Machine-learning aided image recognition and tagging

Ronald Lashley[1], Bo Sun[1], Dantong Yu[2]

[1] Department of Computer Science, Lincoln University, Lincoln University, PA, 19352, USA
[2] Computational Science Initiative, Brookhaven National Laboratory, Upton, NY, 11973, USA

ABSTRACT

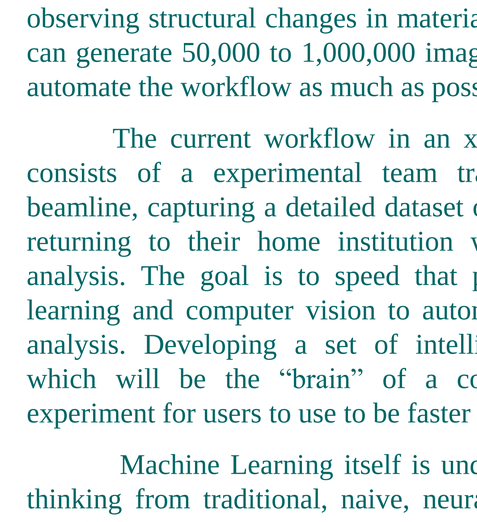
In technology, image recognition software uses various methods to extract information from an image. Seeking to deliver a data analysis pipeline for x-ray synchrotron instruments to assist more ambitious materials discovery experiments, we aimed to build automated analysis pipelines for extracting scientifically meaningful insights from datasets relevant to materials discovery, especially x-ray scattering images. Because users are unfamiliar with the underneath machine learning toolkit, which requires configuring many parameters, developing a graphical interface will greatly improve the usability of machine learning. Previously, the method for image tagging required the use of command line. By introducing a simple button click, allowing users to choose options, run machine learning tools, visually inspect the results, and automatically generate configuration files. Proposing a transformative new paradigm for scientific research , where data analysis tasks (such as pre-process image, extracting features, and tagging image) are massively automated, will thereby liberate scientists to focus on deep scientific questions. This vision can only be realized through a deep integration of machine-learning procedures into all aspects of data interactions. By eliminating the friction inherent in data analysis and pattern recognition, this development will accelerate science discoveries by shorting time to analyze the data with it being automated now. The tag file (.xml) will be stored together with each image. The downstream pipeline relies on this tag information to perform further analysis, such as navigating through all images, searching images with semantic features (tags). All tag information can be used to create an accurate estimation of the distributions of physics property. Users only need to do a few experiment to obtain the optimal solution. From this project, I have gained valuable experience learning and utilizing Python in applications such as Anaconda Navigator, Python IDLE, and QT Designer.

INTRODUCTION

X-ray scattering is a powerful technique for probing the physical structure of materials at the molecular and nanoscale, where strong X-ray beams are shined through a material to learn about its structure at the molecular level. This can be used in a wide variety of applications, from determining protein structure to observing structural changes in materials. Modern x-ray detectors can generate 50,000 to 1,000,000 images/ day, thus it's crucial to automate the workflow as much as possible.

The current workflow in an x-ray scattering experiment consists of a experimental team traveling to a synchrotron beamline, capturing a detailed dataset over several days, and then returning to their home institution with the images for later analysis. The goal is to speed that process up using machine learning and computer vision to automate the process of image analysis. Developing a set of intelligent automated methods, which will be the "brain" of a computer-directed beamline experiment for users to use to be faster and more efficient.

Machine Learning itself is undergoing a shift, with a re-thinking from traditional, naive, neural networks, towards deep learning models where the neural hierarchy is more rational, optimized, and informative. This has already led to clear advances in several fields including computer vision and speech recognition, and we aim to demonstrate similarly transformative gains with respect to scientific image streams. The core idea in deep learning is to design multiple levels of representations corresponding to a hierarchy of features, wherein the high-level concepts and knowledge are derived from the lower layers.



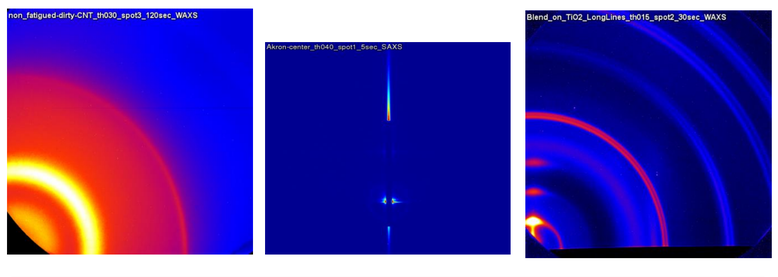
These methods will be used in real-time to extract hierarchical and physically-meaningful insights from scientific datasets collected at NSLS-II beamlines:

1) Low-level: identifying characteristic features in a diffraction image;
2) Intermediate-level: detecting the occurrence of a physical process from a sequence of images; and
3) High-level: learning and predicting scientifically-meaningful trends.

