

Deep Networks for Imaging: Applications towards Automated Experiments

Ayana Ghosh

Postdoctoral Research Associate

*Center for Nanophase Materials Sciences & Computational Sciences &
Engineering Division, Oak Ridge National Laboratory, USA*

Acknowledgments: Maxim Ziatdinov, Sergei V. Kalinin

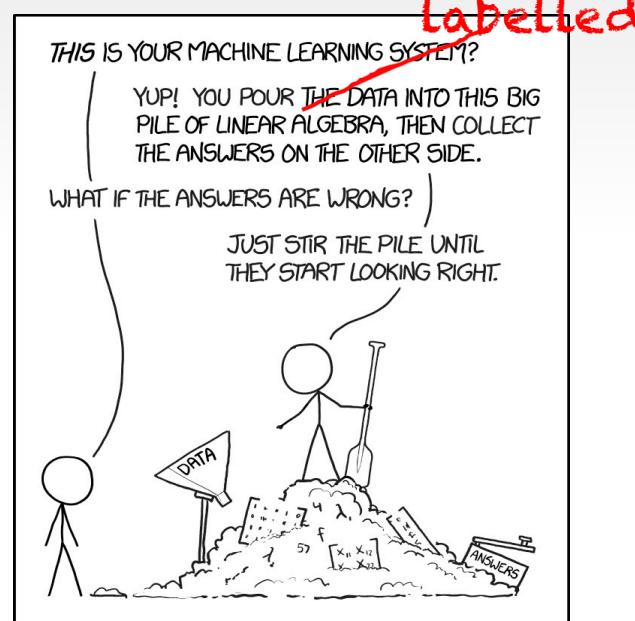
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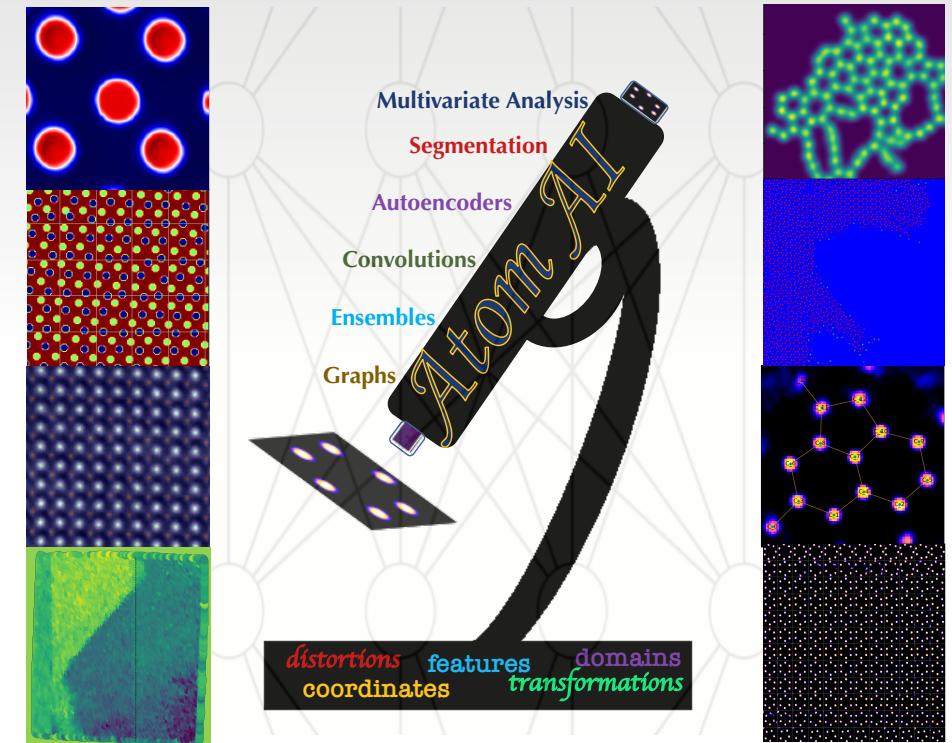
In this presentation...

Introduction to Deep Networks for Imaging

- Traditional Vs. Deep learning
- Usefulness of deep networks
- Working principles
- Semantic segmentation
- Popular deep learning frameworks



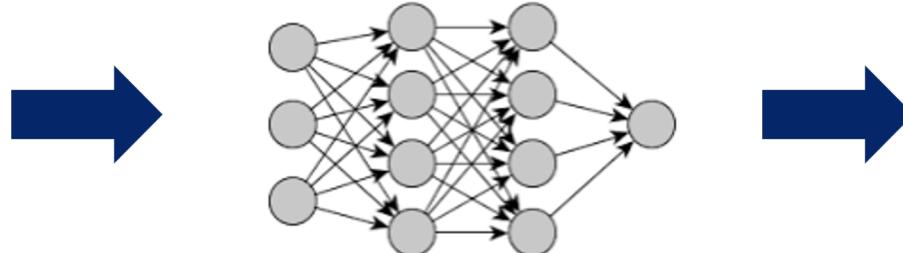
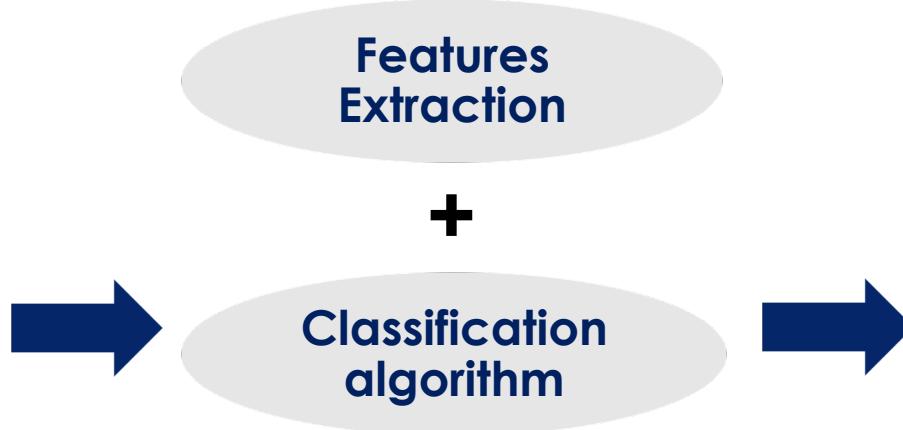
Package we are going to use



