ME 793 - Multiscale Materials Informatics, Discovery and Design

Instructor : A. Alankar

Tutorial 11 - NN Regression and Various Optimisers

For a given learning rate, epochs and other default setup, run the model for RMSProp, Adam and Gradient Descent and compare the loss vs. epochs

Outline:

1. **Getting data**
2. **Processing and Organizing Data**
3. **Creating the Model**
4. **Plotting ## Assignment 05**

0. Import libraries

In [2]:

```
import tensorflow as tf
# You may not be able to install tensorflow using conda install inside pytmatgen.
# use pip install tensorflow

from tensorflow import keras
from tensorflow.keras import initializers
from tensorflow.keras.layers import Dense
from tensorflow.keras.models import Sequential
from tensorflow.keras import optimizers
from sklearn.metrics import mean_absolute_error

import pymatgen.core as pymat
import mendeleev as mendel
import pandas as pd
import numpy as np

import sys
import os
sys.path.insert(0, '../src/')

%matplotlib inline
import matplotlib.pyplot as plt
```

In [ ]:

```
!pip install pymatgen
```

In [ ]:

```
!pip install mendeleev
```

In [ ]:

```

```

1. Getting a dataset

In [3]:

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

elements = fcc_elements + bcc_elements + hcp_elements

querable_mendeleev = ["atomic_number", "atomic_volume", "boiling_point",
                      "en_ghosh",  "evaporation_heat", "heat_of_formation",
                     "lattice_constant", "specific_heat"]

# en_ghosh is Ghosh's scale of electronegativity. See this: https://doi.org/10.1142/S0219
633605001556
# There are many such scale.

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

# Note that in this examples, two different APIs are used and two different sets of featu
res have been collected.
# These features have been collated in a single set of queable values.
#np.shape(elements)
```

Querying the database

In [4]:

```
all_values = [] # Values for Attributes
all_labels = [] # Values for Young's Modulus (Property to be estimated)

# This neural network will produce a virtual function that will give Young's modulus E
#E = E(values)
#E = E(atomic number, atomic mass, boiling point......)

for item in elements:
    element_values = []

    # This section queries Mendeleev
    element_object = mendel.element(item)
    for i in querable_mendeleev:
        element_values.append(getattr(element_object,i))

    # This section queries Pymatgen
    element_object = pymat.Element(item)
    for i in querable_pymatgen:
        element_values.append(getattr(element_object,i))

    all_values.append(element_values) # All lists are appended to another list, creating
a list of lists

# Pandas Dataframe
df = pd.DataFrame(all_values, columns=querable_values)


# The labels (values for Young's modulus) are stored separately for clarity (We drop the
column later)

df.to_csv(os.path.expanduser('element_data.csv'), index=False, compression=None) # this
line saves the data we collected into a .csv file into your home directory

all_labels = df['youngs_modulus'].tolist()

df = df.drop(['youngs_modulus'], axis=1)

#df.head(n=10) # With this line you can see the first ten entries of our database
```

```
df
```

Out[4]:

	atomic_number	atomic_volume	boiling_point	en_ghosh	evaporation_heat	heat_of_formation	lattice_constant	specific_he
0	47	10.30	2435.15	0.147217	254.1	284.90	4.09	0.2
1	13	10.00	2792.15	0.150078	284.1	330.90	4.05	0.8
2	79	10.20	3109.15	0.261370	340.0	368.20	4.08	0.1
3	29	7.10	2833.15	0.151172	304.6	337.40	3.61	0.3
4	77	8.54	4701.15	0.251060	604.0	669.00	3.84	0.1
5	28	6.60	3186.15	0.147207	378.6	430.10	3.52	0.4
6	82	18.30	2022.15	0.177911	177.8	195.20	4.95	0.1
7	46	8.90	3236.15	0.144028	372.4	376.60	3.89	0.2
8	78	9.10	4098.15	0.256910	470.0	565.70	3.92	0.1
9	45	8.30	3968.15	0.140838	494.0	556.00	3.80	0.2
10	90	19.80	5058.15	0.102770	513.7	602.00	5.08	0.1
11	70	24.80	1469.15	0.221190	159.0	155.60	5.49	0.1
12	56	39.00	2118.15	0.158679	142.0	179.10	5.02	0.2
13	24	7.23	2944.15	0.131305	342.0	397.48	2.88	0.4
14	63	28.90	1802.15	0.189935	176.0	177.40	4.61	0.1
15	26	7.10	3134.15	0.139253	340.0	415.50	2.87	0.4
16	3	13.10	1615.15	0.105093	148.0	159.30	3.49	3.5
17	25	7.39	2334.15	0.135284	221.0	283.30	8.89	0.4
18	42	9.40	4912.15	0.131267	590.0	658.98	3.15	0.2
19	11	23.70	1156.09	0.093214	97.9	107.50	4.23	1.2
20	41	10.80	5014.15	0.128078	680.0	733.00	3.30	0.2
21	73	10.90	5728.15	0.234581	758.0	782.00	3.31	0.1
22	23	8.35	3680.15	0.127334	460.0	515.50	3.02	0.4
23	74	9.53	5828.15	0.239050	824.0	851.00	3.16	0.1
24	4	5.00	2741.15	0.144986	309.0	324.00	2.29	1.8
25	20	29.90	1757.15	0.115412	153.6	177.80	5.58	0.6
26	48	13.10	1040.15	0.150407	59.1	111.80	2.98	0.2
27	27	6.70	3200.15	0.143236	389.1	426.70	2.51	0.4
28	66	19.00	2840.15	0.203330	291.0	290.40	3.59	0.1
29	68	18.40	3141.15	0.212261	317.0	316.40	3.56	0.1
30	64	19.90	3546.15	0.194400	398.0	397.50	3.64	0.2
31	72	13.60	4873.15	0.229987	575.0	618.40	3.20	0.1
32	67	18.70	2973.15	0.207795	301.0	300.60	3.58	0.1
33	71	17.80	3675.15	0.225650	414.0	427.60	3.51	0.1
34	12	14.00	1363.15	0.121644	131.8	147.10	3.21	1.0
35	75	8.85	5863.15	0.243516	704.0	774.00	2.76	0.1
36	21	15.00	3109.15	0.119383	332.7	377.80	3.31	0.5
37	65	19.20	3503.15	0.198863	389.0	388.70	3.60	0.1
38	22	10.60	3560.15	0.123364	422.6	473.00	2.95	0.5
39	81	17.20	1746.15	0.173447	162.4	182.20	3.46	0.1
40	69	18.10	2223.15	0.216724	232.0	232.20	3.54	0.1
41	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

	atomic_number	atomic_volume	boiling_point	en_ghosh	evaporation_heat	heat_of_formation	lattice_constant	specific_he
41	39	19.80	3618.15	0.121699	367.0	424.70	3.65	0.2
42	30	9.20	1180.15	0.155152	114.8	130.40	2.66	0.3

2. Processing and Organizing Data

Most machine learning models are trained on a subset of all the available data, called the "training set", and the models are tested on the remainder of the available data, called the "testing set". Model performance has often been found to be enhanced when the inputs are normalized.

SETS

With the dataset we just created, we have 44 entries for our model. We will train with 39 cases and test on the remaining 5 elements to estimate Young's Modulus.

NORMALIZATION

Each one of these input data features has different units and is represented in scales with distinct orders of magnitude. Datasets that contain inputs like this need to be normalized, so that quantities with large values do not bias the neural network, forcing it tune its weights to account for the different scales of our input data. In this tutorial, we will use the Standard Score Normalization, which subtracts the mean of the feature and divide by its standard deviation.

$$\frac{X-\mu}{\sigma}$$

While our model might converge without feature normalization, the resultant model would be difficult to train and would be dependent on the choice of units used in the input.

In [4]:

```
df.to_excel('tut_11_data.xlsx', index=False)
```

In [5]:

```
#We will rewrite the arrays with the patches we made on the dataset by turning the datafr
ame back into a list of lists

all_values = [list(df.iloc[x]) for x in range(len(all_values))]
# all_values is a list of lists.

