Data science for Materials Science & Engineering

Supervised Learning: Neural Networks

In this module

- Introduction to neural networks for materials science
- Hands on tutorial using nanoHUB: neural networks for XX (this file)
- Hands on tutorial using nanoHUB: neural networks for XX
- Homework assignments

Saaketh Desai and Alejandro Strachan
desai61@purdue.edu || strachan@purdue.edu
School of Materials Engineering & Network for Computational Nanotechnology
Purdue University
West Lafayette, Indiana USA

Learning objectives and prerequisites

After completing this lecture you will:

- Be able to create and train a neural network
- Be able to define objective functions for regression and classification tasks
- Know how to determine overfitting and underfitting in training neural networks

Pre-requisites:

- Basic Python programming
- Querying materials repositories
- Linear regression

Launching a Jupyter tool in nanoHUB

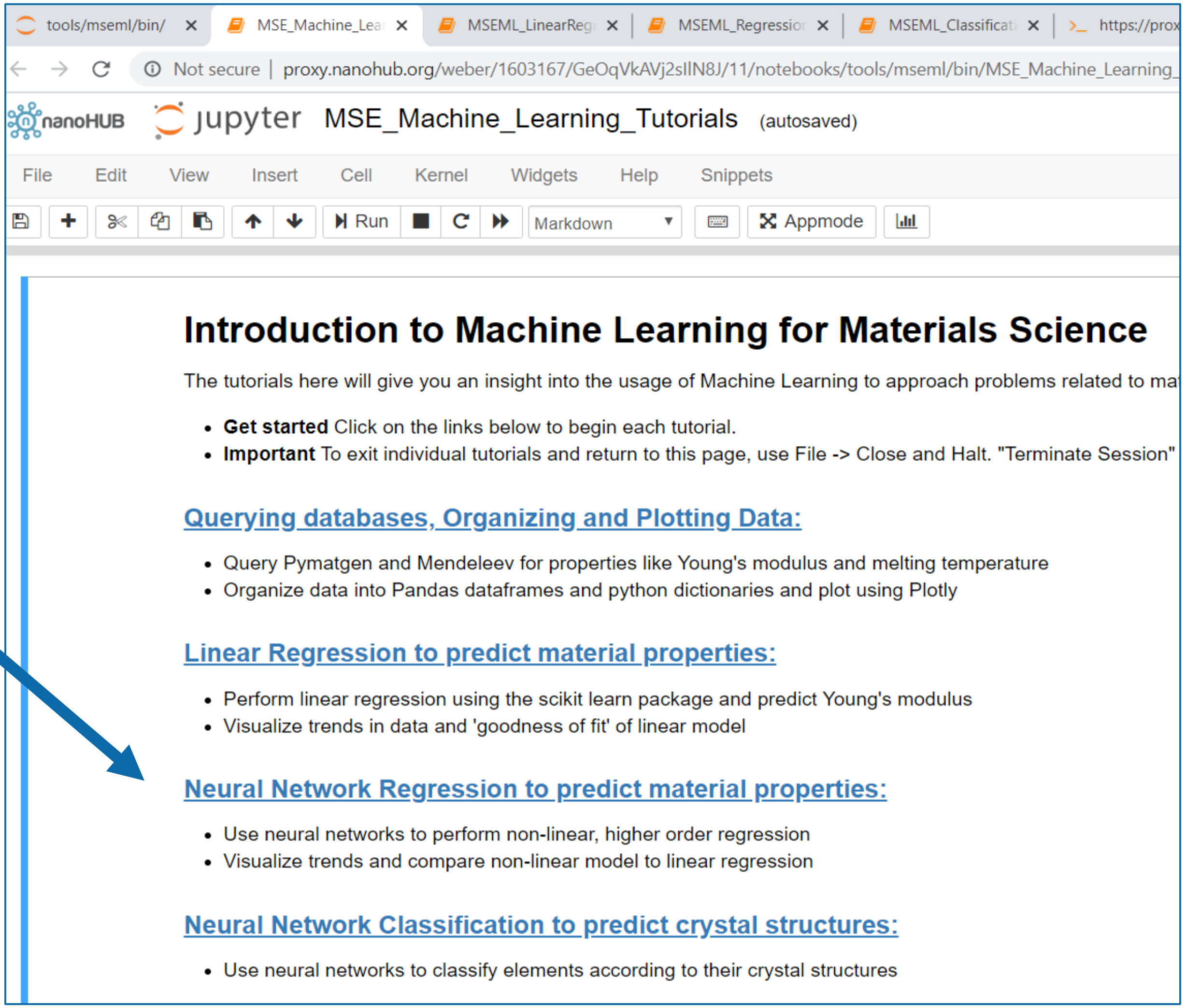
Machine Learning for Materials Science: Part 1

