Applications of Transformer Networks in Bio- and Cheminformatics

Organizational remarks

08.04.2025

Requirements

- Basic Python experience
  - We will use PyTorch
- Basic Machine Learning
  - Training and validation of machine learning models
  - Neural Networks
    - Training and implementation
- No biological / chemical background is required

Course Homepage

- Course material and information will be on https:// www.github.com/AlexanderKroll/DL4Molecules_2025
  - Course information
  - Worksheets
  - Lecture slides (before lecture)
- I will record short lecture videos: https://www.youtube.com/@DL4Molecules
  - Explanations will be less detailed than the actual lectures
- RocketChat channel
  - Send me an email (alexander.kroll@hhu.de) if you are not invited
  - Solutions to worksheets
  - Ask questions regarding lecture and worksheets
    - Help each other
    - I will scan the chat sometimes for unanswered questions
    - Don’t post worksheet solutions!

Lectures and Exercises

- Lectures:
  - Every Tuesday 10:30 – 12:00 (HS 5H)
- Exercises:
  - Every second Tuesday 12:30 – 14:00 (25.02.02.21)
  - First meeting: 29th of April
  - Discussion of worksheet solutions
- Weekly exercise worksheets:
  - Published weekly on Tuesday (starting from 15th of April)
  - Deadline: following Monday 23:59
  - There will be approx. 8 worksheets + one 4-week project
  - Admission to exam: 50% of worksheet and project points
- Exam: Written
  - 1st exam: 01.08.2025
  - 2nd exam: 24.09.2025

Worksheets

- You can discuss and think together
  - Exercises have to be implemented individually
  - No identical solutions!

- You can use chatbots
  - Can be very helpful for small steps such as finding the right python functions
  - If you solve tasks completely with chatbots you will not learn much from the exercises
  - On every worksheet you need to state where you have used chatbots

- Submissions via sciebo:
  - https://uni-duesseldorf.sciebo.de/s/hCt1rTP23EeWmUC
  - Link is on course Homepage

Course Project

- Towards the end of the semester, instead of worksheets you will do a 4-week research project
- Research projects
  - Select one out of multiple research projects
  - Testing a small open research questions
- Motivation:
  - Solving/answering an actual open question instead of only reproducing existing results (worksheets)
  - Learn how to plan the execution of a project
  - Having a project to include in your portfolio for applications
- More information during the semester

Lab Rotations / Master thesis

- Our research group offers Lab Rotations and Master theses
  - This course is a very good preparation
  - If you are interested talk to me (~mid semester)