Machine Learning Fundamentals for Microstructural Analysis

June 2 – 7, 2024

Columbia University, New York, NY

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The Fu Foundation School of Engineering and Applied Science

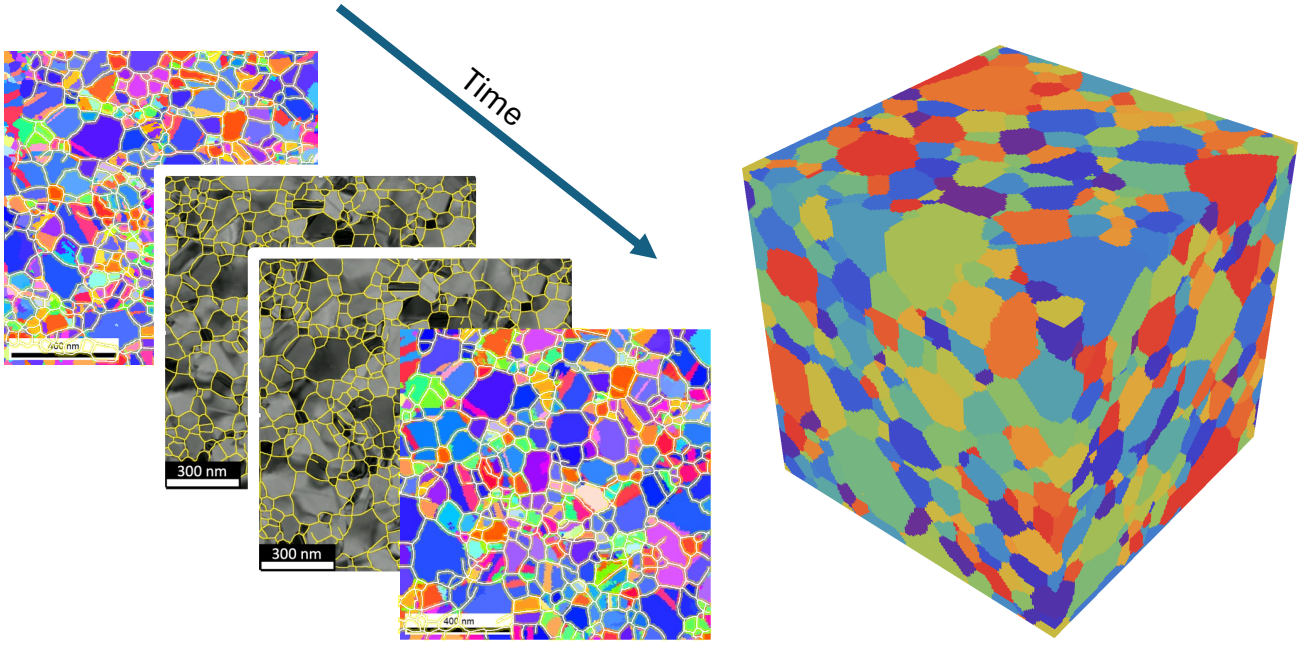
LEHIGH UNIVERSITY

Join us in New York City for a short-course on statistics and machine learning, with case studies from materials science. This NSF sponsored boot camp is intended for students new to data science approaches.

The development of a Materials Genome Initiative (MGI) workforce depends critically on the education of the next generation of scientists and engineers, particularly in modern data science techniques. Unfortunately, when machine learning tools are introduced to beginning students, they are often presented as "black-box" software modules employed without understanding of their statistical underpinning.

This interdisciplinary skills bootcamp seeks to address this shortcoming by providing attendees with both the skills and the requisite understanding of a spectrum of data science tools. As a concrete illustration of the power and utility of these tools, we will take as an example the application of neural networks to problems in microstructural image analysis.

Signup for the bootcamp here!



Housing available, contact organizers for more information.

For more info, contact Jeff Rickman at jmr6@lehigh.edu

Syllabus – Machine Learning for Materials Science Boot Camp

Day 1, Monday June 2

1. Introduction

Overview
Practical information for an Interactive Workshop - Jupyter Notebooks, Google Colaboratory
Description of Software

2. Data Interpretation

Data Wrangling
Clustering Methods, K-means clustering (Example – classifying materials by properties)
Principal Component Analysis – dimensional reduction
Kriging and Interpolation
(Canonical Correlation Analysis)

Day 2, Tuesday June 3

3. Probability and Statistics for Microstructural Interrogation

Probability Distributions and Density Functions
Moments
Analysis of Grain-Size Distributions
Correlation Analysis
Tessellations
Hypothesis Testing
Bayesian Methods

4. Simulation Methodology for Microstructural Evolution

Nucleation and Growth – Voronoi Models
Coarsening – Monte Carlo method

5. Optimization

Genetic Algorithms

Day 3, Wednesday June 4

6. Classification and Regression

Decision Trees
Random Forests
Support Vector Machine

7. Neural Networks for Microstructural Interrogation

Perceptron Models
Deep Learning
Backpropagation
Errors
Generic Examples
Introduction to U-Net
Experimental Imaging of Materials Microstructures
Microstructural Case Study

Day 4, Thursday June 6

8. Practice Time / Work with Your Own Data

Day 5 (Half day), Friday June 7

9. Conclusions