From your browser go to link: https://nanohub.org/tools/mseml/

Click on Launch Tool to begin

Step 1: Landing Page – Notebook: Neural Network Regression

Navigate to the third link in the landing page to access the notebook



Step 2: Let's get some data

1. Getting a dataset

```
import pymatgen as pymat
import mendeleev as mendel
import pandas as pd
import numpy as np
import random
import tensorflow as tf
from tensorflow import keras
from keras import initializers
from keras.layers import Dense
from keras.models import Sequential
%matplotlib inline
import matplotlib.pyplot as plt
import sys

fcc_elements = ["Ag", "Al", "Au", "Cu", "Ir", "Ni", "Pb", "Pd", "Pt", "Rh", "Th", "Yb"]
bcc_elements = ["Ba", "Ca", "Cr", "Cs", "Eu", "Fe", "Li", "Mn", "Mo", "Na", "Nb", "Rb", "Ta", "V", "W" ]
hcp_elements = ["Be", "Cd", "Co", "Dy", "Er", "Gd", "Hf", "Ho", "Lu", "Mg", "Re",
                "Ru", "Sc", "Tb", "Ti", "Tl", "Tm", "Y", "Zn", "Zr"]

elements = fcc_elements + bcc_elements + hcp_elements

random.Random(1).shuffle(elements)

querable_mendeleev = ["atomic_number", "atomic_volume", "boiling_point", "en_ghosh",  "evaporation_heat", "heat_of_formation",
                      "lattice_constant", "melting_point", "specific_heat"]
querable_pymatgen = ["atomic_mass", "atomic_radius", "electrical_resistivity","molar_volume", "bulk_modulus", "youngs_modulus",
                     "average_ionic_radius", "density_of_solid", "coefficient_of_linear_thermal_expansion"]
querable_values = querable_mendeleev + querable_pymatgen
```

	atomic_number	atomic_volume	boiling_point	en_ghosh	evaporation_heat	heat_of_formation	lattice
0	27	6.70	3143.0	0.143236	389.1	426.7	
1	69	18.10	2220.0	0.216724	232.0	232.2	
2	39	19.80	3611.0	0.121699	367.0	424.7	
3	75	8.85	5900.0	0.243516	704.0	774.0	
4	28	6.60	3005.0	0.147207	378.6	430.1	
5	67	18.70	2968.0	0.207795	301.0	300.6	
6	79	10.20	3080.0	0.261370	340.0	368.2	
7	21	15.00	3104.0	0.119383	332.7	377.8	
8	45	8.30	4000.0	0.140838	494.0	556.0	
9	74	9.53	5930.0	0.239050	824.0	851.0	

Use Keras to train neural networks

Keras: https://keras.io/

Query Pymatgen and Mendeleev for atomic number, melting point etc.