Traditional Vs. Deep Learning



Both could be supervised or unsupervised



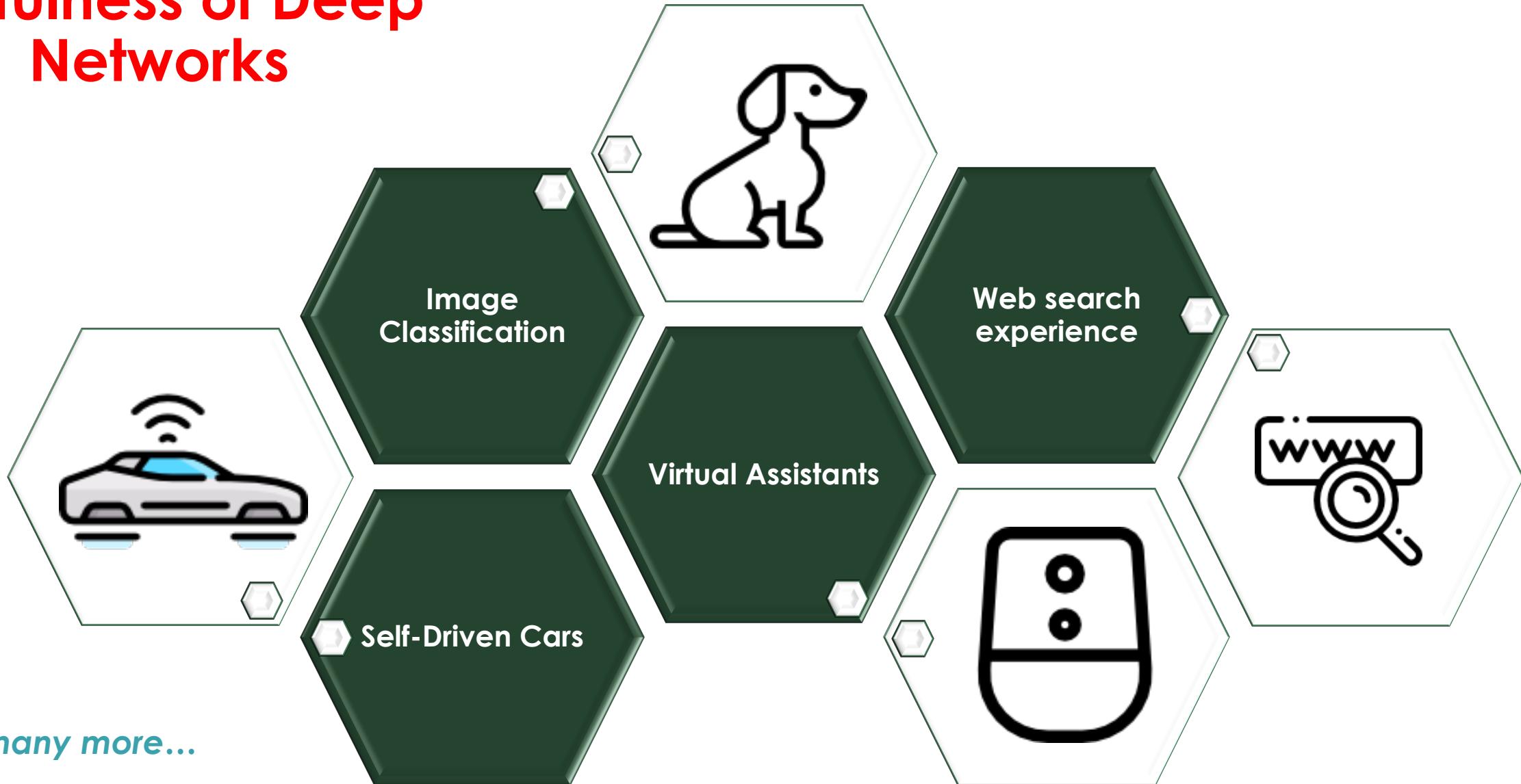
Large number of layers

Small Datasets
Feature Engineering
Interpretability

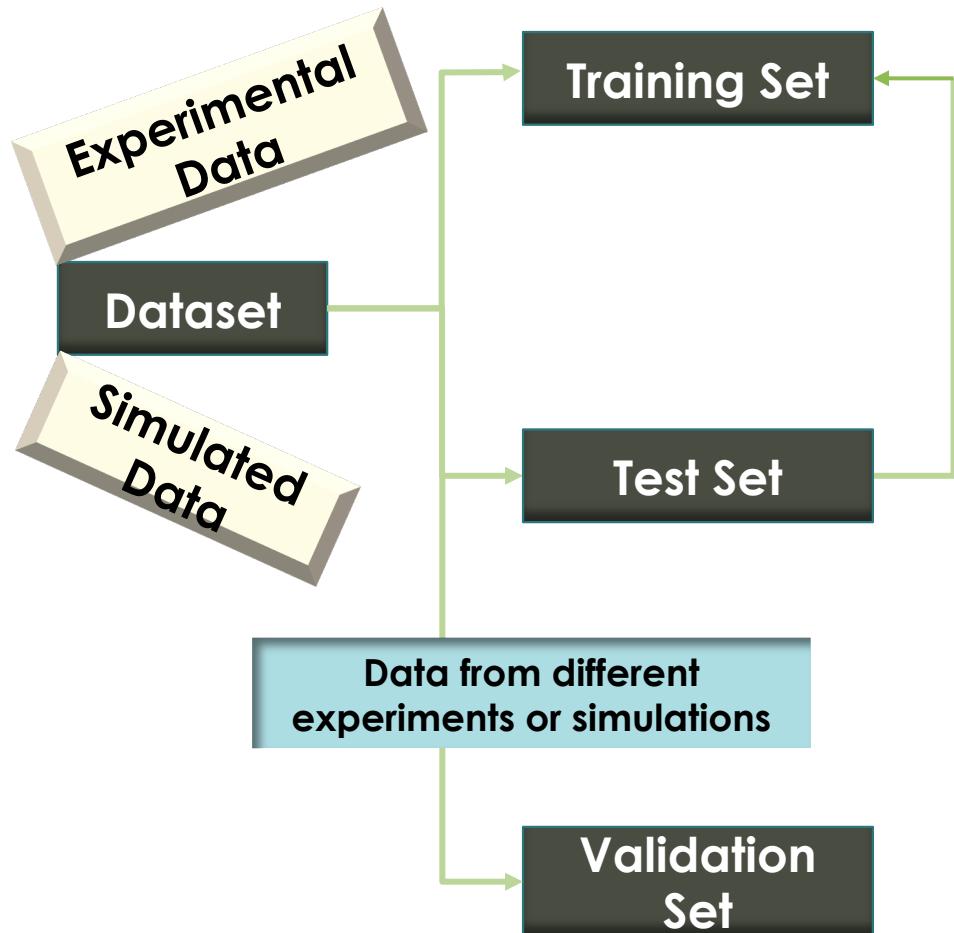


Large Datasets
Avoids the crucial step of feature engineering

Usefulness of Deep Networks



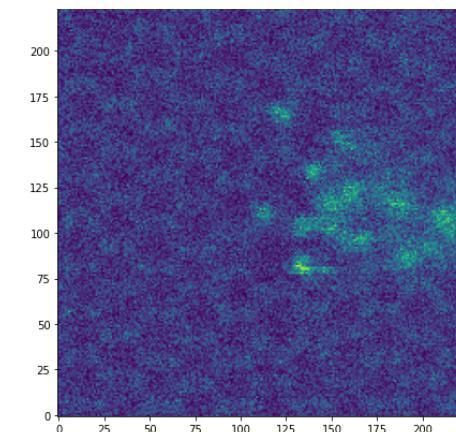
Input data



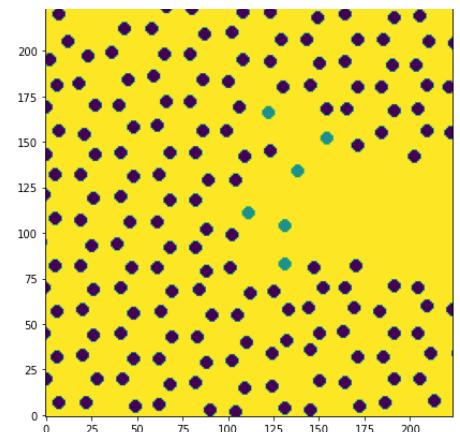
Types of data labels



Image

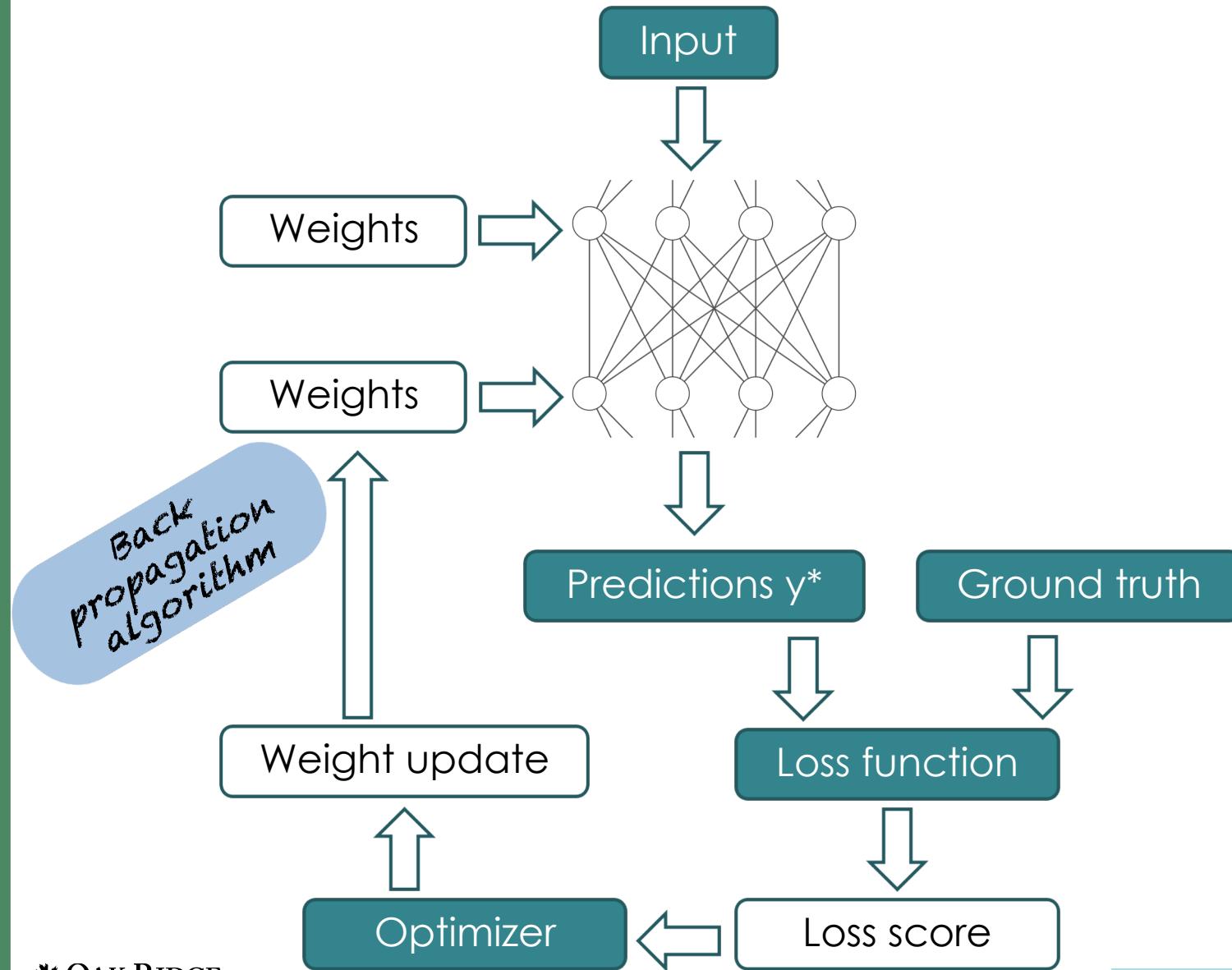


