

Machine Learning in Sciences

Mendoza-Cortes Group

September 19, 2018

Contents

| | Page |
|-------------------------------|------|
| List of Contents | i |
| List of Tables | ii |
| List of Figures | iii |
| 1 Introduction and Background | 1 |
| 2 Results | 1 |
| 3 Conclusions | 2 |
| Appendix | 2 |
| A Scripts | 3 |
| B Extra plots | 4 |
| C Inputs | 5 |
| D Things to be careful with | 6 |

List of Tables

Page

List of Figures

Page

Chapter 1

Introduction and Background

Abstract

The following guide is intended for non CS majors that wonder if there will be any use of Machine Learning on their field. It contains applications to Art, Engineering, Physics and Chemistry.

Software required: This guide will require a basic knowledge of python 3, we recommend to install it with Anaconda. We also have an introduction to Python. We will use Sklearn and Keras for most of the introductory part and Tensorflow, Pytorch for the advanced parts.

Chapter 2

Results

Chapter 3

Conclusions

Here we will put the most significant results over time

Appendix A

Scripts

Appendix B

Extra plots

Appendix C

Inputs

Appendix D

Things to be careful with

- Remember to update the path and home in constants when trying to run the create_MOF script from a folder outside of scratch.
- Remember to change the time step in the in.lammps file from 2 to 1.
- Some of the nets in the database are just named according to shape and not by shape and symmetry.
- Make sure there is at least one SBU of the correct symmetry for a framework to be created from a net.

Bibliography