Organize data into a Pandas Dataframe

Pandas: https://pandas.pydata.org/

Step 3: Preprocess data and create network

2. Processing and Organizing Data

```
all_values = [list(df.iloc[x]) for x in range(len(all_values))]

# List of lists are turned into Numpy arrays to facilitate calculations in steps to follow (Normalization).
all_values = np.array(all_values, dtype = float)
print("Shape of Values:", all_values.shape)
all_labels = np.array(all_labels, dtype = int)
print("Shape of Labels:", all_labels.shape)

# Training Set
train_values = all_values[:40, :]
train_labels = all_labels[:40, :]

# Testing Set
test_values = all_values[-7:, :]
test_labels = all_labels[-7:, :]

# NORMALIZATION

mean = np.nanmean(train_values, axis = 0) # mean
std = np.nanstd(train_values, axis = 0) # standard deviation

train_values = (train_values - mean) / std # input scaling
test_values = (test_values - mean) / std # input scaling

print(train_values[0]) # print a sample entry from the training set
#print(train_labels[0])
```

Divide data into training and testing sets

Standard Score normalization

32 = # of neurons

Activation = activation function

https://en.wikipedia.org/wiki/Activation_function

3. Creating the Model

```
model = Sequential()
model.add(Dense(32, activation='relu', input_shape=(train_values.shape[1], ), kernel_initializer=kernel_init))
model.add(Dense(64, activation='relu', kernel_initializer=kernel_init))
#model.add(Dense(64, activation='relu', kernel_initializer=kernel_init))
model.add(Dense(1, kernel_initializer=kernel_init))

# DEFINITION OF THE OPTIMIZER

optimizer = optimizers.RMSprop(0.002) # Root Mean Squared Propagation

# This line matches the optimizer to the model and states which metrics will evaluate the model's accuracy
model.compile(loss='mae', optimizer=optimizer, metrics=['mae'])
model.summary()
```

Define a model with two hidden layers and an output layer: Uncomment the line to add a third hidden layer

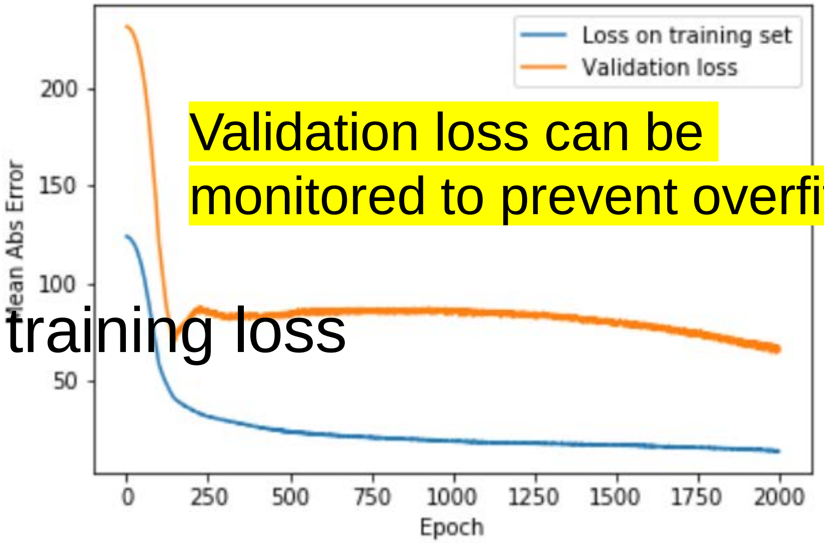
Loss function: Mean absolute error

Step 4: Train and evaluate network

TRAINING

```
# EPOCH REAL TIME COUNTER CLASS
class PrintEpNum(keras.callbacks.Callback): # This is a function for the Epoch Counter
    def on_epoch_end(self, epoch, logs):
        sys.stdout.flush()
        sys.stdout.write("Current Epoch: " + str(epoch+1) + " Training Loss: " + "%4f" %logs.get('loss') + '

EPOCHS = 2000 # Number of EPOCHS

# HISTORY Object which contains how the model learned

# Training Values (Properties), Training Labels (Known Young's Moduli)
history = model.fit(train_values, train_labels, batch_size=train_values.shape[0],
                    epochs=EPOCHS, verbose = False, validation_split=0.1, callbacks=[PrintEpNum()])


# PLOTTING HISTORY USING MATPLOTLIB

plt.figure()
plt.xlabel('Epoch')
plt.ylabel('Mean Abs Error')
plt.plot(history.epoch, np.array(history.history['mean_absolute_error']),label='Loss on training set')
plt.plot(history.epoch, np.array(history.history['val_mean_absolute_error']),label = 'Validation loss')
plt.legend()
plt.show()
```