Ground truth



For models constructed on simulated data, it then becomes important to perform experiment-theory matching !

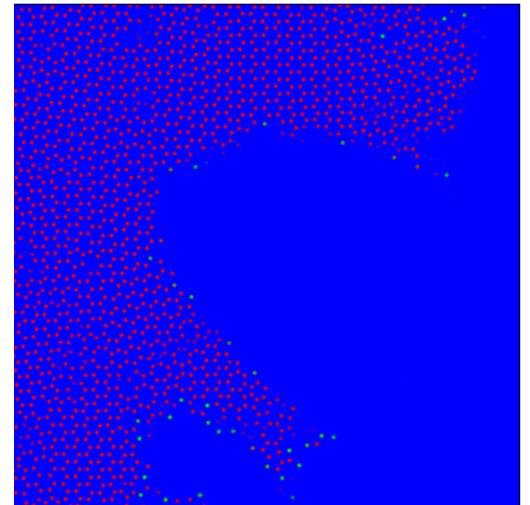
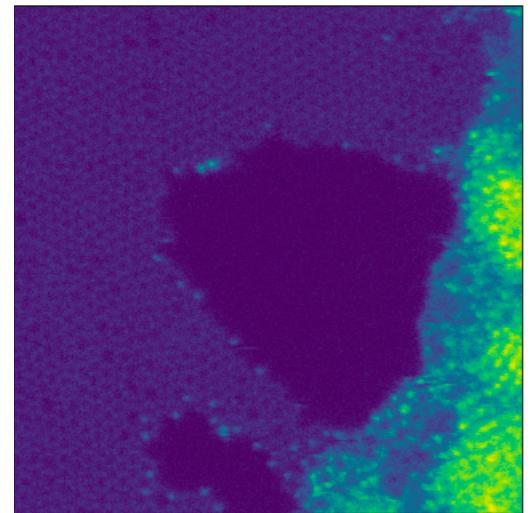
Primary Working Principles



- The network is parameterized by its weights
- A loss function measures the quality of the network's output
- The gradient of the loss is computed for the network's parameters using back propagation algorithm
- The loss score is used as a feedback to adjust the weights