# read about df.iloc here: https://pandas.pydata.org/docs/reference/api/pandas.DataFrame.
iloc.html

# SETS

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

# Uncomment the line below to shuffle the dataset (we do not do this here to ensure consi
stent results for every run)
#order = np.argsort(np.random.random(all_labels.shape)) # This numpy argsort returns the
indexes that would be used to shuffle a list
order = np.arange(43)
all_values = all_values[order]
all_labels = all_labels[order]

# Training Set, this is a manual partition. If we do the above shuffling, there will be d
ifferent training set
# for each training set.
# We have 43 elements in our dataframe i.e. numpy dataset now. Our of those, 38 are used
for training.
```

```
# Training data includes actual training or 'fitting' and validation. This validation is
done on-the-fly using
# some of the data from training data set. It is called validation dataset. In this examp
les we have 10 % data
# used for validation.
# So, training data. = actual training data + validation data

train_labels = all_labels[:38]
train_values = all_values[:38]

# Testing Set. This dataset is not seen at all by the model before it is fitted.
test_labels = all_labels[-5:]
test_values = all_values[-5:]

# This line is used for labels in the plots at the end of the tutorial - Testing Set
labeled_elements = [elements[x] for x in order[-5:]]
elements = [elements[x] for x in order]

# NORMALIZATION

mean = np.mean(train_values, axis = 0) # mean, calculating mean for each row.
std = np.std(train_values, axis = 0) # standard deviation

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

mean_all = np.mean(all_values, axis = 0) # mean, calculating mean for each row.
std_all = np.std(all_values, axis = 0) # standard deviation
all_values_normalized = (all_values - mean_all) / std_all # input scaling

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

```
Shape of Values: (43, 16)
Shape of Labels: (43,)
[-0.04080514 -0.50673999 -0.61573665 -0.48000707 -0.59640276 -0.57914974
  0.23007252 -0.34851127 -0.1169633   0.27242314 -0.74442966 -0.50761875
 -0.23457382  0.8715687   0.20497176  0.23990096]
[-1.03477644 -0.46692446  0.25397834 -0.97359468  0.30431353  0.3650567
 -0.78177941  0.11430967 -1.03412225 -0.62775766  0.23766706 -0.45697574
 -0.13693109 -0.39396025 -0.84271597 -0.55854493]
[ 0  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42]
```

3. Defining the Model, Training, Testing and Predictions

.Q1 For learning rate 0.001, epochs 20000 and other default setup, run the model for RMSProp, Adam and Gradient Descent and compare the accuracy vs. epochs. Write your observation and reasoning.

RMSProp Optimiser

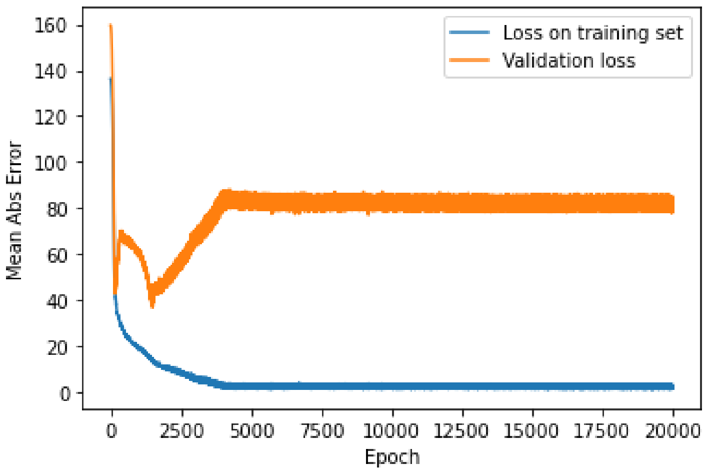
In [6]:

```
# DEFINITION OF THE MODEL
# The weights of our neural network will be initialized in a random manner, using a seed
allows for reproducibility
kernel_init = initializers.RandomNormal(seed=0) # initialization of seed will always pro
duce same result.
bias_init = initializers.Zeros()

model = Sequential() # one input layer and one output layer
# https://keras.io/guides/sequential_model/
```

```
model.add(Dense(16, activation='relu', input_shape=(train_values.shape[1], ), kernel_ini
tializer=kernel_init,
                bias_initializer=bias_init))
model.add(Dense(32, activation='relu', kernel_initializer=kernel_init, bias_initializer=
bias_init))
model.add(Dense(128, activation='relu', kernel_initializer=kernel_init, bias_initializer=
bias_init))
# model.add(Dense(128, activation='relu', kernel_initializer=kernel_init, bias_initialize
r=bias_init))
model.add(Dense(1, kernel_initializer=kernel_init, bias_initializer=bias_init))

EPOCHS = 20000 # Number of EPOCHS
my_learning_rate = 0.001
my_decay_rate = my_learning_rate / EPOCHS

# CHOOSING THE OPTIMIZER

optimizer = optimizers.RMSprop(learning_rate=my_learning_rate,decay=my_decay_rate) # RMSP
rop. Initial learning rate has been set to 0.001
# optimizer = optimizers.Adam(0.001) # AdaM
# optimizer = optimizers.SGD(0.001) # SGD
#
# 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'])
# mae is Mean Absolute Error
# Read more about regression losses: https://keras.io/api/losses/regression_losses/

model.summary() # this will show a chart of the 'architecture' of the model i.e. arrangem
ent of layers etc.

#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')
                         + " Validation Loss: " + "%4f" %logs.get('val_loss')
                         + '                                         \r') # Updates curre
nt Epoch Number
# 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, shuffle=False, validation_split=0.1,
callbacks=[PrintEpNum()])

# Validation split is the 10 % of training data which will be used for on-the-fly 'verifi
cation' of fit.

# PLOTTING HISTORY USING MATPLOTLIB

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

```
Model: "sequential"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dense (Dense)               (None, 16)                272

 dense_1 (Dense)             (None, 32)                544

 dense_2 (Dense)             (None, 128)               4224

 dense_3 (Dense)             (None, 1)                 129
```

```
=================================================================
Total params: 5,169
Trainable params: 5,169
Non-trainable params: 0
_________________________________________________________________
Current Epoch: 20000 Training Loss: 1.255679 Validation Loss: 78.393318
```



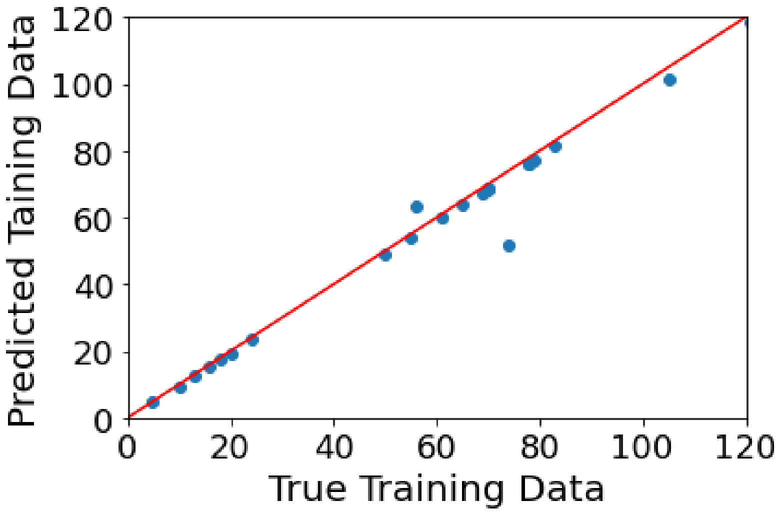
RMSProp is an optimization algorithm that adapts the learning rate for each parameter based on the average of the squared gradients for that parameter. It can improve the convergence of the model by decreasing the learning rate for parameters with high variance

However after certain number of epochs the validation loss shoots up again due to overfitting of the data and not actually capturing the pattern of the data. We can also see that loss on training dataset continuously decreases due to minimisation of biasness of the data but the variance shoots up as both are inversely proportion

In [7]:

```
# Check the predictions of training data by the model
train_labels_predict=model.predict(train_values)
#
plt.scatter(train_labels,train_labels_predict)
plt.ylabel('Predicted Taining Data',fontsize=20)
plt.xlabel('True Training Data',fontsize=20)
plt.xticks(fontsize=18)
plt.yticks(fontsize=18)
plt.xlim(0,120)
plt.ylim(0,120)
plt.axline([0, 0], [1, 1],color='red')
plt.show()
```

