Applications of Transformer Networks in Bio- and Cheminformatics

Organisational remarks

09.04.2024

Course content

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- Biological / chemical background
- Transformer Networks
  - Architecture
  - Training
    - Self-Supervised
    - Supervised: Fine-tuning pre-trained models
- Transformer Networks for proteins (large molecules) and small molecules
- Multimodal Transformer Networks:
  - Applying a single Transformer to multiple types of input data
- Visualizing what Transformer Networks learn
- Many different biological applications
  - Achieving state-of-the art results for biological prediction tasks

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 github.com/AlexanderKroll/DL_for_Molecules_Course
  - Course Information
  - Worksheets
  - Solution to Worksheets
  - Lecture Slides (before Lecture)

- RocketChat Channel
  - Send me an email if you are not invited
  - 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 12:30 – 2:00 pm (25.02.02.21)
- Exercises:
  - Every Tuesday 4:30 – 6:00 pm (25.02.02.21)
  - First meeting: 23rd of April
- Weekly exercise worksheets:
  - Published weekly on Tuesday (starting from 16th of April)
  - Deadline: following Monday 11:59 pm
  - Admission to exam: 50% of worksheet points
- Exam: Oral or written

Worksheets

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- You can discuss and think together
  - Exercises have to be done 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

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)