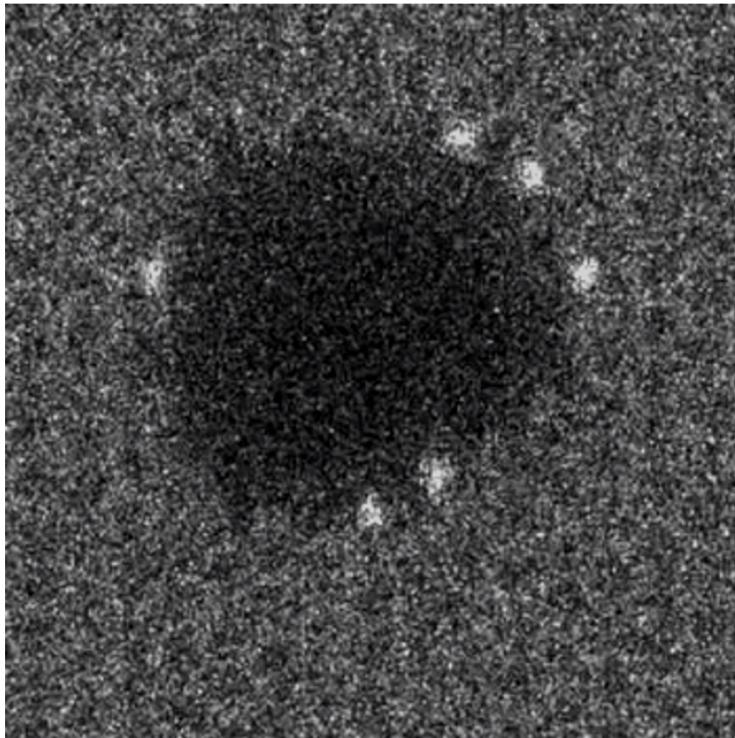
Semantic Segmentation

- Deep learning strategies applied to categorize natural images into different classes, e.g., CIFAR, MNIST datasets
- Each class generally contains thousands of samples with large variability
- Image segmentation: Atom/particle/defect identification in STEM/SPM
 - Find nearly identical objects
 - Significant variations in image acquisition parameters
 - Difficult for a neural network trained on a broad distribution of parameters to recognize subtle features
 - Feature finding is much challenging

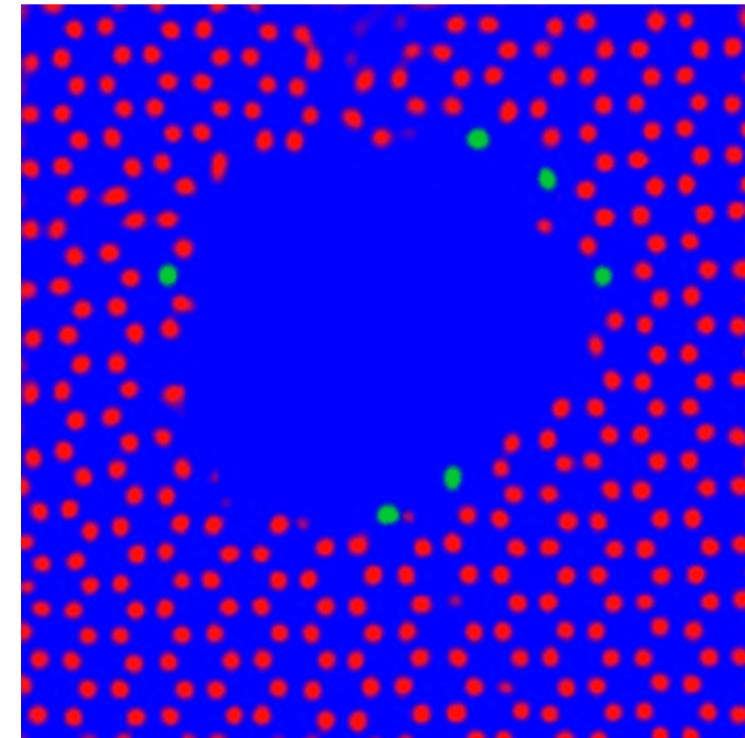


Application to real data: Semantic segmentation of noisy images (“denoising” + atom finding)

Experiment



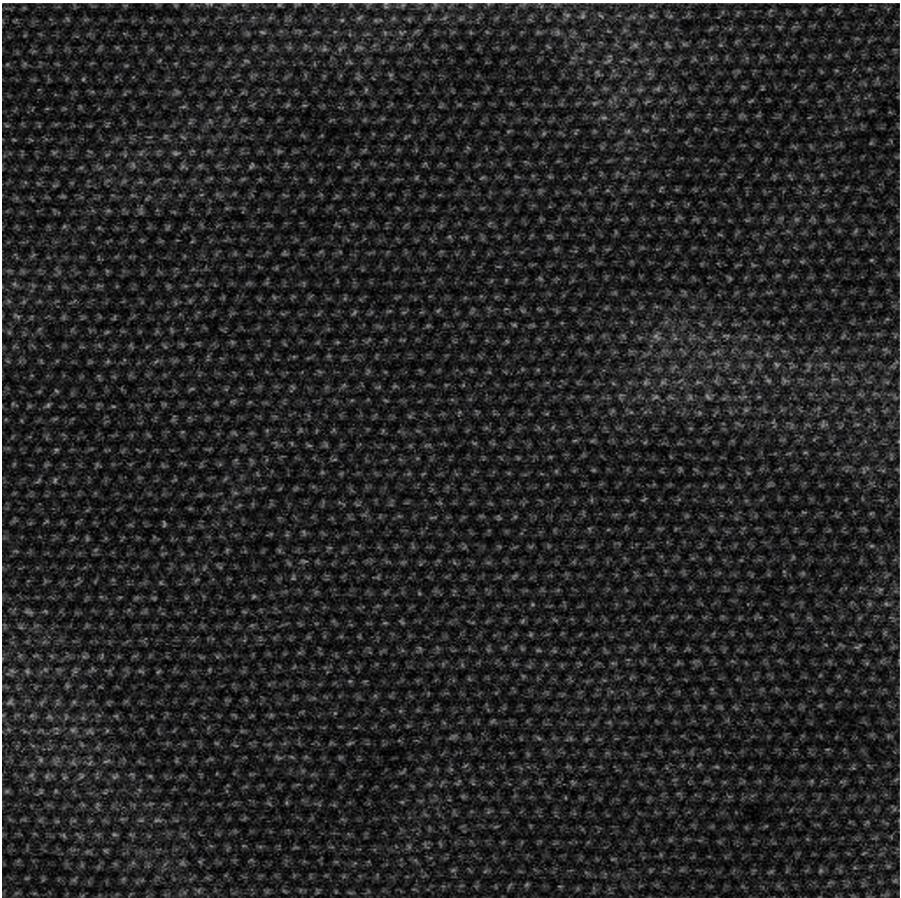
Neural network output



- U-Net-based models typically work well for noisy data
- The neural network accomplishes two goals:
 - Removes noise
 - Separate different atom/defect types into different classes