```
2/2 [==============================] - 0s 5ms/step
```



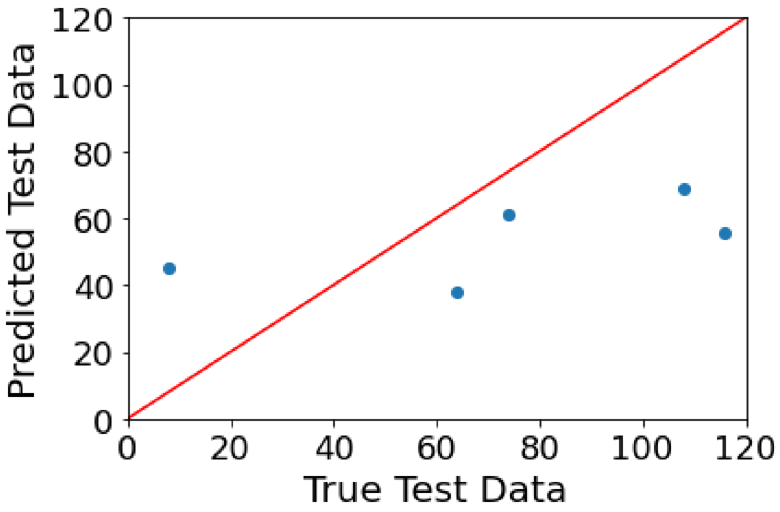
In [ ]:

In [ ]:

In [8]:

```
# Check the predictions of only test data by the model
test_labels_predict=model.predict(test_values)
#np.shape(test_labels_predict)
#np.shape(test_labels)
# Plot the predictions of only test data by the model
plt.scatter(test_labels,test_labels_predict)
plt.ylabel('Predicted Test Data',fontsize=20)
plt.xlabel('True Test Data',fontsize=20)
plt.xticks(fontsize=18)
plt.yticks(fontsize=18)
plt.xlim(0,120)
plt.ylim(0,120)
plt.axline([0, 0], [1, 1],color='red')
plt.show()
```

```
1/1 [==============================] - 0s 80ms/step
```



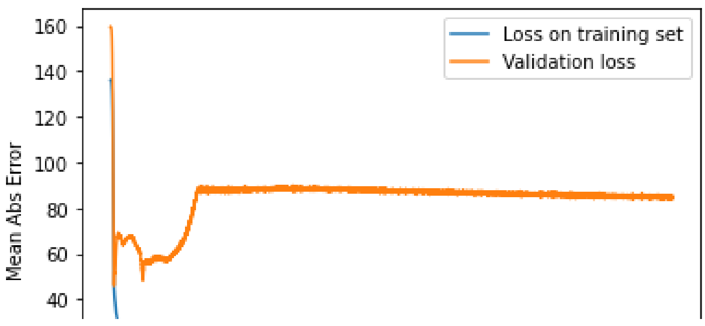
Adam Optimiser

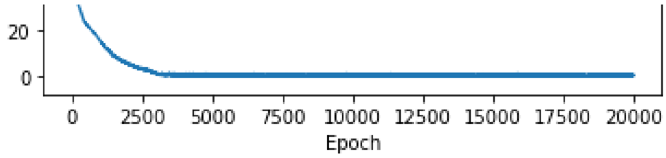
In [10]:

```
# DEFINITION OF THE MODEL
# The weights of our neural network will be initialized in a random manner, using a seed
allows for reproducibility
kernel_init = initializers.RandomNormal(seed=0)
bias_init = initializers.Zeros()

model = Sequential()
model.add(Dense(16, activation='relu', input_shape=(train_values.shape[1], ), kernel_ini
tializer=kernel_init,
                bias_initializer=bias_init))
model.add(Dense(32, activation='relu', kernel_initializer=kernel_init, bias_initializer=
bias_init))
model.add(Dense(128, activation='relu', kernel_initializer=kernel_init, bias_initializer=
bias_init))
# model.add(Dense(128, activation='relu', kernel_initializer=kernel_init, bias_initialize
r=bias_init))
model.add(Dense(1, kernel_initializer=kernel_init, bias_initializer=bias_init))

# DEFINITION OF THE OPTIMIZER
EPOCHS = 20000 # Number of EPOCHS
my_learning_rate = 0.001
my_decay_rate = my_learning_rate / EPOCHS
```

```
# optimizer = optimizers.RMSprop(0.001) # RMSProp
optimizer = optimizers.Adam(learning_rate=my_learning_rate,decay=my_decay_rate)#0.001) #
AdaM
# optimizer = optimizers.SGD(0.001) # SGD

# 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()

#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')
                         + " Validation Loss: " + "%4f" %logs.get('val_loss')
                         + '                                          \r') # Updates curre
nt Epoch Number

EPOCHS = 20000 # 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, shuffle=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['loss']),label='Loss on training set')
plt.plot(history.epoch, np.array(history.history['val_loss']),label = 'Validation loss')
plt.legend()
plt.show()
```

```
Model: "sequential_2"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dense_8 (Dense)             (None, 16)                272

 dense_9 (Dense)             (None, 32)                544

 dense_10 (Dense)            (None, 128)               4224

 dense_11 (Dense)            (None, 1)                 129

=================================================================
Total params: 5,169
Trainable params: 5,169
Non-trainable params: 0
_________________________________________________________________
Current Epoch: 20000 Training Loss: 0.423276 Validation Loss: 84.223587
```





The Adam optimizer is a popular optimization algorithm used for training neural networks. It is an adaptive learning rate optimization algorithm that combines the advantages of two other optimization techniques: AdaGrad and RMSProp. During the training process, the Adam optimizer updates the model's weights by taking into account the gradients of the loss function with respect to the weights. The optimizer uses a combination of the first and second moments of the gradients to update the weights. of the first and second moments of the gradients to update the weights..

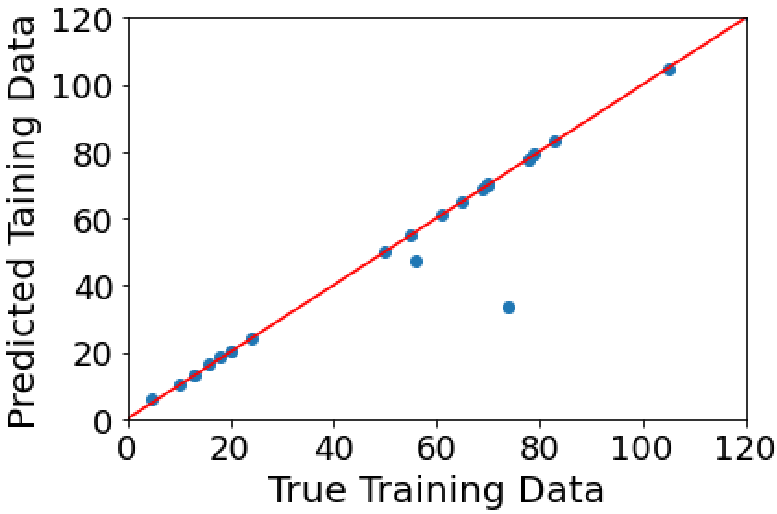
In some cases, after a certain number of epochs, the validation loss may increase while the training loss continues to decrease. This phenomenon is called overfitting. Overfitting occurs when the model becomes too complex and starts to fit the training data too closely, resulting in poor performance on new data (i.e., the validation set). One possible explanation for this behavior is that the model has learned to fit the noise in the training data instead of the underlying patterns. As a result, the model becomes less generalizable to new data, which leads to an increase in the validation loss

Predictions by ADAM optimizer

In [11]:

```
# Check the predictions of training data by the model
train_labels_predict=model.predict(train_values)
#
plt.scatter(train_labels,train_labels_predict)
plt.ylabel('Predicted Taining Data',fontsize=20)
plt.xlabel('True Training Data',fontsize=20)
plt.xticks(fontsize=18)
plt.yticks(fontsize=18)
plt.xlim(0,120)
plt.ylim(0,120)
plt.axline([0, 0], [1, 1],color='red')
plt.show()
```

