Lecture Data Science for Electron Microscopy Winter 2024

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Abstract

This is the website for the Data Science for Electron Microscopy Lecture

Plain Language Summary

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- Pelz Lab website
- Studon Link

1 Lecture 1: Intro (25.10.2024)

- Introduction
- d2l Chapter 2: Preliminaries

2 Lecture 2: Regression and Sensor Fusion (8.11.2024)

- d2l Chapter 3: Regression
- Sensor Fusion Slides

3 Lecture 3: CNNs (15.11.2024)

- d2l Chapter 7: CNNs
- d2l Chapter 8: CNNs

4 Lecture 4: Classification, Segmentation, AutoEncoders (22.11.2024)

- d2l Chapter 4: Classification
- d2l Chapter 14.9: Segmentation
- Segmentation
- Dimensionality Reduction
  - PCA
  - Autoencoder
  - Variational Autoencoder

5 Miniproject (29.11. - 13.12.2024)

In the miniproject, you will test multiple deep neural network architectures on one of four microscopy-related tasks. You should summarize your results in a short presentation (5 minutes + 2 minutes discussion) and deliver a Jupyter Notebook with your code and results. The miniproject will be graded and will count as 40% towards your final grade.

1. Segmentation Task

   We will use the HRTEM dataset from "A robust synthetic data generation framework for machine learning in high-resolution transmission electron microscopy (HRTEM)" by Rangel DaCosta et al. (2024) to implement a segmentation model. The goal is to segment nanoparticles in HRTEM images.

   Please use the article "A robust synthetic data generation framework for machine learning in high-resolution transmission electron microscopy (HRTEM)" by Rangel DaCosta et al. (2024) as a starting point for your implementation.

   The datast contains pairs of HRTEM images and ground truth segmentations.

2. VAE & Dimensionality Reduction

   We will use the dataset from "Uncovering material deformations via machine learning combined with four-dimensional scanning transmission electron microscopy" by Shi et al. (2022) to implement a dimensionality reduction model and cluster 4DSTEM data.

The goal is to learn a mapping from 4DSTEM data to a lower-dimensional embedding where you can perform clustering to identify different deformation modes.

Please use the article "Uncovering material deformations via machine learning combined with four-dimensional scanning transmission electron microscopy" by Shi et al. (2022) as a starting point for your implementation.

3. Denoising

   We will use the dataset from "Unsupervised deep denoising for four-dimensional scanning transmission electron microscopy" by Sadri et al. (2024) to implement a denoising model for 4DSTEM data.

   The goal is to learn a mapping from noisy to clean 4DSTEM data.

   Please use the article "Unsupervised deep denoising for four-dimensional scanning transmission electron microscopy" by Sadri et al. (2024) as a starting point for your implementation.

   The article contains pytorch code for the model.

   Learn how to adapt it to your needs and try to replicate the results on the SrTiO3_High_mag_Low_dose.npy and SrTiO3_High_mag_High_dose.npy datasets.

4. Image-to-Image Translation

   We will use a simulated X-ray image dataset with pairs of projected thickness and phase contrast images to implement an Image to image translation model.

   The goal is to learn a mapping from phase contrast images to projected thickness images.

   This is usually a task that is solved with multiple measurements and a physical model of the imaging process.

   Here we will try to learn this mapping from simulated data. Please use the article "Multi-resolution convolutional neural networks for inverse problems" by Wang et al. (2020) as a starting point for your implementation.

6 Lecture 5: Mixed Bag (10.1.2025)

- Project presentation
- Generative Adversarial Networks
- Gaussian Processes 1

7 Lecture 6: Gaussian Processes Introduction (17.1.2025)

- Introduction to Gaussian Processes

8 Lecture 7: Gaussian Processes Applications (24.1.2025)

- Bayesian Optimization
- Active Learning
- Deep Kernel Learning

9 Lecture 8: Inverse Imaging Problems 1: Linear Problems (31.1.2025)

- Algorithms for linear inverse problems
- Tomography
- Deconvolution

10 Lecture 9: Inverse Imaging Problems 2: Nonlinear Problems (7.2.2025)

- Phase Contrast Imaging

- Superresolution Imaging
- Inverse Problems in Electron Microscopy

References

Rangel DaCosta, L., Sytwu, K., Groschner, C., & Scott, M. (2024). A robust synthetic data generation framework for machine learning in high-resolution transmission electron microscopy (HRTEM). *Npj Computational Materials*, *10*(1), 165.

Sadri, A., Petersen, T. C., Terzoudis-Lumsden, E. W., Esser, B. D., Etheridge, J., & Findlay, S. D. (2024). Unsupervised deep denoising for four-dimensional scanning transmission electron microscopy. *Npj Computational Materials*, *10*(1), 243.

Shi, C., Cao, M. C., Rehn, S. M., Bae, S.-H., Kim, J., Jones, M. R., et al. (2022). Uncovering material deformations via machine learning combined with four-dimensional scanning transmission electron microscopy. *Npj Computational Materials*, *8*(1), 114.

Wang, F., Eljarrat, A., Müller, J., Henninen, T. R., Erni, R., & Koch, C. T. (2020). Multi-resolution convolutional neural networks for inverse problems. *Scientific Reports*, *10*(1), 5730.