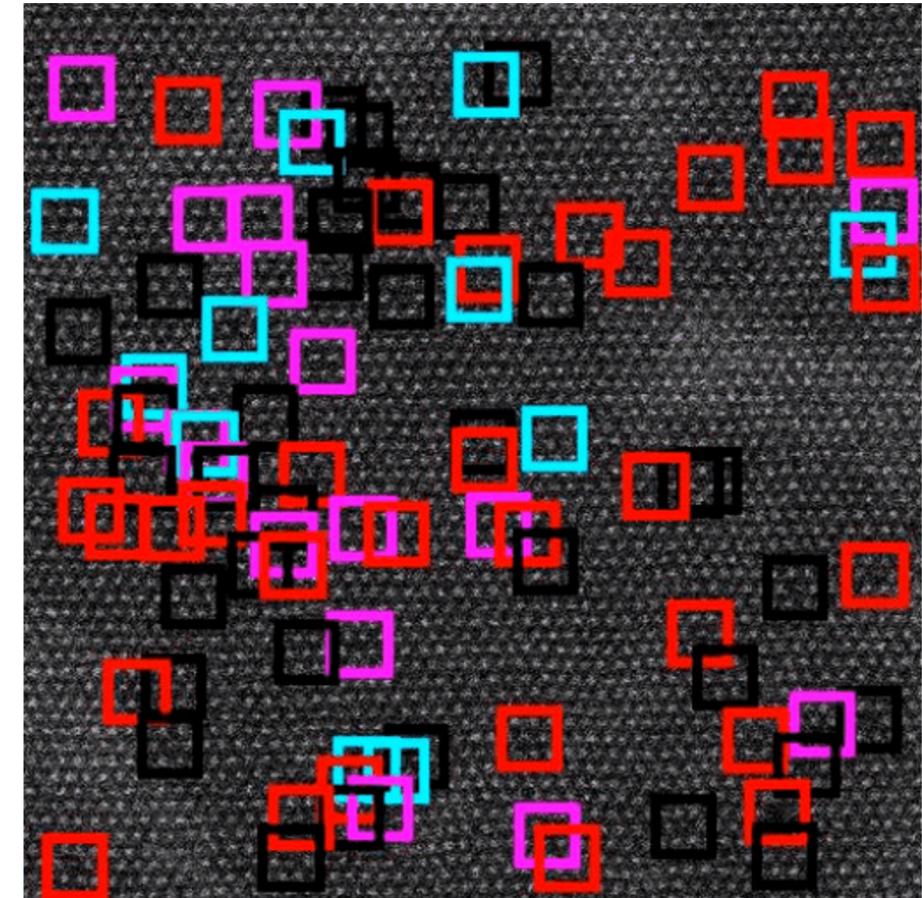
Application to real data: Finding complex defects

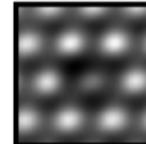
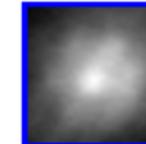
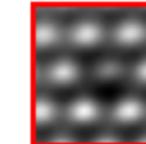
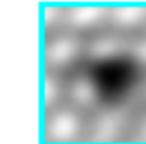
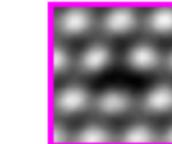
Experimental



Sample: WS2
E-beam energy: 60 kV

Decoded



Class 1 Count: 2078	Class 2 Count: 1055	Class 3 Count: 1687	Class 4 Count: 2123	Class 5 Count: 1166
				

Popular Deep Learning Frameworks

TensorFlow (2.x)

```
# Import tensorflow
import tensorflow as tf

# Define a model
class NNRegressor(tf.keras.Model):
    """2-layer neural network for regression"""
    def __init__(self, nb_neurons):
        """Initialization of model parameters"""
        super(NNRegressor, self).__init__()
        self.layer1 = tf.keras.layers.Dense(nb_neurons)
        self.layer2 = tf.keras.layers.Dense(nb_neurons)
        self.output_layer = tf.keras.layers.Dense(1)
        self.relu = tf.keras.activations.relu

    def call(self, x):
        """Forward path"""
        l1 = self.relu(self.layer1(x))
        l2 = self.relu(self.layer2(l1))
        return self.output_layer(l2)

# Initialize model
model = NNRegressor(nb_neurons=100)

# Specify weights optimizer and loss function (criterion)
optimizer = tf.keras.optimizers.Adam(learning_rate=5e-4)
criterion = tf.keras.losses.MeanSquaredError()
```

