Computational Modeling, Statistical Analysis and Machine Learning in Science

38-615 & 09-615, Fall 2024

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Outline

- Course logistics
- Course objectives
- Course overview
- Anaconda Python& Jupyter notebook ecosystem

Intro!

- Introduce yourself in a few sentences.

- What do you expect from this course?

- Tell one fact about yourself!

Class schedule

Tue & Thu 11:00- 12:20 AM

Canvas: https://canvas.cmu.edu/courses/37306

Slack or Discord channel ?

Piazza ?

TAs

Ilkwon Cho <ilkwonc@andrew.cmu.edu>,

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Kamal Singh Nayal <knayal@andrew.cmu.edu>

Course requirements

Designed for STEM master students & MCS recent graduates

Open to senior–year undergraduate students (with permission)

This is **practical**, application-oriented course, requiring skill in algorithmic problem solving.

We will use **Python** based tools and libraries. Prior programming experience with Python is needed.

Prerequisites: probability, linear algebra, statistical thermodynamics. If you took quantum mechanics and related quantitative courses it’s a plus

Programming experience

ML experience

Stats and Probability

Linear Algebra

Jupyter Notebook / Lab

M.S. in Data Analytics for Science (MS-DAS) program

- New program, 3rd year
- Please gave your feedback. olexandr@cmu.edu
- Job market is tough, but we are here to help!

Learning objectives

- Know how to explore and visualize scientific data
- Compare and contrast different types of data and representations.
- Understand core components of data analytics pipeline: visualization, exploratory data analysis, classification, regressions, prediction etc.
- Be able to analyze scientific data using a variety of machine learning approaches.
- Implement and analyze well-known existing ML algorithms.
- Integrate multiple components of practical machine learning in a single system: data preprocessing, learning, regularization, model selection and be familiar with programming tools to accomplish it.
- Hands on experience with real-world cases on how ML could address challenges in STEM sciences.

Course Outline

- Exploratory data analysis and visualization
- Unsupervised learning, clustering, dimensionality reduction
- Supervised learning, model training and evaluation
- Linear and nonlinear models
- Classification, SVM, kernel methods
- Decision trees and RF
- Probabilistic methods

Lectures

- EDA – exploratory data analysis
- Clustering
- Model training, bias and variance
- Probabilistic methods
- Linear methods, regularization, LASSO, Ridge regression
- Classification, SVM
- Decision trees
- RF, boosting, GBDT, etc
- Databases of scientific data
- Time series analysis
- Application of ML in science

Course Structure

Tuesday

- Lecture materials

Thursday

- Recital/practice
- Tutorials
- Lab discussions

Reading

No textbook

Readings will be provided on Canvas portal and lectures.

The readings for this course are required.

We recommend you read them **before** the lecture.

- Optional topics
- Very useful in practice
- Extend skills

Course Grades

5% for attendance

5% for class participation

50% for Lab assignments

40% for final open-ended class project

Bonus points for Top Kaggle leaderboard score

Final Project

- Work in teams 3-4 people.
- Open-ended project!
- Solve a science related problem with machine learning! Use your domain expertise
- Encourage to use your data
- Jupyter notebook, which mixes together written markdown and code portions or python script and report.
  - ~2000 words (2-3 pages of text)
  - ~500-1000 lines of code
- All text and code must be your own work

Final Project

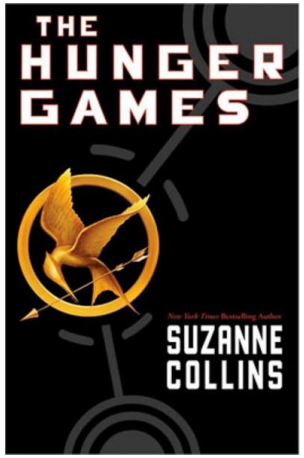
- Submit one paragraph project proposal (September)
- Short project talk (Pitch! 1-2 slides) (~Early Oct)
- Presentation during last week & also project final report
- You will be graded by the course instructor and other students taking the course (peers)

Lab Exercises / Home Assignments

- Lab1: EDA
- Lab2: Clustering
- Lab3: Linear Methods
- Lab4: Classification
- Lab 5: Regression

Lab auto-grading

Brought to you by



- Five Labs per semester
- Short solution discussions after each Lab
- Assignments will include 2 parts: *programming* component and *kaggle* component (autoscoring)
- Sometimes you will compete with each other…

Dashboard | Public Leaderboard - Heritage Health Prize

This leaderboard is calculated on approximately 30% of the test data.
The final results will be based on the other 70%, so the final standings may be different.

#	Δ1w	Team Name * in the money	Score	Entries
1	–	EXL Analytics *	0.443793	555
2	–	POWERDOT	0.447651	671
3	–	Dolphin	0.450403	555
4	↑1	jack3	0.451425	455
5	↓1	Hopkins Biostat	0.451569	444
6	–	Xing Zhao	0.453081	161
7	–	Old Dogs With New Tricks	0.454096	370
8	–	Areté Associates	0.454424	112
9	–	Alice Sasandr	0.454670	376
10	↑9	J.A. Guerrero	0.454728	173

Grading Policies

Late-work policy/Flex days: You will have 5 flex days for the entire semesters that you can use for homework submission. You can chose to divide the days up the way you want. After that, submissions will not be accepted.