```
2/2 [==============================] - 0s 4ms/step
```



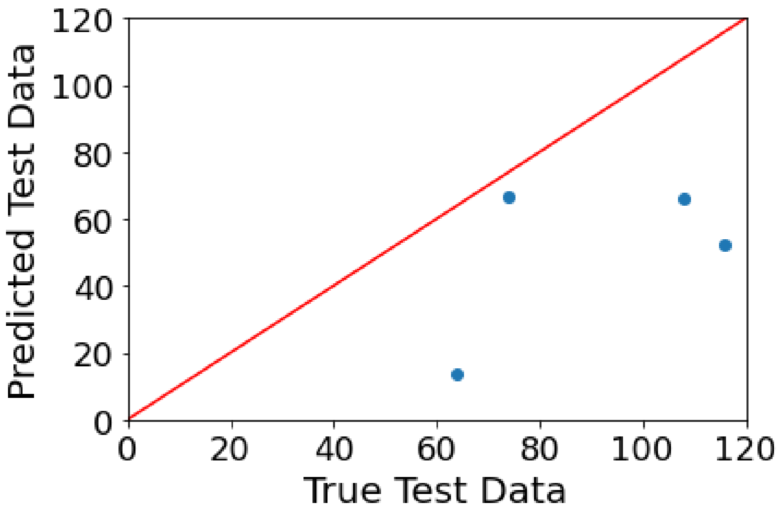
Due to the overfitting the training data fits best with almost zero loss

In [12]:

```
# Check the predictions of only test data by the model
test_labels_predict=model.predict(test_values)
#np.shape(test_labels_predict)
```

```
#np.shape(test_labels)
# Plot the predictions of only test data by the model
plt.scatter(test_labels,test_labels_predict)
plt.ylabel('Predicted Test Data',fontsize=20)
plt.xlabel('True Test Data',fontsize=20)
plt.xticks(fontsize=18)
plt.yticks(fontsize=18)
plt.xlim(0,120)
plt.ylim(0,120)
plt.axline([0, 0], [1, 1],color='red')
plt.show()
```

```
1/1 [==============================] - 0s 55ms/step
```



The Model fails to capture the test data which is the alien data for the model and hence validation loss is huge

In [ ]:

```

```

Gradient Descent Optimiser

In [ ]:

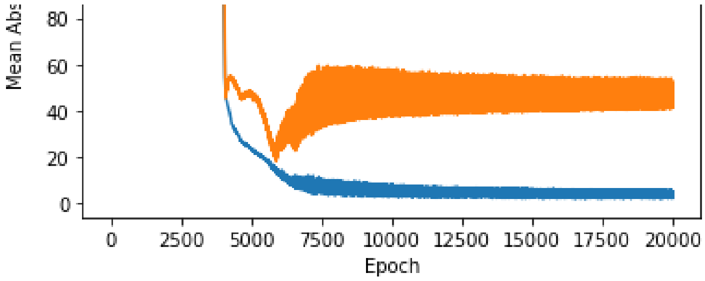
```

```

In [13]:

```
# DEFINITION OF THE MODEL
# The weights of our neural network will be initialized in a random manner, using a seed
allows for reproducibility
kernel_init = initializers.RandomNormal(seed=0)
bias_init = initializers.Zeros()

model = Sequential()
model.add(Dense(16, activation='relu', input_shape=(train_values.shape[1], ), kernel_ini
tializer=kernel_init,
                bias_initializer=bias_init))
#model.add(Dense(32, activation='relu', kernel_initializer=kernel_init, bias_initializer=
bias_init))
model.add(Dense(16, activation='relu', kernel_initializer=kernel_init, bias_initializer=
bias_init))

#model.add(Dense(128, activation='relu', kernel_initializer=kernel_init, bias_initializer
=bias_init))
model.add(Dense(16, activation='relu', kernel_initializer=kernel_init, bias_initializer=
bias_init))

# model.add(Dense(128, activation='relu', kernel_initializer=kernel_init, bias_initialize
```

```
r=bias_init))
model.add(Dense(1, kernel_initializer=kernel_init, bias_initializer=bias_init))

# DEFINITION OF THE OPTIMIZER
EPOCHS = 20000 # Number of EPOCHS
my_learning_rate = 0.001
my_decay_rate = my_learning_rate / EPOCHS

# optimizer = optimizers.RMSprop(0.001) # RMSProp
# optimizer = optimizers.Adam(0.001) # AdaM
optimizer = optimizers.SGD(learning_rate=my_learning_rate,decay=my_decay_rate) # SGD

# 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()

#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')
                         + " Validation Loss: " + "%4f" %logs.get('val_loss')
                         + '                                          \r') # Updates curre
nt Epoch Number

# 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, shuffle=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['loss']),label='Loss on training set')
plt.plot(history.epoch, np.array(history.history['val_loss']),label = 'Validation loss')
plt.legend()
plt.show()
```

```
Model: "sequential_3"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dense_12 (Dense)            (None, 16)                272

 dense_13 (Dense)            (None, 16)                272

 dense_14 (Dense)            (None, 16)                272

 dense_15 (Dense)            (None, 1)                 17

=================================================================
Total params: 833
Trainable params: 833
Non-trainable params: 0
_________________________________________________________________
Current Epoch: 20000 Training Loss: 2.615557 Validation Loss: 44.193333
```



Gradient descent optimizes the training process by iteratively adjusting the model parameters to minimize the training loss. As the number of epochs (i.e., training iterations) increases, the optimization process attempts to further minimize the training loss by finding the optimal set of parameters for the given training data. However, minimizing the training loss alone does not guarantee good performance on unseen data. This is where the validation loss comes into play. The validation loss measures the model's performance on a separate validation set, which consists of data that the model has not been trained on

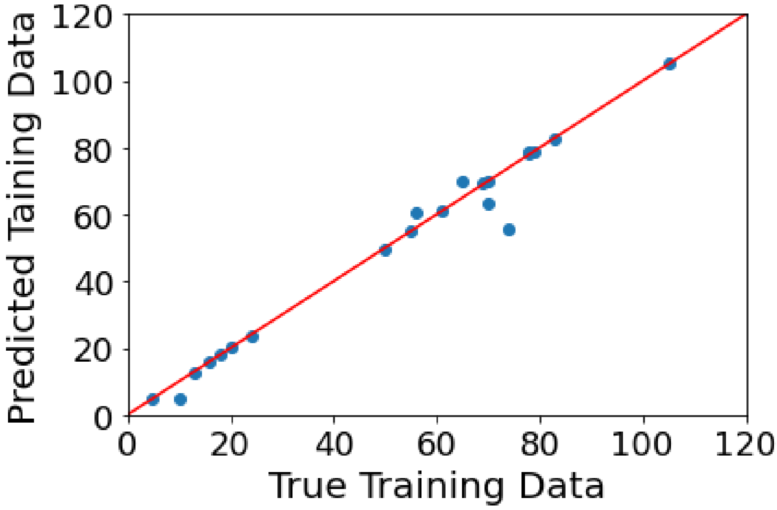
here again at certain nummber of epochs the validation loss gets minimised but after the epochs increased the validation loss shoots up and the validation loss kept on increasing because of the overfitting

Predictions by GD

In [19]:

```
# Check the predictions of training data by the model
train_labels_predict=model.predict(train_values)
#
plt.scatter(train_labels,train_labels_predict)
plt.ylabel('Predicted Taining Data',fontsize=20)
plt.xlabel('True Training Data',fontsize=20)
plt.xticks(fontsize=18)
plt.yticks(fontsize=18)
plt.xlim(0,120)
plt.ylim(0,120)
plt.axline([0, 0], [1, 1],color='red')
plt.show()
```

```
2/2 [==============================] - 0s 6ms/step
```



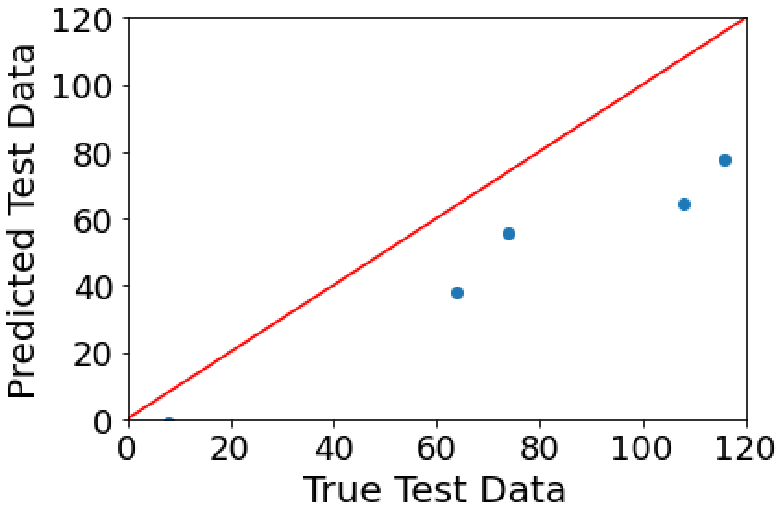
Due to the overfitting the training data fits best with loss minimised

In [20]:

