

Handout Introduction to Machine learning in Chemistry

Github repo with Jupyter notebooks and Colab links:

https://github.com/meyresearch/ML_for_chemistry

Additional resources links:

<https://pubs.rsc.org/en/content/ebook/978-1-78801-789-3>

<https://www.nature.com/articles/s41557-021-00716-z>

<https://pubs.acs.org/doi/book/10.1021/acsinfocus.7e5017>

<https://www.amazon.co.uk/Deep-Learning-Sciences-Bharth-Ramsundar/dp/1492039837>

<https://dmol.pub>

<https://www.amazon.co.uk/Deep-Learning-Adaptive-Computation-Machine/dp/0262035618>

<https://pubs.rsc.org/en/content/ebook/978-1-78801-547-9>

Google tutorial:

<https://developers.google.com/machine-learning/crash-course/ml-intro>

ML Python libraries:

<https://pytorch.org>

<https://scikit-learn.org/stable/>

<https://rdkit.org>

<https://www.tensorflow.org>

<https://deeptime-ml.github.io/latest/index.html>