PyTorch

```
# Import pytorch
import torch

# Define a model
class NNRegressor(torch.nn.Module):
    """2-layer neural network for regression"""
    def __init__(self, nb_neurons):
        """Initialization of model parameters"""
        super(NNRegressor, self).__init__()
        self.layer1 = torch.nn.Linear(1, nb_neurons)
        self.layer2 = torch.nn.Linear(nb_neurons, nb_neurons)
        self.output_layer = torch.nn.Linear(nb_neurons, 1)
        self.lrelu = torch.nn.functional.leaky_relu

    def forward(self, x):
        """Forward path"""
        l1 = self.lrelu(self.layer1(x))
        l2 = self.lrelu(self.layer2(l1))
        return self.output_layer(l2)

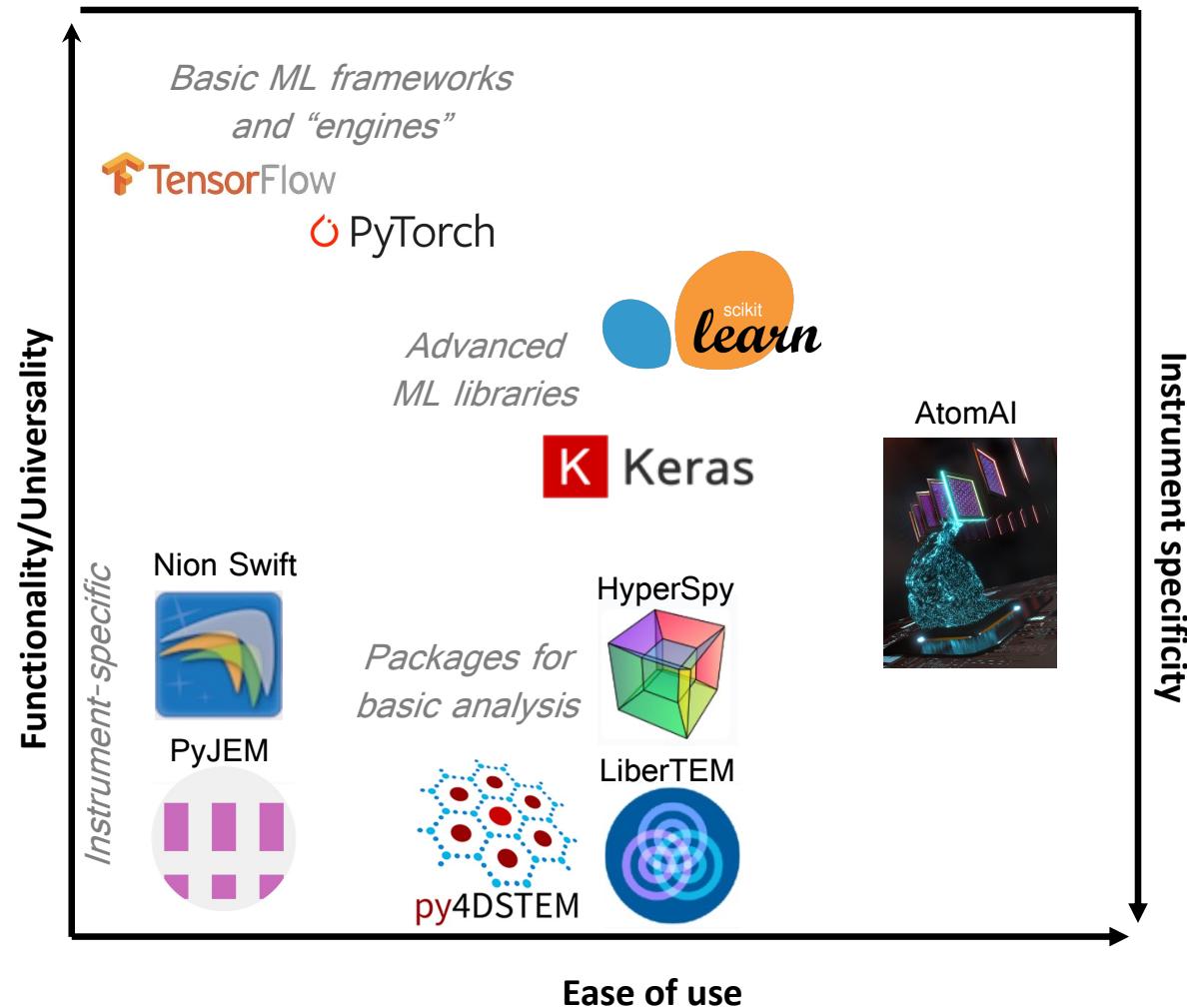
# Initialize model
model = NNRegressor(nb_neurons=100)

# Specify weights optimizer and loss function (criterion)
optimizer = torch.optim.Adam(model.parameters(), lr=5e-4)
criterion = torch.nn.MSELoss()
```

AtomAI: Microscopic Images to Atomistic Simulations to Learning and Discovering Physics

- Python-based infrastructure bridging instruments and HPC
- Microscopic and mesoscopic data analysis and beyond
- Neural Networks and other machine learning methods

<https://arxiv.org/abs/2105.07485>



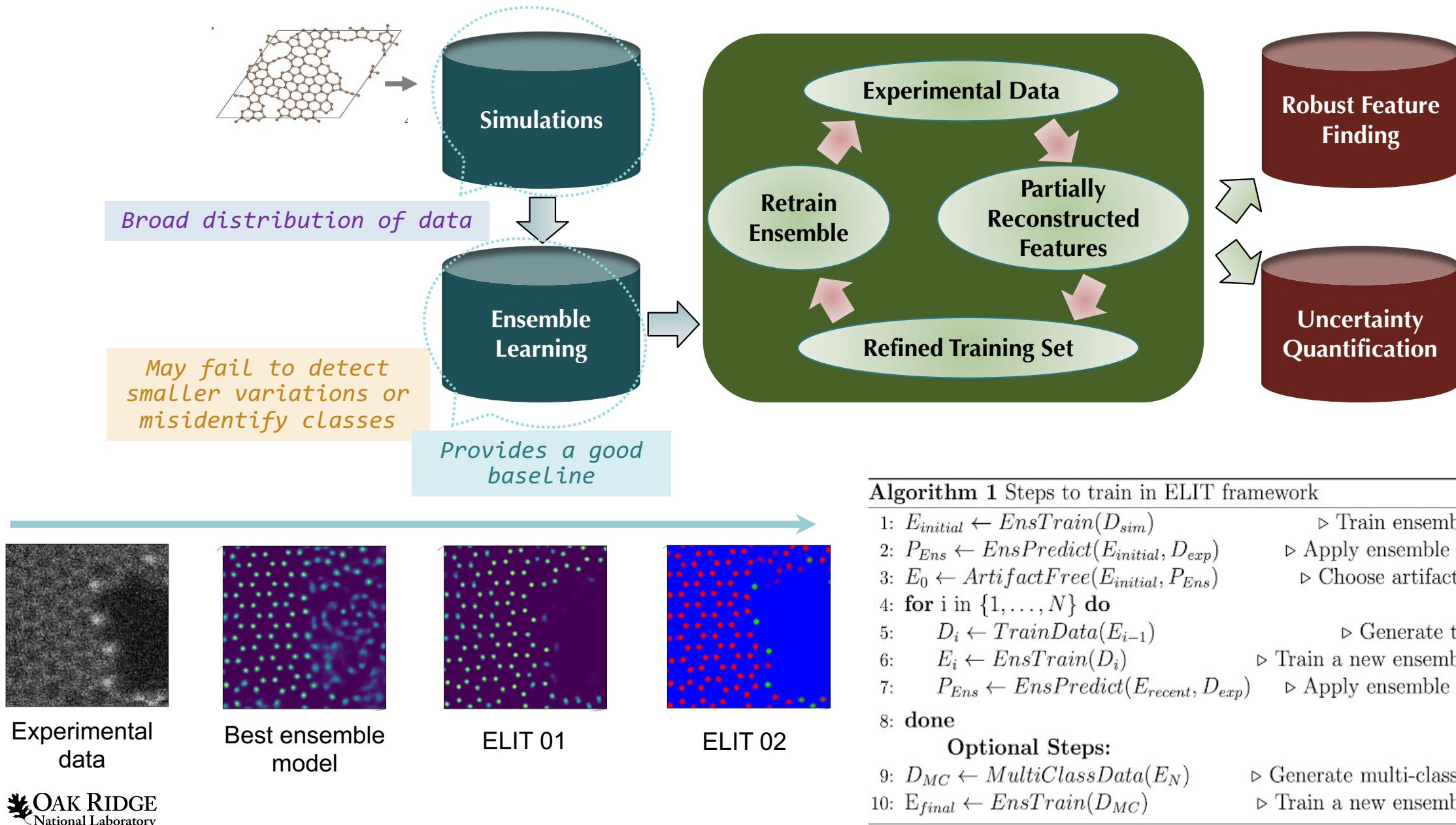
AtomAI: Extensive List of Interactive Examples & Tutorials