METHODS

The Graphical User Interface has four buttons and a combo box for the user to use. The combo box allows the user to choose which tag they would like to use for the images. The load button allows the user to select a directory of images and scan the record to determine which images have the current tag selected. With this being done in the background, up front, the images with the current tag are displayed in the left panel and the images that do not have that attribute are displayed in the right panel. The predict button triggers the automated analysis tasks (pre-process image, extracting features, and tagging images) allowing the scientist to focus on deep scientific questions. The save button allows the user to save a tag file as a .xml that will be stored with each image. The downstream pipeline relies on this tag information to perform This only needs the user to do a few experiments to obtain optimal solution.

For machine-learning, there are two types of datasets that are used. The first is real dataset, which is collected by shining powerful x-rays through a particular material and the attribute is labeled by material experts. The second type dataset is synthetic scattering dataset, where the data is generated by simulation software. The simulation software is able to synthetic scattered images based on physics laws. Tags can include a diverse selection of images, which makes classification of x-ray scattering images difficult.

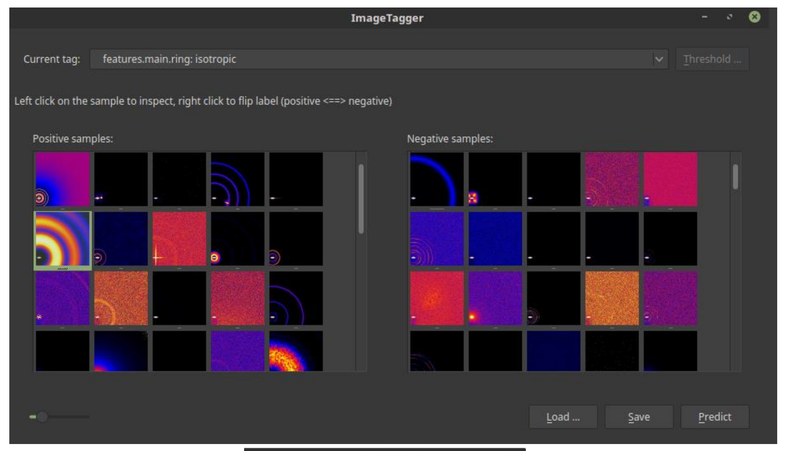


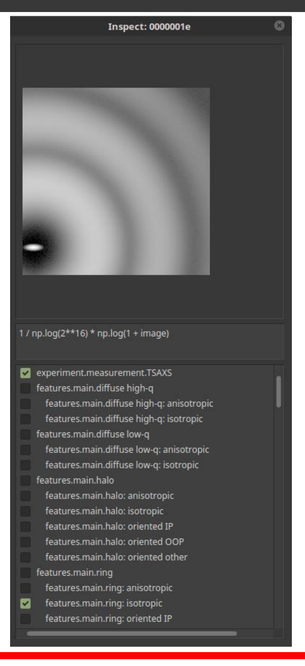
Example of false color images with the "Ring" tag. Tags can include a diverse selection of images, which makes classification of x-ray scattering images difficult