Re-grade policy: Requests for re-grades must be submitted within 1 week of receiving the grades assignment, paper, or test.

Attendance policy: Attending lectures is mandatory and class attendance will be kept. Each student is allowed two absences (no questions asked) for the entire semester

Disability/ Accommodation Policy

Please see me for specific cases

There is no Final Exam

Homework assignments – you can’t more than 5 extra days

Rough plan for next few weeks

Aug 27: Lecture 0 Intro & Class logistics
Aug 29: Lecture 1 - Data, data types, formats, basic analysis

Sep 03: Lecture 2 - Data Visualization
Sep 03: Lab 1 released
Sep 05: Recital time - time for setup, refresher/sci tutorial?

Sep 10: Lecture 3 - Dimensionality reduction
Sep 12: Recital time
~Sep 17: Lab 1 Due
Sep 17: Lecture 4 – Unsupervised Learning
Sep 19: Lab1 discussions; Lab 2 released

ChatGPT Policy

ChatGPT, the chatbot developed by OpenAI that can write cogent essays, solving science and math problems and producing working computer code.

Embrace ChatGPT, if you find it useful for this class. Learn from it, but please clearly attribute ChatGPT, if used to comply with university policies on Ethics and Academic Integrity:

https://www.cmu.edu/policies/student-and-student-life/academic-integrity.html

Questions?

Anaconda Python

- For the class, we strongly recommend you use Anaconda Python

- This distribution of Python, includes most libraries and tools

https://www.anaconda.com/download/

Installing additional packages

There are two general ways to install additional packages

```
conda install <package name>

     conda search <package name>
     conda list


pip install <package name>
```

Jupyter notebook

- Notebook documents (are documents produced by the Jupyter Notebook App, which contain both computer code (python) and rich text elements (paragraph, equations, figures, links, etc…).

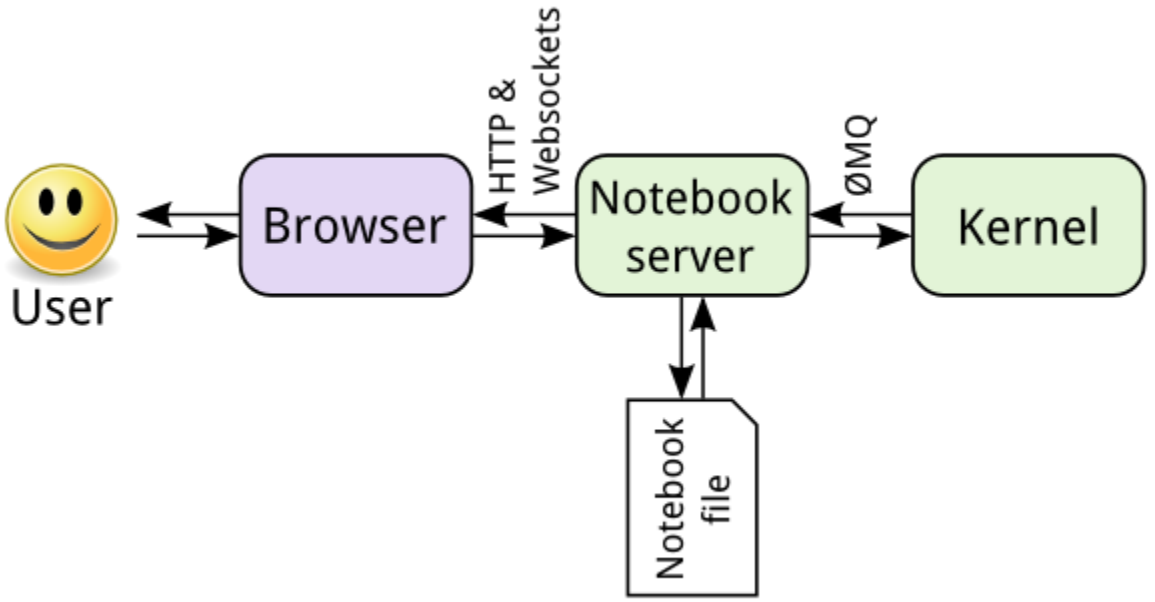
- Notebook documents are both human-readable documents containing the analysis description and the results (figures, tables, etc..) as well as executable documents which can be run to perform data analysis.

- More info about Jupyter here: http://www.jupyter.org

Kernels

Behind every notebook runs a kernel. When you run a code cell, that code is executed within the kernel and any output is returned back to the cell to be displayed.

The kernel's state persists over time and between cells — it pertains to the document as a whole and not individual cells.



Jupyter notebook

Launch jupyter via the command:

```
jupyter notebook
```

Open in browser: http://localhost:8888

New (alternative) environment: `jupyter lab`

Windows PC vs MAC

Any decent laptop should work for this class

This is NOT the case for 38-616/09-616

HPC Resources for 2025 (38-616/09-616)

Pittsburgh Supercomputing Center (PSC) is a joint effort of Carnegie Mellon University and the University of Pittsburgh. Established in 1986, PSC is supported by several federal agencies, the Commonwealth of Pennsylvania, and private industry.

Bridges-2 Supercomputer:

V100 and A100 GPUs