MS43040: General Project Instructions

1 Important dates

- Mid-term presentation: March 21, 2024, 3:45 pm (as per Regular Course Schedule)
- Final presentation: April 4, 2024, 3:45 pm (as per Regular Course Schedule)
- Report deadline: April 18, 2024, 5:00 pm

2 Group

- Each group will consist of 2 MSc students.
- Projects will be assigned on a first-come-first-serve basis.
- It is expected that each group member will contribute equally. Individual participation will be tested in the presentation.

3 Assessment

- The assessment is based on your understanding and approach towards solving the project problem, and evaluating the outcomes of your method. The assessment is NOT based on how accurately your machine learning models are performing. We expect your model to produce predictions which are better than random or mean prediction. On the contrary, we will not reward time- and resource-consuming efforts to optimize hyper-parameters and model architectures to obtain incremental gains in accuracy.
- The assessment breakdown is as follows:
  - Mid-term presentation: no grade
  - Final presentation: 50% of grade
  - Final report: 50% of grade
- Submit the report by the announced deadline. Extensions may only be provided for serious reasons and only upon prior consultation with the instructors.

4 Office hours

- Note that as part of each project, you will develop through self-exploration a novel concept in machine learning that has not been taught in the lab sessions so far. Groups are suggested to exploit the office hours dedicated to the course to exchange feedback, discuss ideas, identify bottlenecks and their resolution, with the course instructors and TAs.
- The presence of challenges in the development of the project is expected, and is part of the learning process. When facing a challenge, we suggest you to discuss with the instructors and/or TAs. To maximize the efficiency of these discussions, please prepare beforehand:
  - a brief recap of the context in which the problem occurred,
  - a clear recap of the approaches you have been attempting to solve it.
- You may directly visit the instructors or the TAs in their office (location listed in the document) during the dedicated office hours. Walk-in consultations outside of the dedicated office hours is not possible without appointments in advance.

5   Report

- While there are no requirements or restrictions on the number of pages or words, an ideal report should be anywhere between 10-20 pages in length.

- Fully working code (without errors) and data should be submitted along with the report as a digital attachment with the report.

- The codes should be concisely but fully documented with comments.

- The following items shall be discussed in the report:
    - Problem description
    - Data description
    - Modeling goals
    - Approach. E.g., model architecture, inductive biases, physical constraints, loss function, if any.
    - Results. E.g., model accuracy, computational cost, prediction plots. Note: The results should be accompanied by sufficient analysis and discussion (beyond just plotting the figures).
    - **The Big Picture.** What are the potential applications of your project? How has this already been deployed in existing scientific literature (tip: refer to papers in the project description). How can your approach be further improved?

- Proper scientific writing (including citations, figure captions, axes labels, plot legends, etc.) is expected throughout the report.

6   Mid-term and Final Presentation

- Each group will present along the format: 10 minutes presentation + 5 minutes for discussion (informal discussion in mid-term presentation; questions and answers in the final presentation).

- The content of the oral presentation should be equally divided between the two group members. A suggested scheme for the final presentation could be, for example, Speaker A - introduction, method; Speaker B - results, future works.

- Attendance of all project groups are mandatory in both mid-term and final presentation.

- The presentation should discuss the following aspects of your project:

    Mid-term presentation: (NOTE: The mid-term presentation is not graded. However, this a crucial chance for you to get critical feedback and potential ideas from the instructors, TAs, as well as other groups and projects.)
    - Problem description
    - Data description
    - Modeling goals
    - Preliminary approach. E.g., model architecture, inductive biases, physical constraints, loss function, if any.

    Final presentation:
    - Problem description
    - Data description
    - Modeling goals
    - Approach. E.g., model architecture, inductive biases, physical constraints, loss function, if any.
    - Results. E.g., model accuracy, computational cost, prediction plots
    - **The Big Picture.** What are the potential applications of your project? How has this already been deployed in existing scientific literature (tip: refer to papers in the project description). How can your approach be further improved?

- **Target audience:** In both presentations, assume that the audience knows all the concepts of machine learning taught in the lab sessions, so there is no need to go over the basics of neural network. However, the audience does not know anything about your project and the materials science context of it. Consequently, your presentation must aim to present the project in a manner that fellow students of the course can understand it.

7 Conflict resolution

- Members in a group shall develop an ability to share opinion regularly, communicate effectively needs, and express concerns. We suggest to set-up clear expectations and timelines from the project's start, so as to help managing expectations and minimize misunderstandings.

- Swift intervention is crucial when conflicts arise. Do not hesitate to contact the course instructors if mediation is necessary to facilitate constructive dialogue and guide the team towards a successful outcome.

- In case of unbalanced project work distribution between group members, please reach out to us confidentially. The instructors will also uphold confidentiality.

8 Contacts

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