Tentative lecture plan (May 23, 2023)

**Virtual Summer School: Machine Learning in Electron Microscopy**

Sergei V. Kalinin and Gerd Duscher, University of Tennessee, Knoxville

Maxim Ziatdinov and Rama Vasudevan, Oak Ridge National Laboratory

1. Outline and structure of the course (June 6)
   1. Goals, team, resources
   2. Introduce STEM, SPM, STM
   3. Analysis and automated experiment workflows
   4. Python ecosystem: scikit-learn and scikit-image
   5. Introduce resources: PyCroscopy, AtomAI, GPax
   6. **Colab:** Basic introduction into Python
2. Imaging in Scanning Transmission Electron Microscopy (June 9)
   1. STEM Instrumentation
   2. Physics of STEM
   3. Similarities and Differences between TEM and STEM
   4. Structure of STEM data files
   5. **Colab:** STEM analysis
3. Spectroscopy in STEM (June 13)
   1. Analytical Microscopy
   2. Spectroscopy Methods in STEM: EELS, EDX, CL
   3. **Colab**: STEM Analysis of Spectroscopy Data
4. Linear methods and dimensionality reduction for spectral data (June 16)
   1. Analysis workflow
   2. Supervised regression
   3. PCA, NMF
   4. K-means clustering, GMM, dbscan, UMAP
   5. **Colab:** Analysis of spectroscopic data
5. High-resolution and Z-Contrast Imaging (June 20)
   1. Contrast Transfer Functions in TEM and STEM
   2. Aberrations and Their Corrections
   3. Ronchigram and Electron Probe Shape
   4. Blob-Finders
   5. **Colab:** Ronchigram Simulation
6. Image registration methods (June 23)
   1. Reasons for Image Registration
   2. Rigid and Non-Rigid Registration
   3. Analysis of Distortion and Stress
   4. **Colab:** Image Registration and Analysis
7. Linear methods and dimensionality reduction for imaging data (June 27)
   1. Building descriptors: sliding windows, feature centric, time-delayed
   2. Analysis workflows for images and videos
   3. Case studies for image analysis
   4. **Colab:** Analysis of the imaging and video data
8. Diffraction and 4D STEM (June 30)
   1. Very Basic Crystallography
   2. Indexing Convergent Beam Electron Diffraction (CBED)
   3. Determination of Angles from CBED
   4. Simulation of CBED
   5. Simulation of Z-contrast Imaging and 4D STEM data
   6. **Colab:** Indexing and simulating CBED pattern;
9. Bringing Cloud and Edge to STEM: from tool to ecosystem (Wednesday - July 5)
   1. Cloud, edge, and code ecosystems
   2. Versions and code ecosystems
   3. **Colab:** Using PyCroscopy
10. Image simulations (July 7)
    1. Simulating images, spectra, and 4D STEM
    2. **Colab:** The world of simulations: STEM, SPM, STM
11. Deep convolutional networks (July 11)
    1. What are DCNN
    2. DCNN for segmentation and classification
    3. **Colab:** DCNN for MNIST data
12. DCNN for image data (July 14)
    1. Building the DCNNs: UNet
    2. Ensemble DCNNs
    3. Direct STEM to HPC workflows
    4. DCNN denoising
    5. **Colab:** DCNN atom finding and denoising
13. DCNN case studies (July 18)
    1. UNet
    2. Mask RCNNs
    3. **Colab:** UNet and RCNN
14. Gaussian processes and Bayesian Optimization (July 21)
    1. Gaussian Processes
    2. Bayesian Optimization
    3. **Colab:** GP and BO
15. Bayesian Inference, Structured GP, and Hypothesis Learning (July 25)
    1. LMFIT vs BI
    2. Use cases: spectroscopy
    3. Use case: how good a microscope do we need?
    4. sGP
    5. Hypothesis learning
    6. **Colab:** BI
    7. **Colab:** sGP and hypothesis learning
    8. **Colab:** GP, BO, and HL in 2D
16. Variational Autoencoders – 1 (July 28)
    1. What is VAE
    2. Why invariant VAE
    3. VAE workflows for spectral and structural data
    4. **Colab:** VAE on cards
17. Variational Autoencoders – 2 (August 1)
    1. Joint, conditional, and semisupervised VAE
    2. **Colab:** j, ss, cVAE for cards and spectral data
    3. VAE case studies
    4. Graphene, particles, crystallogrpahy
    5. Colab: VAE on graphene and 4D STEM
18. Encoders-decoders and structure-property relationships (August 4)
    1. Case studies
    2. Colab: im2spec, spe2im
19. Special topic: VAE for any tasks (August 8)
    1. Engineering the loss function
    2. Engineering architecture: dual VAE
    3. Injecting physics
    4. **Colab:** build your own VAE
20. Deep kernel learning: EELS and 4D STEM (August 11)
    1. Deep Kernel Learning introduction
    2. Multichannel DKL
    3. Hypothesis DKL
    4. **Colab**: DKL plasmonics
    5. Deep kernel learning: 4D STEM
    6. **Colab:** DKL 4D STEM
21. DKL forensics and human in the loop (August 15)
    1. Forensic workflow
    2. **Colab:** Forensic workflow STEM-EELS
22. Special topics: Reinforcement learning (August 18)
    1. Reinforcement learning
    2. **Colab:** RL for SPM
23. Special topics: Learning physics form images (August 22)
    1. Learning statistical physics from images
    2. **Colab:** physics from images
24. Special topic: Causality (August 25)
    1. Why causality matters
    2. **Colab:** ANNI and LinGAM