

# NANOx81- Data Science in Materials Science

## Course Admin

Shyue Ping Ong

University of California, San Diego

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## Course Objectives

To provide a comprehensive introduction into the application of data science to materials science.

# What will you learn in this course?

- Enough data science (including the mathematics) to understand how to apply them to solve materials science problems.
- Best practices in using various data science techniques.
- Practical use of open-source Python packages to do data science in materials science.

## What this course is **not**

- A probability and statistics course.
- A replacement for a rigorous data science course.
- A replacement for a materials science course.

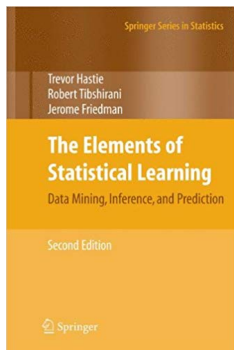
# Course Plan

- Weeks 1 and 2: Introduction to Data Science, Python and Data Wrangling
- Week 3: Lab 1 (Introduction to Python for Data Science and Data Wrangling)
- Weeks 4 and 5: Linear Methods and Unsupervised Learning
- Week 6: Lab 2 (Exercises in linear methods and clustering for materials science)
- Weeks 7 and 8: Kernel Methods, Trees and Neural Networks
- Weeks 9 and 10: Final Lab (Kaggle competition)

# Instructors

- Lecturer: Shyue Ping Ong ([ongsp@ucsd.edu](mailto:ongsp@ucsd.edu))
- Teaching Assistant: Keivan Rahmani ([kerahmani@ucsd.edu](mailto:kerahmani@ucsd.edu))

# Recommended Textbooks (All Free)



**Figure:** The Elements of Statistical Learning: Data Mining, Inference, and Prediction, Second Edition [Amazon][Free PDF]



**Figure:** Python Data Science Handbook [Amazon][Free web version]

# Course Structure

- Lectures/Labs (Tues/Thurs @ 1230-1350) in person.
- Note: Please ignore scheduled lab sessions - all labs are held in lecture times, not in a separate time.
- Recordings will be available online after the class.
- **Please bring your laptops.**
- Grading:
  - Lab 1: 25% - Same for NANO181 and NANO281
  - Lab 2: 25% - Same for NANO181 and NANO281
  - Lab 3: 50% - Different for NANO181 and NANO281



# Lab Assessment Criteria

|                            |     |
|----------------------------|-----|
| Model performance          | 30% |
| Materials Science Insights | 30% |
| Data Science Technique     | 30% |
| Programming Style          | 10% |

- **Collaboration policy:** Working together is highly encouraged, but each student must submit his / her own work.
- To make the best use of this course, you should make sure you can do the exercises and not over-rely on your course mates.

# Class etiquette

- Interaction preferred - interruptions with questions highly encouraged.
- Please be punctual. Lectures will start on time.
- Use of laptop to follow class examples is encouraged, but please be respectful of your lecturer and classmates by not using devices for non-class applications. All devices must be on silent mode.

# Prerequisites

- Knowledge of basic statistics (e.g., Gaussian distributions, Bayes theorem, etc.)
- Knowledge of basic linear algebra (e.g., matrix multiplication, eigenvalue decomposition, inverse)
- Some programming experience. Ideally, experience in the Python programming language would be helpful.
- 1st Homework (ungraded):
  - ① Go to [Google Colab](#).
  - ② Create a new notebook.
  - ③ Go through items 1-3 in the [official Python tutorial](#) – please run through the actual tutorial line by line. It should not take you more than 30 mins to do the whole thing.
  - ④ Extra: Briefly read through item 4 in the tutorial on flow control (if and for statements, especially).

# Course Admin

- Canvas for all course admin, including announcements/communications and submission of labs.
- **NANOx81 website** for all materials, including labs with instructions.



# Questions and Feedback

- Questions welcomed at any time during or after lectures
- NANOx81 is relatively very new - the instructors will try their best, but I would ask for you to be tolerant of any issues while we continue to improve the curriculum and labs.
- Your **feedback** is invaluable for shaping the current course as well as future courses.
- Email all feedback directly to [ongsp@ucsd.edu](mailto:ongsp@ucsd.edu).

# The End