Quickstart: AtomAI in the Cloud

The easiest way to start using AtomAI is via [Google Colab](#), which is a free research tool from Google for machine learning education and research built on top of Jupyter Notebook. The following notebooks can be executed in Google Colab by simply clicking on "Open in Colab" icon:

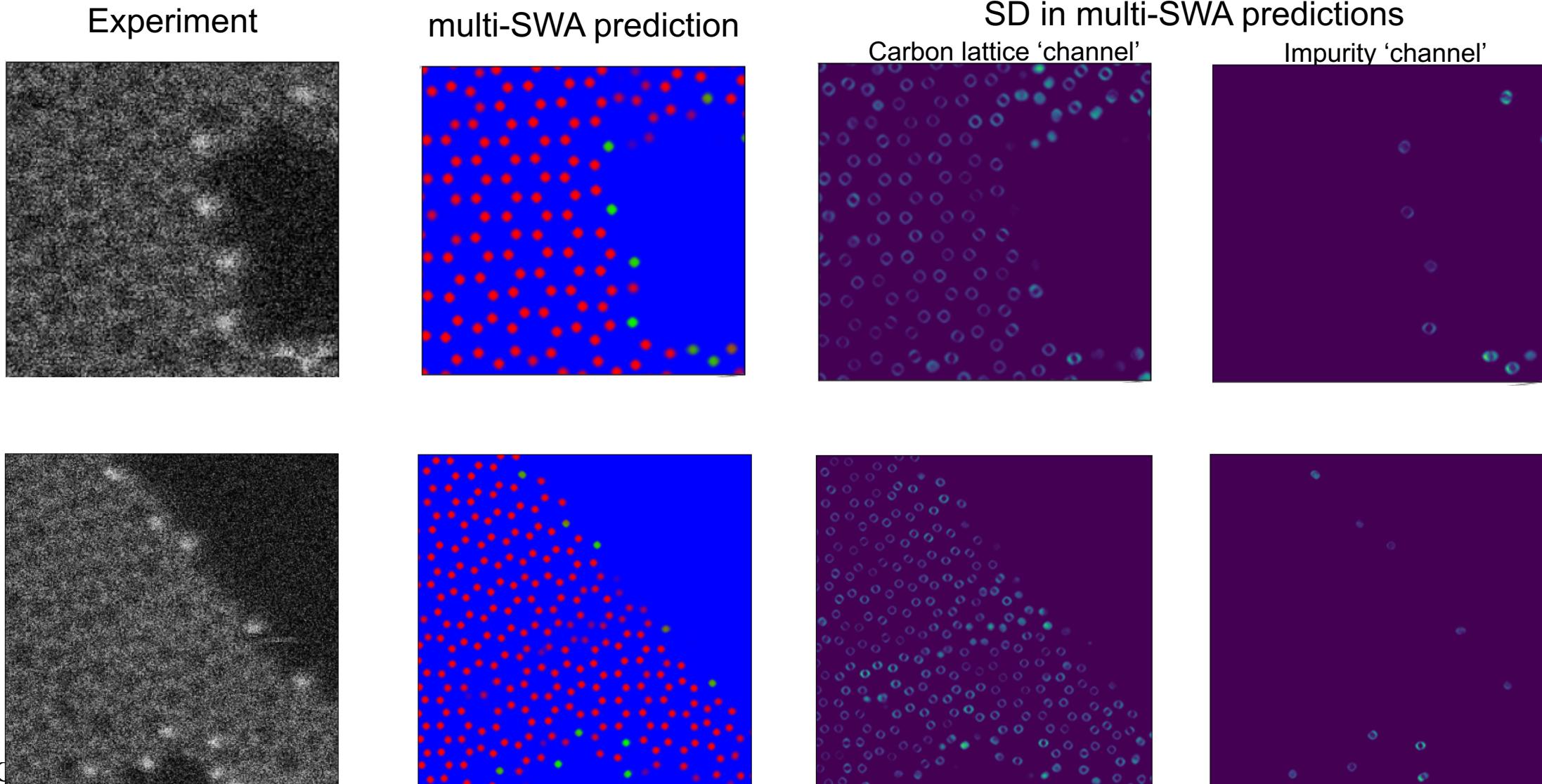
- 1) Train a Deep Fully Convolutional Neural Network for Atom Finding [!\[\]\(f0fdb60b777eb11b66cba545acf146fa_img.jpg\) Open in Colab](#)
- 2) Multivariate Statistical Analysis of Distortion Domains in a Single Atomic Image [!\[\]\(3081bcc7c327f2189a2e87fbbfba0d83_img.jpg\) Open in Colab](#)
- 3) Variational Autoencoders I: Learning Disentangled Representations of Arbitrarily Rotated Handwritten Digits [!\[\]\(e1b24ca8c6cfcc73d77e9423094927ff_img.jpg\) Open in Colab](#)
- 4) Variational Autoencoders II: Simple Analysis of Structural Transformations in Atomic Movies [!\[\]\(a0119c114202c9efb7c4df11970c17bd_img.jpg\) Open in Colab](#)
- 5) Implementation of Custom Image Denoiser in AtomAI [!\[\]\(2054bdb83284824c3f0040a980572239_img.jpg\) Open in Colab](#)
- 6) Prepare Training Data from Experimental Image with Atomic Coordinates [!\[\]\(9a485dbd23c8c9825730d15f14d33e45_img.jpg\) Open in Colab](#)

Ensemble Learning and Iterative Training (ELIT)