Attribute	#	Attribute	#
Thin film [G5]	1646	Silicon [G7]	130
Specular rod [G3]	1597	GTSAXS [G1]	127
Beam off image[G2]	1591	MWCNT [G7]	125
Photonics CCD[G2]	1591	Nanoporous [G5]	125
Ordered [G5]	1462	Theta sweep [G1]	109
GIWAXS [G1]	1439	PDMS [G7]	107
MarCCD [G2]	1241	Saturation artifacts [G3]	97
Horizon[G4]	1171	Peaks: Line z [G4]	90
Linear beamstop [G2]	1156	Circular beamstop [G2]	85
Peaks: Isolated[G4]	1099	Peaks: Line xy [G4]	79
GISAXS[G1]	870	Diffuse low-q: Anisotropic [G4]	78
Ring: Oriented z [G4]	856	Many rings [G4]	78
Polymer [G6]	821	Diffuse low-q: Oriented z [G4]	76
Halo: Isotropic [G4]	791	Misaligned [G3]	76
Ring: Isotropic [G4]	604	Beam streaking [G3]	70
Ring: Textured [G4]	528	Diffuse low-q: Oriented xy [G4]	69
Higher orders: 2 to 3 [G4]	513	Blocked [G3]	62
P3HT [G7]	505	Diffuse specular rod [G4]	62
Ring: Oriented xy [G4]	491	Smeared horizon [G4]	55
SiO2 [G7]	467	Symmetry ring: 4-fold [G4]	55
Vertical streaks [G4]	434	Higher orders: 10 to 20 [G4]	53
Single crystal [G5]	430	Ring doubling [G4]	53
Block-copolymer [G6]	416	Halo: Anisotropic [G4]	46
Peaks: Many/field [G4]	396	Powder [G5]	44
Grating [G5]	375	Specular rod peaks [G4]	41
PCBM [G7]	369	AgBH [G7]	40
Diffuse high-q: Isotropic [G4]	357	Ring: Oriented other [G4]	33
Higher orders: 4 to 6 [G4]	351	Peaks: Line [G4]	23
Weak scattering [G3]	318	Diffuse high-q: Oriented z [G4]	20
Rubrene [G7]	266	Bad beam shape [G3]	19
TSAXS [G1]	264	LaB6 [G7]	16
Higher orders: 7 to 10 [G4]	260	Phi sweep [G1]	16
2D detector obstruction [G3]	224	Peak doubling [G4]	15
Bragg rods [G4]	211	Halo: Oriented xy [G4]	14
Ring: Anisotropic [G4]	205	Polycrystalline [G5]	14
Peaks: Along ring [G4]	201	Diffuse high-q: Oriented xy [G4]	11
Amorphous [G5]	197	Direct [G3]	11
Saturation [G2]	193	Object obstruction [G3]	9
PS-PMMA [G7]	190	Peaks: Line other [G4]	9
Composite [G5]	179	Waveguide streaks [G4]	8
Diffuse low-q: Isotropic [G4]	170	Higher orders: 20 or more [G4]	4
Yoneda [G4]	167	Substrate streaks/Kikuchi [G4]	4
Strong scattering [G3]	159	Diffuse low-q: Oriented other [G4]	3
TWAXS [G1]	152	Halo: Spotted [G4]	3
Halo: Oriented z [G4]	148	Diffuse low-q: Spotted [G4]	2
High background [G4]	142	Diffuse high-q: Spotted [G4]	1
Asymmetric (left/right) [G2]	138	Empty cell [G3]	1
Ring: Spotted [G4]	136	Parasitic slit scattering [G3]	1
Superlattice [G6]	136	Point detector obstruction [G3]	1

List of the 104 tags used in this experiment

Graphical User Interface for image tagging. A simple button click, allowing users to choose options, run machine learning tools, visually inspect the results, and automatically generate configuration files.





CONCLUSIONS

In this work, we addressed the development of a graphical user interface that is simple for an experimenter that is unfamiliar with the underneath machine learning toolkit which requires configuring parameters. Previously being required to use command line clients to tag image files and having to manually inspect each image, and use editor to inspect the corresponding tag file, users can now use a GUI to choose options, run machine learning tools, visually inspect the results, and automatically generate configuration files.

Experimenters can now maximize their beam time by focusing on deep scientific questions and not having to travel back and forth to the synchrotron beam line to interact with the data of the images. This elimination of friction inherited in data analysis and pattern recognition, this development will accelerate science discoveries.

Machine-learning will continue to improve and grow therefore requiring the GUI to be flexible. The GUI being flexible allows changes to be made without having to make a new one.

ACKNOWLEDGEMENT

"This project was supported in part by the National Science Foundation, Louis Stokes Alliance(s) for Minority Participation (LSAMP) at Lincoln University of Pennsylvania under the LSAMP Internship Program at Brookhaven National Laboratory." I wish to thank my host, Dr. Dantong Yu, for his professionalism and generosity during the NSF program. I also wish to thank my visiting faculty member and mentor, Dr. Bo Sun, for the support and adding me to her team. Further, I would express my gratitude to the Office of Science Education Programs, and all who continue to so willingly assist interns in that branch. I very much appreciate the efforts of the National Science Foundation, LSAMP at Lincoln University of Pennsylvania with regard to their support. Finally, I wish to acknowledge the hospitality and kindness of Brookhaven National Laboratory and the Department of Energy.