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Hands-on Tutorials

Tutorial Lecture:

Structural descriptors and atomic cluster expansion basis

Dr. Anton Bochkarev – Ruhr-Universität Bochum, Germany

Link to Google Colab: <https://colab.research.google.com/drive/1avJoULLhrGGPQdLdMlb73vkCe41v7sCW>

Tutorial Lecture:

Materials structure-property mapping with kernel-based methods

Dr. Milica Todorović – Turku University, Finland

Links to Google Colab:

Introduction to KRR: <https://colab.research.google.com/drive/12eV4CJctJYbITM1YwqAnn-Ynoz8hsYKz?usp=sharing>

Introduction to GPR

<https://colab.research.google.com/drive/1HbvBmNjTdHPsn6ZxvG6ejn-tnJ2Podhk?usp=sharing>

Introduction to BO

https://colab.research.google.com/drive/1vOCULuq_1_IjiC3JRgtvgQUIPRQX-J_r?usp=sharing

BO structure search

<https://colab.research.google.com/drive/1pUpXgM17vpcEtd1gge5Z15EeP38yxcoa?usp=sharing>

Tutorial Lecture:

Data-manifold characterisation: Estimating intrinsic dimension, density, and density peaks with DADApy

Dr. Aldo Glielmo – SISSA and Banca d'Italia, Italy

Links to Google Colab:

Tutorial 0: Visualising the curse of dimensionality

https://colab.research.google.com/drive/1v7hE2Vy8H2yqhb_6A3Aw5_Y2pFDSH_TG?usp=sharing

Tutorial 1: Intrinsic dimension estimation

<https://colab.research.google.com/drive/1tW6PsTOiWfDFqi5mIV2k9l7zSvsvTaLW?usp=sharing>

Tutorial 2: Density and density peaks estimation

https://colab.research.google.com/drive/1eOZLPr-sEegujRSYNQ2oJL52_LEDwLko?usp=sharing

Link to optional dataset:

Tutorial 3: Free experimentation with DADApy. <https://drive.google.com/drive/folders/1zmVYwNCbnpMtlRFnplZB4pYWmxLdG1cG?usp=sharing>

Tutorial Lecture:

Training neural network potentials with PANNA

Dr. Franco Pellegrini – SISSA, Italy

Link to Google Colab:

<https://bit.ly/ML4M22PANNA>

Young Researcher's Workshop on Machine Learning for Materials 2022, Blog at WordPress.com.