```
# Check the predictions of only test data by the model
test_labels_predict=model.predict(test_values)
#np.shape(test_labels_predict)
#np.shape(test_labels)
# Plot the predictions of only test data by the model
plt.scatter(test_labels,test_labels_predict)
```

```
plt.ylabel('Predicted Test Data',fontsize=20)
plt.xlabel('True Test Data',fontsize=20)
plt.xticks(fontsize=18)
plt.yticks(fontsize=18)
plt.xlim(0,120)
plt.ylim(0,120)
plt.axline([0, 0], [1, 1],color='red')
plt.show()
```

```
1/1 [==============================] - 0s 56ms/step
```



The Model fails to capture the test data which is the alien data for the model and hence validation loss is huge

Q2 . For epochs 20000 and other default setup, run the model for Adam Optimizer for learning rate 0.01, 0.001 and 0.0001 and compare the accuracy vs. epochs. Write your observation and reasoning.

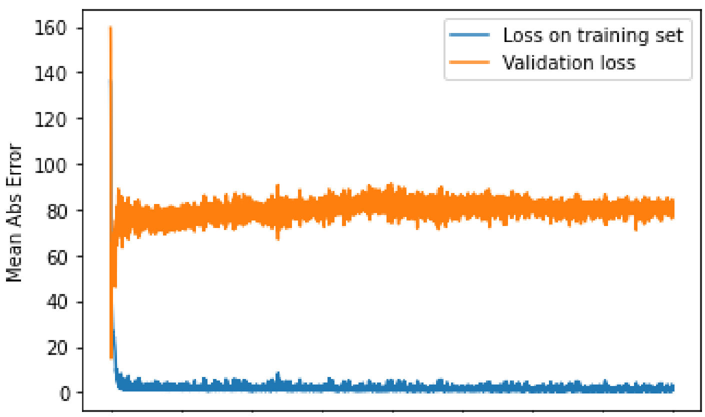
For 0.01

In [14]:

```
# DEFINITION OF THE MODEL
# The weights of our neural network will be initialized in a random manner, using a seed allows for reproducibility
kernel_init = initializers.RandomNormal(seed=0)
bias_init = initializers.Zeros()

model = Sequential()
model.add(Dense(16, activation='relu', input_shape=(train_values.shape[1], ), kernel_initializer=kernel_init,
                bias_initializer=bias_init))
model.add(Dense(32, activation='relu', kernel_initializer=kernel_init, bias_initializer=bias_init))
model.add(Dense(128, activation='relu', kernel_initializer=kernel_init, bias_initializer=bias_init))
# model.add(Dense(128, activation='relu', kernel_initializer=kernel_init, bias_initializer=bias_init))
model.add(Dense(1, kernel_initializer=kernel_init, bias_initializer=bias_init))

# DEFINITION OF THE OPTIMIZER
EPOCHS = 20000 # Number of EPOCHS
my_learning_rate = 0.01
my_decay_rate = my_learning_rate / EPOCHS


# optimizer = optimizers.RMSprop(0.001) # RMSProp
optimizer = optimizers.Adam(learning_rate=my_learning_rate,decay=my_decay_rate)#0.001) #
```

```
AdaM
# optimizer = optimizers.SGD(0.001) # SGD

# 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()

#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')
                         + " Validation Loss: " + "%4f" %logs.get('val_loss')
                         + '                                    \r') # Updates curre
nt Epoch Number

EPOCHS = 20000 # 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, shuffle=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['loss']),label='Loss on training set')
plt.plot(history.epoch, np.array(history.history['val_loss']),label = 'Validation loss')
plt.legend()
plt.show()
```

```
Model: "sequential_4"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dense_16 (Dense)            (None, 16)                272

 dense_17 (Dense)            (None, 32)                544

 dense_18 (Dense)            (None, 128)               4224

 dense_19 (Dense)            (None, 1)                 129

=================================================================
Total params: 5,169
Trainable params: 5,169
Non-trainable params: 0
_________________________________________________________________
Current Epoch: 20000 Training Loss: 2.308318 Validation Loss: 80.562935
```



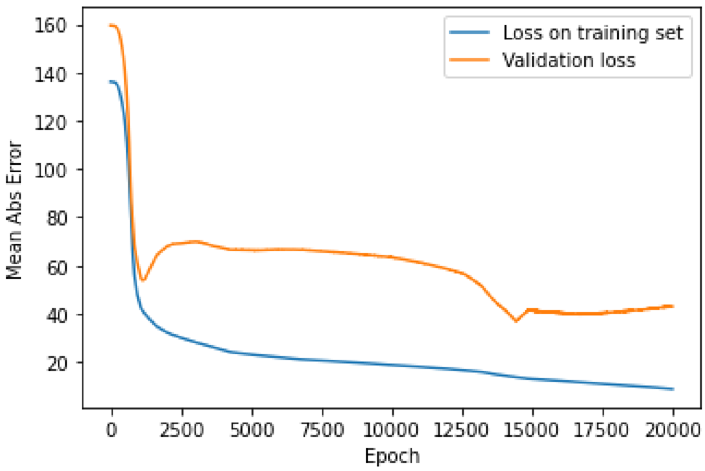
for learning rate = 0.0001

In [15]:

```
# DEFINITION OF THE MODEL
# The weights of our neural network will be initialized in a random manner, using a seed
allows for reproducibility
kernel_init = initializers.RandomNormal(seed=0)
bias_init = initializers.Zeros()

model = Sequential()
model.add(Dense(16, activation='relu', input_shape=(train_values.shape[1], ), kernel_ini
tializer=kernel_init,
                bias_initializer=bias_init))
model.add(Dense(32, activation='relu', kernel_initializer=kernel_init, bias_initializer=
bias_init))
model.add(Dense(128, activation='relu', kernel_initializer=kernel_init, bias_initializer=
bias_init))
# model.add(Dense(128, activation='relu', kernel_initializer=kernel_init, bias_initialize
r=bias_init))
model.add(Dense(1, kernel_initializer=kernel_init, bias_initializer=bias_init))

# DEFINITION OF THE OPTIMIZER
EPOCHS = 20000 # Number of EPOCHS
my_learning_rate = 0.0001
my_decay_rate = my_learning_rate / EPOCHS


# optimizer = optimizers.RMSprop(0.001) # RMSProp
optimizer = optimizers.Adam(learning_rate=my_learning_rate,decay=my_decay_rate)#0.001) #
AdaM
# optimizer = optimizers.SGD(0.001) # SGD

# 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()

#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')
                         + " Validation Loss: " + "%4f" %logs.get('val_loss')
                         + '                                        \r') # Updates curre
nt Epoch Number

EPOCHS = 20000 # 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, shuffle=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['loss']),label='Loss on training set')
plt.plot(history.epoch, np.array(history.history['val_loss']),label = 'Validation loss')
plt.legend()
```

```
plt.show()
```

```
Model: "sequential_5"
_________________________________________________________________
 Layer (type)                Output Shape              Param #   
=================================================================
 dense_20 (Dense)            (None, 16)                272       
                                                                 
 dense_21 (Dense)            (None, 32)                544       
                                                                 
 dense_22 (Dense)            (None, 128)               4224      
                                                                 
 dense_23 (Dense)            (None, 1)                 129       
                                                                 
=================================================================
Total params: 5,169
Trainable params: 5,169
Non-trainable params: 0
_________________________________________________________________
Current Epoch: 20000 Training Loss: 8.705514 Validation Loss: 42.888947
```



In [ ]:

```

```

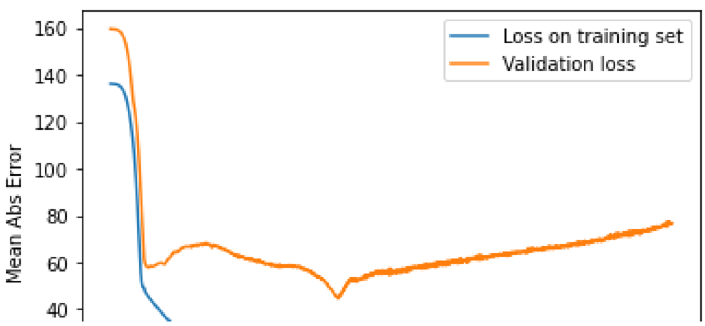
for 0.001

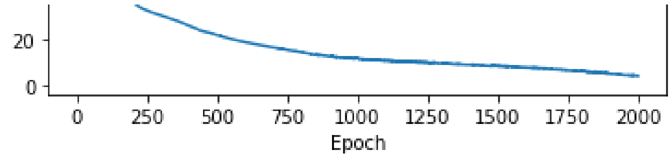
In [24]:

