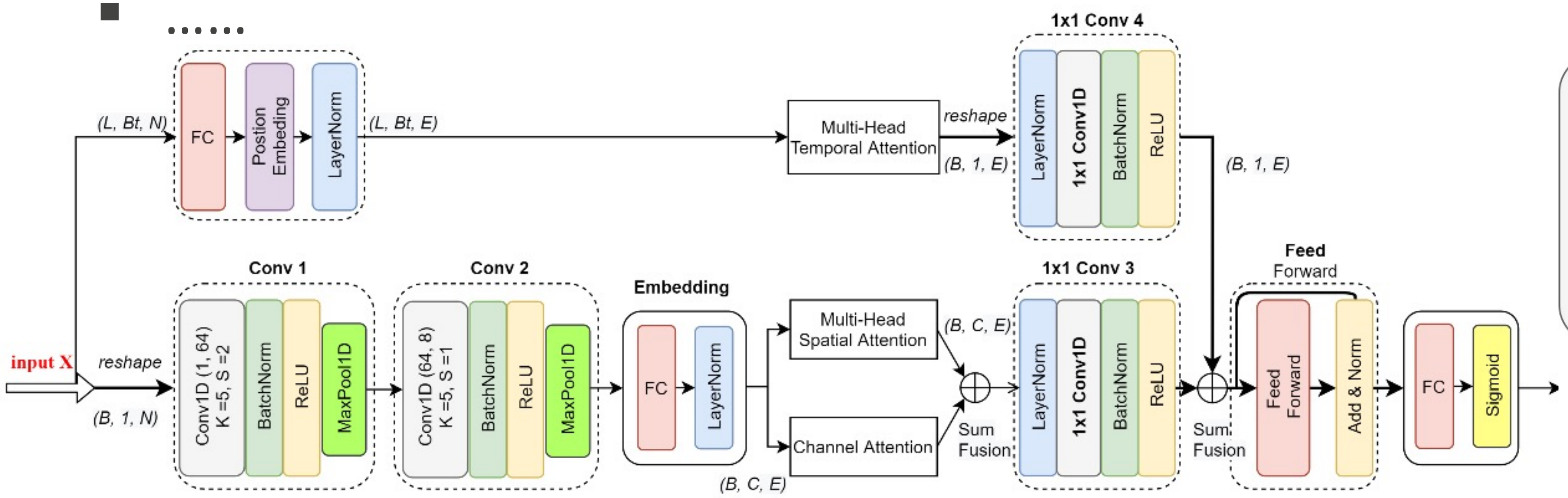
Training epochs decreases;

Training time decreases.

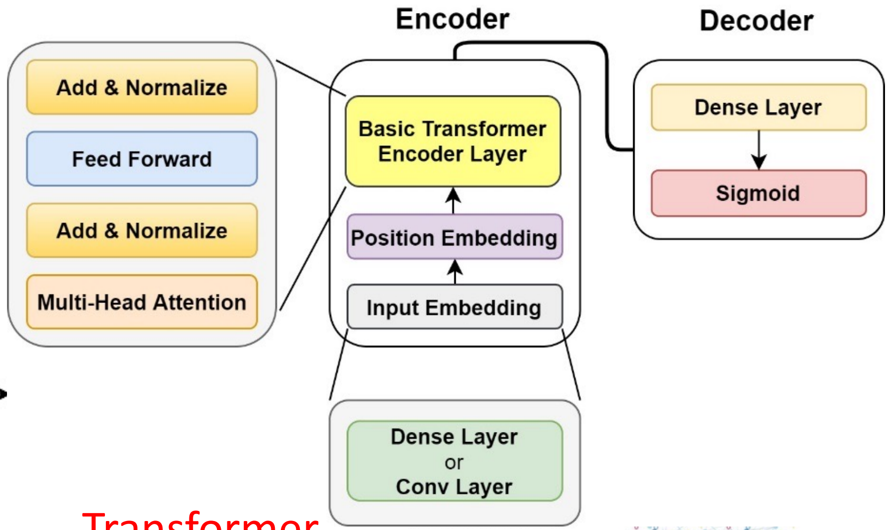
Other classification models

Under the setting of 1D spectral time series classification:

- 1D Fully Connected NN (FCNN)
- Convolutional Neural Network (CNN) solution, ResNets solution
- LSTM-based solution
- Transformer-based solution
- CNN+Multi-head Attention
- ……



CNN+Attention



Transformer

Conclusion and Perspectives

- The process of selecting/creating the training set is still limited, because the data is not properly annotated and some key information (such as the pressure value for each diffractogram) is missing.
- Appropriate NeXus Application Definitions needs to be developed.
- PaN portal is enabling 'FAIR' principle:
  - Data search;
  - Download / Data Analysis and Visualization cloud environment;
  - Automatic data interpretation via NeXus ontologies for
    - interoperability, and
    - reusability

Thank you

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