model.fit(…) trains the network



Validation loss can be monitored to prevent overfitting

Plot training loss

TESTING

```
[loss, mae] = model.evaluate(test_values, test_labels, verbose=0)

print("Testing Set Mean Absolute Error: {:2.2f} GPa".format(mae))
```

```
Testing Set Mean Absolute Error: 34.38 GPa
```

```
test_predictions = model.predict(test_values).flatten()
```

model.evaluate(…) evaluates the network

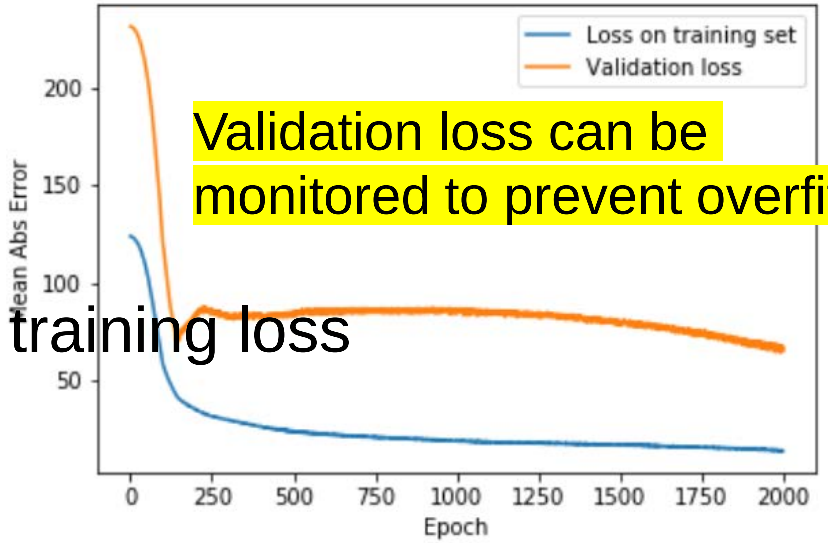
model.predict(…) makes predictions for a given dataset

Step 4: Train and evaluate network

TRAINING

```
# EPOCH REAL TIME COUNTER CLASS
class PrintEpNum(keras.callbacks.Callback): # This is a function for the Epoch Counter
    def on_epoch_end(self, epoch, logs):
        sys.stdout.flush()
        sys.stdout.write("Current Epoch: " + str(epoch+1) + " Training Loss: " + "%4f" %logs.get('loss') + '

EPOCHS = 2000 # Number of EPOCHS

# HISTORY Object which contains how the model Learned

# Training Values (Properties), Training Labels (Known Young's Moduli)
history = model.fit(train_values, train_labels, batch_size=train_values.shape[0],
                    epochs=EPOCHS, verbose = False, validation_split=0.1, callbacks=[PrintEpNum()])


# PLOTTING HISTORY USING MATPLOTLIB

plt.figure()
plt.xlabel('Epoch')
plt.ylabel('Mean Abs Error')
plt.plot(history.epoch, np.array(history.history['mean_absolute_error']),label='Loss on training set')
plt.plot(history.epoch, np.array(history.history['val_mean_absolute_error']),label = 'Validation loss')
plt.legend()
plt.show()
```

model.fit(…) trains the network



Validation loss can be monitored to prevent overfitting

Plot training loss

TESTING

```
[loss, mae] = model.evaluate(test_values, test_labels, verbose=0)

print("Testing Set Mean Absolute Error: {:2.2f} GPa".format(mae))
```

```
Testing Set Mean Absolute Error: 34.38 GPa
```

```
test_predictions = model.predict(test_values).flatten()
```

model.evaluate(…) evaluates the network

model.predict(…) makes predictions for a given dataset

Plot results