```
# DEFINITION OF THE MODEL
# The weights of our neural network will be initialized in a random manner, using a seed
allows for reproducibility
kernel_init = initializers.RandomNormal(seed=0)
bias_init = initializers.Zeros()

model = Sequential()
model.add(Dense(16, activation='relu', input_shape=(train_values.shape[1], ), kernel_ini
tializer=kernel_init,
                bias_initializer=bias_init))
model.add(Dense(32, activation='relu', kernel_initializer=kernel_init, bias_initializer=
bias_init))
model.add(Dense(128, activation='relu', kernel_initializer=kernel_init, bias_initializer=
bias_init))
# model.add(Dense(128, activation='relu', kernel_initializer=kernel_init, bias_initialize
r=bias_init))
model.add(Dense(1, kernel_initializer=kernel_init, bias_initializer=bias_init))

# DEFINITION OF THE OPTIMIZER
EPOCHS = 20000 # Number of EPOCHS
my_learning_rate = 0.001
my_decay_rate = my_learning_rate / EPOCHS
```

```
# optimizer = optimizers.RMSprop(0.001) # RMSProp
optimizer = optimizers.Adam(learning_rate=my_learning_rate,decay=my_decay_rate)#0.001) #
AdaM
# optimizer = optimizers.SGD(0.001) # SGD

# 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()

#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')
                         + " Validation Loss: " + "%4f" %logs.get('val_loss')
                         + '                                          \r') # Updates curre
nt Epoch Number

EPOCHS = 20000 # 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, shuffle=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['loss']),label='Loss on training set')
plt.plot(history.epoch, np.array(history.history['val_loss']),label = 'Validation loss')
plt.legend()
plt.show()
```

```
Model: "sequential_9"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dense_32 (Dense)            (None, 16)                272

 dense_33 (Dense)            (None, 32)                544

 dense_34 (Dense)            (None, 128)               4224

 dense_35 (Dense)            (None, 1)                 129

=================================================================
Total params: 5,169
Trainable params: 5,169
Non-trainable params: 0
_________________________________________________________________
Current Epoch: 2000 Training Loss: 4.340346 Validation Loss: 76.706619
```





In [ ]:

```

```

For Learning rate = 0.01 --- Training Loss: 1.758114 Validation Loss: 74.715210

Here the bias variance trade off is not maintained training loss is very less but the validation loss is very high. Overfitting case

For Learning rate = 0.001 ---- Training Loss: 32.577240 Validation Loss: 49.114491

Here the bias variance trade off is maintained and training loss and valiation loss are comparable with each other.. Also with epochs increasing the validaton loss kept on decreasing indicating the model performed better here and learning the data pattern

For Learning rate = 0.0001 ---- Training Loss: 4.340346 Validation Loss: 76.706619

Here , the bias variance trade off is not maintained training loss is very less but the validation loss is very high.This implies model is overfitting

In [ ]:

```

```

In [ ]:

```

```

Q 3 For learning rate 0.01, epochs 2000 and other default setup, run the model for Adam Optimizer for 16 units, 32 units and 64 units in the first layer and compare the loss vs. epochs. Write your observation and reasoning.

In [ ]:

```

```

In [ ]:

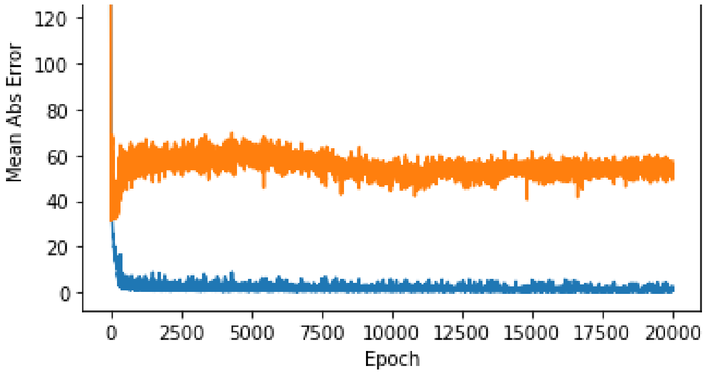
```

```

In [16]:

```
# DEFINITION OF THE MODEL
# The weights of our neural network will be initialized in a random manner, using a seed
allows for reproducibility
kernel_init = initializers.RandomNormal(seed=0)
bias_init = initializers.Zeros()

model = Sequential()
model.add(Dense(16, activation='relu', input_shape=(train_values.shape[1], ), kernel_ini
tializer=kernel_init,
                bias_initializer=bias_init))
model.add(Dense(32, activation='relu', kernel_initializer=kernel_init, bias_initializer=
bias_init))
model.add(Dense(128, activation='relu', kernel_initializer=kernel_init, bias_initializer=
bias_init))
# model.add(Dense(128, activation='relu', kernel_initializer=kernel_init, bias_initialize
r=bias_init))
```

```
model.add(Dense(1, kernel_initializer=kernel_init, bias_initializer=bias_init))

# DEFINITION OF THE OPTIMIZER
EPOCHS = 20000  # r of EPOCHS
my_learning_rate = 0.01
my_decay_rate = my_learning_rate / EPOCHS


# optimizer = optimizers.RMSprop(0.001) # RMSProp
optimizer = optimizers.Adam(learning_rate=my_learning_rate,decay=my_decay_rate)#0.001) #
AdaM
# optimizer = optimizers.SGD(0.001) # SGD

# 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()

#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')
                         + " Validation Loss: " + "%4f" %logs.get('val_loss')
                         + '                                    \r') # Updates curre
nt Epoch Number

EPOCHS = 20000# 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, shuffle=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['loss']),label='Loss on training set')
plt.plot(history.epoch, np.array(history.history['val_loss']),label = 'Validation loss')
plt.legend()
plt.show()
```

```
Model: "sequential_6"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dense_24 (Dense)            (None, 16)                272

 dense_25 (Dense)            (None, 32)                544

 dense_26 (Dense)            (None, 128)               4224

 dense_27 (Dense)            (None, 1)                 129

=================================================================
Total params: 5,169
Trainable params: 5,169
Non-trainable params: 0
_________________________________________________________________
Current Epoch: 20000 Training Loss: 2.543922 Validation Loss: 57.465054
```



In [ ]:

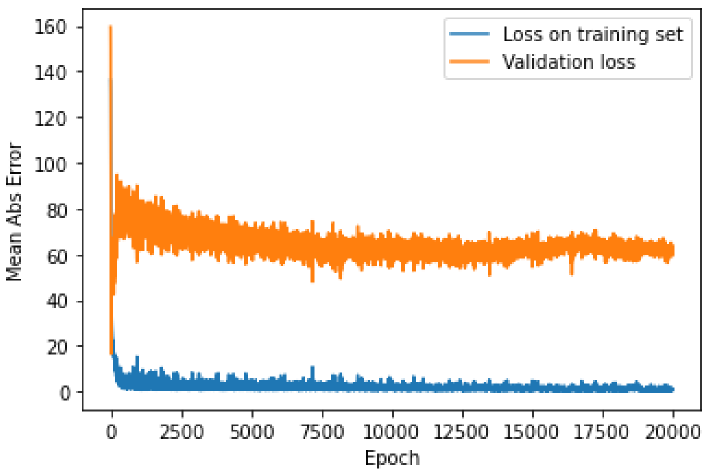
for 32 units in the first layer

In [17]:

```
# DEFINITION OF THE MODEL
# The weights of our neural network will be initialized in a random manner, using a seed
allows for reproducibility
kernel_init = initializers.RandomNormal(seed=0)
bias_init = initializers.Zeros()

model = Sequential()
model.add(Dense( 32,activation='relu', input_shape=(train_values.shape[1], ), kernel_ini
tializer=kernel_init,
                bias_initializer=bias_init))
model.add(Dense(32, activation='relu', kernel_initializer=kernel_init, bias_initializer=
bias_init))
model.add(Dense(128, activation='relu', kernel_initializer=kernel_init, bias_initializer=
bias_init))
# model.add(Dense(128, activation='relu', kernel_initializer=kernel_init, bias_initialize
r=bias_init))
model.add(Dense(1, kernel_initializer=kernel_init, bias_initializer=bias_init))

