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Freie Universität Berlin

Machine Learning for Molecular Physics

WiSe 2021/22

L01 - Introduction

General Setup

Lectures - Fridays 16-18, online

Tutorials - Wednesdays 16-18, in person (Félix Musil); computational in the computer pool and on your own laptop/computer

Whiteboard - exchange information, assignments

Chat channel - https://meet.physik.fu-berlin.de (Machine Learning for Molecular Physics (WiSe 21/22)

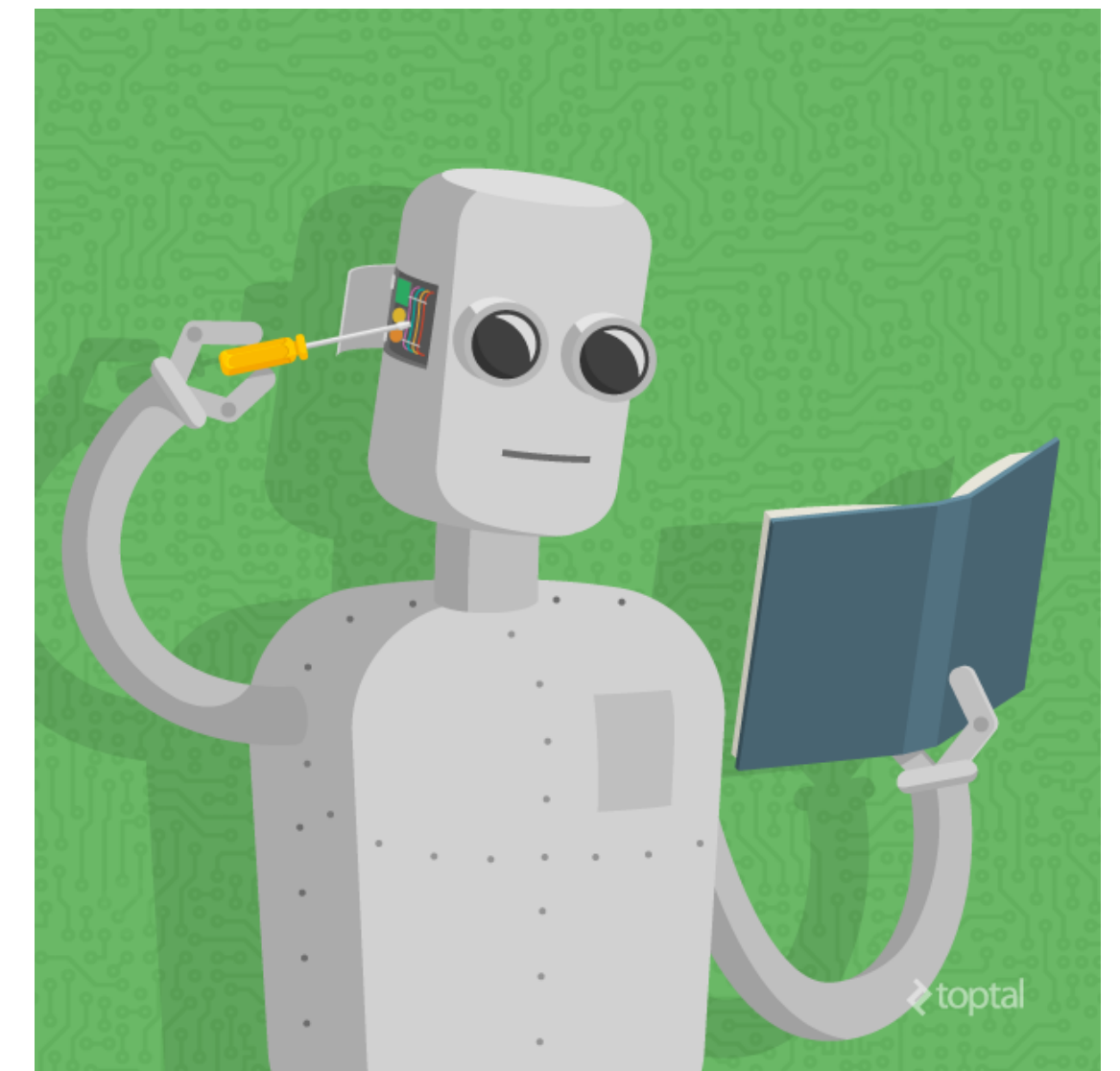Examination - project work (need to pass 50% of tutorial)

Topics

Image Credit: Toptal

Poll: Technical skills

1. How do you rank your python skills?

   • What is python? Never heard of it

   • Beginner with basic knowledge of python commands

   • Medium knowledge, have worked with python several times

   • Expert, working with python on a regular basis

2. Have you worked with Jupyter Notebooks?

   • Yes

   • No

Poll: Technical skills

3. Have you worked with Anaconda/Miniconda?

   - No

   - Yes, I know some conda basics

   - Yes, I use conda regularly

4. Have you worked with Visual Studio Code or other integrated development environments? (multiple)

   - No

   - Yes, I know Visual Studio Code

   - Yes, I have worked with other IDEs

Poll: ML and Molecular Simulations

1. How do you rate you knowledge about machine learning? (multiple)

   • My knowledge is based on popular media

   • I have attended lectures about ML

   • I have already programmed some ML code

2. How do you rate your knowledge about molecular simulations? (multiple)

   • I only have a very rough idea about this

   • I have attended lectures on molecular simulations

   • I have run molecular simulations myself

   • I have programmed my own MD or MC code (or something comparable)

Poll: Computer pool/laptops

1. Do you have a laptop or desktop that you can use for the tutorial?

   • Yes

   • No

2. Where would you prefer to work?

   • Only on my laptop

   • Only in the computer pool

   • Both on my laptop and in the computer pool

3. Which is your preferred operating system?

   • Linux

   • Windows

   • Mac

Questions?