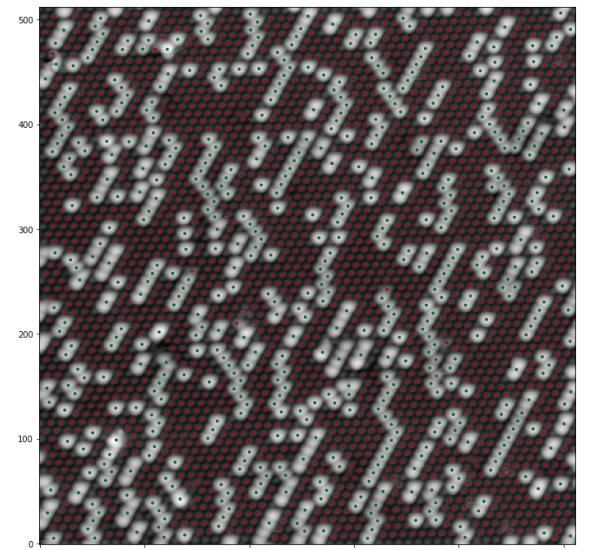
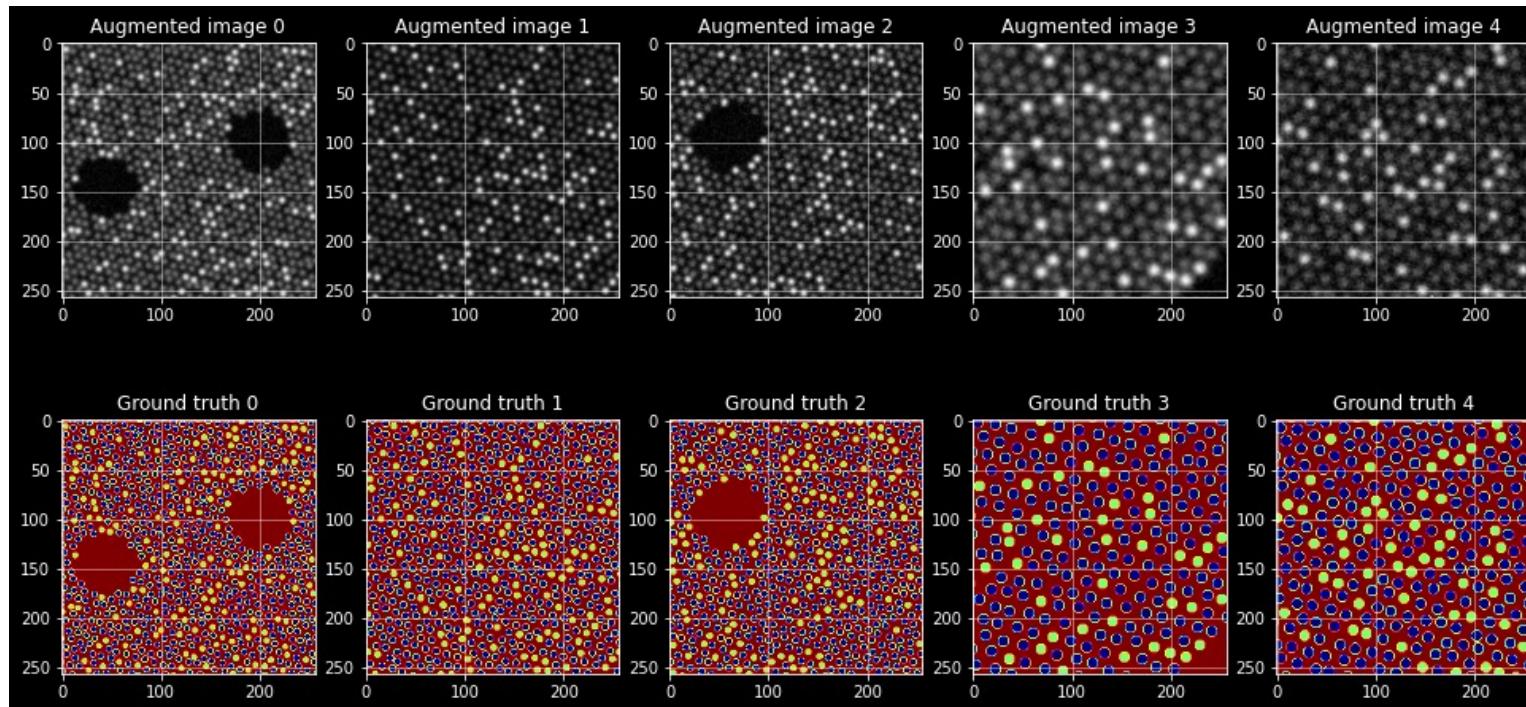
ELIT produces meaningful uncertainty estimates

The shapes in “uncertainty maps” could be associated with specific events (e.g., “unstable” atoms)



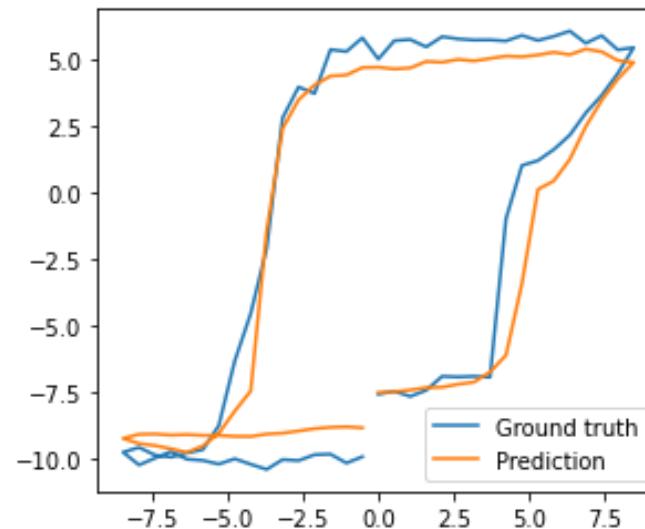
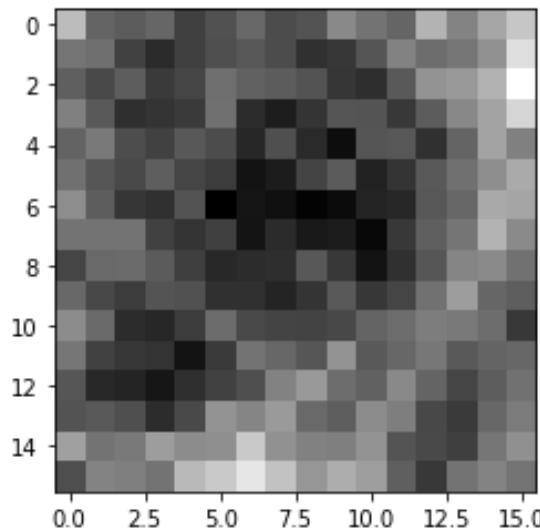
In Today's Tutorials

- Perform semantic segmentation on an STM image
- We use simulated data to train a DL U-Net type of model
- Use that to find atoms, coordinates from the experimental image



In Today's Tutorials

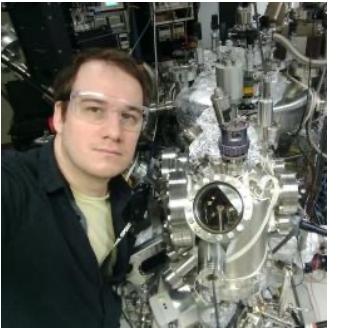
- Predict functional property (spectrum) from input image
- im2spec models
 - Use (2D CNN layers) to embed input images into a latent vector
 - Decoder for generating one-dimensional signals from the embedded features
 - Encoder part consists of three back-to-back two-dimensional convolutional layers
 - Decoder part represents a cascade of one-dimensional dilated convolutions



<https://pubs.acs.org/doi/pdf/10.1021/acsami.0c15085>

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Acknowledgments



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- DOE, Office of Science, Basic Energy Sciences (BES), Materials Sciences and Engineering Division
- Oak Ridge National Laboratory's Center for Nanophase Materials Sciences (CNMS)



Link to Tutorials!

https://github.com/pycroscopy/SPM_ML_School_2021/tree/main/Day01/Notebooks