# DEFINITION OF THE OPTIMIZER
EPOCHS =20000# Number of EPOCHS
my_learning_rate = 0.01
my_decay_rate = my_learning_rate / EPOCHS


# optimizer = optimizers.RMSprop(0.001) # RMSProp
optimizer = optimizers.Adam(learning_rate=my_learning_rate,decay=my_decay_rate)#0.001) #
AdaM
# optimizer = optimizers.SGD(0.001) # SGD

# 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()

#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')
                         + " Validation Loss: " + "%4f" %logs.get('val_loss')
                         + '                                        \r') # Updates curre
nt Epoch Number

EPOCHS = 20000 # 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, shuffle=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['loss']),label='Loss on training set')
plt.plot(history.epoch, np.array(history.history['val_loss']),label = 'Validation loss')
plt.legend()
plt.show()
```

```
Model: "sequential_7"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dense_28 (Dense)            (None, 32)                544

 dense_29 (Dense)            (None, 32)                1056

 dense_30 (Dense)            (None, 128)               4224

 dense_31 (Dense)            (None, 1)                 129

=================================================================
Total params: 5,953
Trainable params: 5,953
Non-trainable params: 0
_________________________________________________________________
Current Epoch: 20000 Training Loss: 0.664293 Validation Loss: 60.765953
```



In [ ]:

For 64 units in the first layer

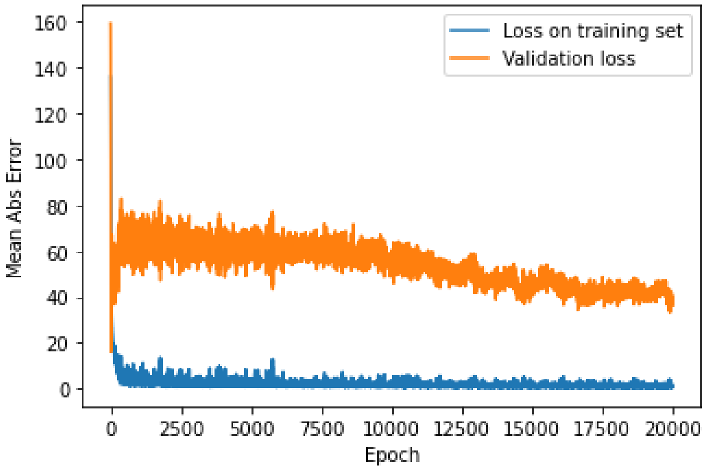
In [18]:

```
# DEFINITION OF THE MODEL
# The weights of our neural network will be initialized in a random manner, using a seed
allows for reproducibility
kernel_init = initializers.RandomNormal(seed=0)
bias_init = initializers.Zeros()

model = Sequential()
model.add(Dense(64, activation='relu', input_shape=(train_values.shape[1], ), kernel_ini
tializer=kernel_init,
                bias_initializer=bias_init))
```

```
model.add(Dense(32, activation='relu', kernel_initializer=kernel_init, bias_initializer=
bias_init))
model.add(Dense(128, activation='relu', kernel_initializer=kernel_init, bias_initializer=
bias_init))
# model.add(Dense(128, activation='relu', kernel_initializer=kernel_init, bias_initialize
r=bias_init))
model.add(Dense(1, kernel_initializer=kernel_init, bias_initializer=bias_init))

# DEFINITION OF THE OPTIMIZER
EPOCHS = 20000 # Number of EPOCHS
my_learning_rate = 0.01
my_decay_rate = my_learning_rate / EPOCHS


# optimizer = optimizers.RMSprop(0.001) # RMSProp
optimizer = optimizers.Adam(learning_rate=my_learning_rate,decay=my_decay_rate)#0.001) #
AdaM
# optimizer = optimizers.SGD(0.001) # SGD

# 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()

#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')
                         + " Validation Loss: " + "%4f" %logs.get('val_loss')
                         + '                                          \r') # Updates curre
nt Epoch Number

EPOCHS = 20000 # 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, shuffle=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['loss']),label='Loss on training set')
plt.plot(history.epoch, np.array(history.history['val_loss']),label = 'Validation loss')
plt.legend()
plt.show()
```

```
Model: "sequential_8"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dense_32 (Dense)            (None, 64)                1088

 dense_33 (Dense)            (None, 32)                2080

 dense_34 (Dense)            (None, 128)               4224

 dense_35 (Dense)            (None, 1)                 129

=================================================================
Total params: 7,521
Trainable params: 7,521
Non-trainable params: 0
_________________________________________________________________
```

```
Current Epoch: 20000 Training Loss: 0.509566 Validation Loss: 39.504852
```



In [ ]:

```

```

In [ ]:

```

```

for units 16 = --- Training Loss: 2.537484 Validation Loss: 57.663315

For 32 units = - -- Training Loss: 0.664293 Validation Loss: 60.765953

For 64 Units = - ---- Training Loss: 0.509566 Validation Loss: 39.504852

There is no effect on increasing the units in the first layer ,increasing the number of units in the first layer could increase the risk of overfitting, where the model becomes too complex and starts to memorize the training data instead of learning generalizable patterns. This lead to poor performance on new, unseen data.

In [ ]:

```

```

Q4 For learning rate 0.01, epochs 20000 and other default setup, run the model for Adam Optimizer for ReLU, tanh and softmax activation functions in the hidden layer and compare the accuracy vs. epochs. Write your observation and reasoning?

using only 1000 epochs due to inability of juoyter to perform at faster rate

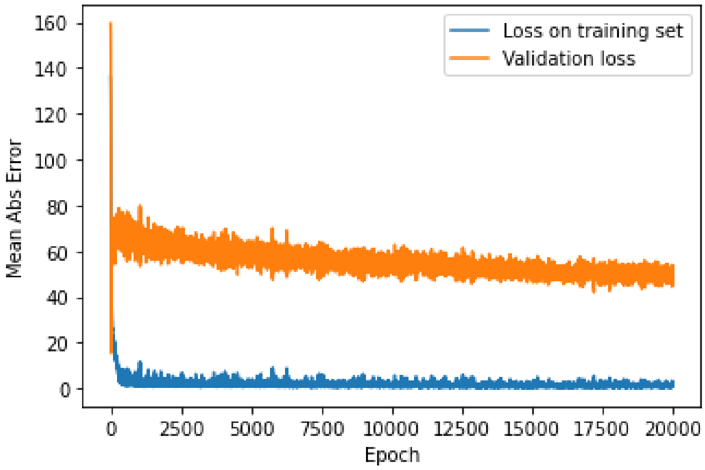
FOr ReLU activation function

In [19]:

```
# DEFINITION OF THE MODEL
# The weights of our neural network will be initialized in a random manner, using a seed
allows for reproducibility
kernel_init = initializers.RandomNormal(seed=0)
bias_init = initializers.Zeros()

model = Sequential()
model.add(Dense(16, activation='relu', input_shape=(train_values.shape[1], ), kernel_ini
tializer=kernel_init,
                bias_initializer=bias_init))
model.add(Dense(32, activation='relu', kernel_initializer=kernel_init, bias_initializer=
bias_init))
```

```
model.add(Dense(128, activation='relu', kernel_initializer=kernel_init, bias_initializer=
bias_init))
# model.add(Dense(128, activation='relu', kernel_initializer=kernel_init, bias_initialize
r=bias_init))
model.add(Dense(1, kernel_initializer=kernel_init, bias_initializer=bias_init))

# DEFINITION OF THE OPTIMIZER
EPOCHS = 20000 # Number of EPOCHS
my_learning_rate = 0.01
my_decay_rate = my_learning_rate / EPOCHS


# optimizer = optimizers.RMSprop(0.001) # RMSProp
optimizer = optimizers.Adam(learning_rate=my_learning_rate,decay=my_decay_rate)#0.001) #
AdaM
# optimizer = optimizers.SGD(0.001) # SGD

# 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()

#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')
                         + " Validation Loss: " + "%4f" %logs.get('val_loss')
                         + '                                         \r') # Updates curre
nt Epoch Number

EPOCHS = 20000 # 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, shuffle=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['loss']),label='Loss on training set')
plt.plot(history.epoch, np.array(history.history['val_loss']),label = 'Validation loss')
plt.legend()
plt.show()
```

```
Model: "sequential_9"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dense_36 (Dense)            (None, 16)                272

 dense_37 (Dense)            (None, 32)                544

 dense_38 (Dense)            (None, 128)               4224

 dense_39 (Dense)            (None, 1)                 129

=================================================================
Total params: 5,169
Trainable params: 5,169
Non-trainable params: 0
_________________________________________________________________
Current Epoch: 20000 Training Loss: 2.388709 Validation Loss: 46.047752
```



In [ ]:

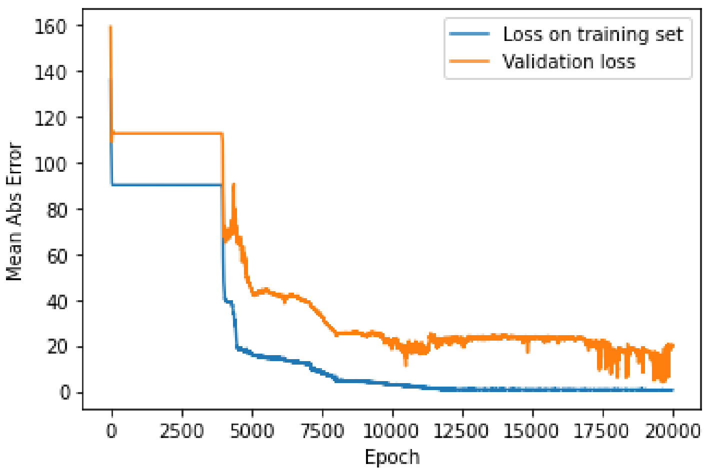
In [ ]:

In [20]:

```
# DEFINITION OF THE MODEL
# The weights of our neural network will be initialized in a random manner, using a seed
allows for reproducibility
kernel_init = initializers.RandomNormal(seed=0)
bias_init = initializers.Zeros()

model = Sequential()
model.add(Dense(16, activation='relu', input_shape=(train_values.shape[1], ), kernel_ini
tializer=kernel_init,
                bias_initializer=bias_init))
model.add(Dense(32, activation='tanh', kernel_initializer=kernel_init, bias_initializer=
bias_init))
model.add(Dense(128, activation='tanh', kernel_initializer=kernel_init, bias_initializer=
bias_init))
# model.add(Dense(128, activation='relu', kernel_initializer=kernel_init, bias_initialize
r=bias_init))
model.add(Dense(1, kernel_initializer=kernel_init, bias_initializer=bias_init))

# DEFINITION OF THE OPTIMIZER
EPOCHS = 20000 # Number of EPOCHS
my_learning_rate = 0.01
my_decay_rate = my_learning_rate / EPOCHS


# optimizer = optimizers.RMSprop(0.001) # RMSProp
optimizer = optimizers.Adam(learning_rate=my_learning_rate,decay=my_decay_rate)#0.001) #
AdaM
# optimizer = optimizers.SGD(0.001) # SGD

# 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()

#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')
                         + " Validation Loss: " + "%4f" %logs.get('val_loss')
                         + '                                    \r') # Updates curre
nt Epoch Number
```

```
EPOCHS = 20000 # 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, shuffle=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['loss']),label='Loss on training set')
plt.plot(history.epoch, np.array(history.history['val_loss']),label = 'Validation loss')
plt.legend()
plt.show()
```

```
Model: "sequential_10"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dense_40 (Dense)            (None, 16)                272

 dense_41 (Dense)            (None, 32)                544

 dense_42 (Dense)            (None, 128)               4224

 dense_43 (Dense)            (None, 1)                 129

=================================================================
Total params: 5,169
Trainable params: 5,169
Non-trainable params: 0
_________________________________________________________________
Current Epoch: 20000 Training Loss: 0.561918 Validation Loss: 19.856144
```



In [ ]:

```

```

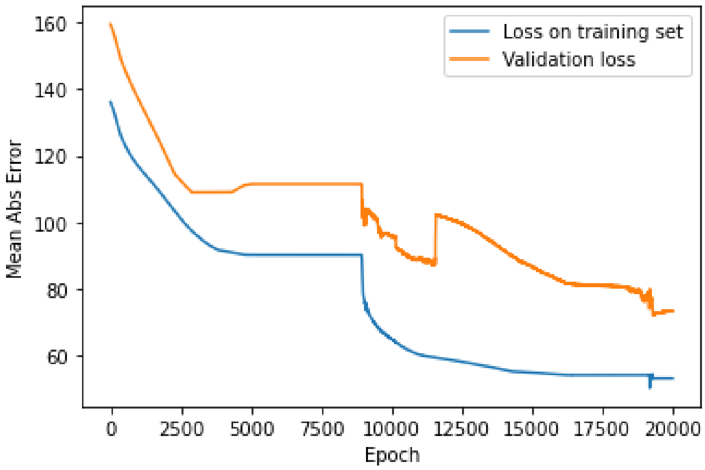
In [21]:

```
# DEFINITION OF THE MODEL
# The weights of our neural network will be initialized in a random manner, using a seed
allows for reproducibility
kernel_init = initializers.RandomNormal(seed=0)
bias_init = initializers.Zeros()

model = Sequential()
model.add(Dense(16, activation='relu', input_shape=(train_values.shape[1], ), kernel_ini
```

```
tializer=kernel_init,
                bias_initializer=bias_init))
model.add(Dense(32, activation='softmax', kernel_initializer=kernel_init, bias_initialize
r=bias_init))
model.add(Dense(128, activation='softmax', kernel_initializer=kernel_init, bias_initializ
er=bias_init))
# model.add(Dense(128, activation='relu', kernel_initializer=kernel_init, bias_initialize
r=bias_init))
model.add(Dense(1, kernel_initializer=kernel_init, bias_initializer=bias_init))

# DEFINITION OF THE OPTIMIZER
EPOCHS = 20000 # Number of EPOCHS
my_learning_rate = 0.01
my_decay_rate = my_learning_rate / EPOCHS


# optimizer = optimizers.RMSprop(0.001) # RMSProp
optimizer = optimizers.Adam(learning_rate=my_learning_rate,decay=my_decay_rate)#0.001) #
AdaM
# optimizer = optimizers.SGD(0.001) # SGD

# 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()

#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')
                         + " Validation Loss: " + "%4f" %logs.get('val_loss')
                         + '                                         \r') # Updates curre
nt Epoch Number

EPOCHS = 20000 # 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, shuffle=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['loss']),label='Loss on training set')
plt.plot(history.epoch, np.array(history.history['val_loss']),label = 'Validation loss')
plt.legend()
plt.show()
```

```
Model: "sequential_11"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dense_44 (Dense)            (None, 16)                272

 dense_45 (Dense)            (None, 32)                544

 dense_46 (Dense)            (None, 128)               4224

 dense_47 (Dense)            (None, 1)                 129

=================================================================
Total params: 5,169
Trainable params: 5,169
```

```
Non-trainable params: 0
_________________________________________________________________
Current Epoch: 20000 Training Loss: 53.099979 Validation Loss: 73.350121
```



In [ ]:

```

```

For ReLU function - - ---- Training Loss: 2.388709 Validation Loss: 46.047752

wRectified Linear Unit (ReLU) does so by outputting x for all x >= 0 and 0 for all x < 0. In other words, it equals max(x, 0). This simplicity makes it more difficult than the Sigmoid activation function and the Tangens hyperbolicus (Tanh) activation function, which use more difficult formulas and are computationally more expensive. In addition, ReLU is not sensitive to vanishing gradients, whereas the other two are, slowing down learning in the network. For ReLU , the validationn loss became lesser than training loss once.

For tanh function ------ Training Loss: 0.561918 Validation Loss: 19.856144

For Softmax function ----- Training Loss: 53.099979 Validation Loss: 73.350121

Softmax and Tanh essentially produce non-sparse models because their neurons pretty much always produce an output value: when the ranges are (0, 1)and (-1, 1), respectively, the output either cannot be zero or is zero with very low probabilit Both have a vanishing Gradient Problem which is also seen in the Validation and training losses in each of the cases. for Tanh the model is performing better than the other two maintaining the good bias- variance trade off.

In [ ]:

```

```

In [ ]:

```
------------------------------------------------------------END-----------------------------
-----------------------------------
```

In [ ]:

```

```