

Python Exercises for Petroleum Engineers: Set 2

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Welcome to the second homework for your "Introduction to Machine Learning" course. In this assignment, you will be working with a real well-logging dataset. Your task is to build a machine learning model that can predict water saturation using the appropriate set of logs.

In this homework, you will have the opportunity to solve a realistic machine learning problem step by step. To begin, you will need to import your well-logging data into Python and use appropriate tools to describe the data. You will then perform several preprocessing steps, such as

1. data cleaning,
2. normalization,
3. exploratory data analysis,
4. and feature selection,

to ensure that the data is ready to be used in a machine learning model.

Next, you should design an ANN model using Keras or Pytorch Lightning libraries. You will then train the neural network with different configurations, including varying the number of layers, number of neurons, learning rates, activation functions, and number of epochs.

During training, you will analyze the loss versus iteration curves to determine the best configuration for your model. You will also need to identify cases of overfitting and underfitting, which can negatively impact the performance of your model. Through this process, you will gain valuable experience in designing and training neural networks, and learn how to optimize their performance for a specific problem.

This homework will provide you with a hands-on experience in solving a realistic machine learning problem and help you develop important skills in data preprocessing, neural network training, and performance analysis. By completing this assignment, you will be well-prepared to tackle more complex machine learning problems in your future career as a petroleum engineer.

So, let's get started and dive into the exercises!

Task 1: Data Import

You have been provided with a well logging data set *FullSet_HW2.las*. This file is an *ASCII* file, which means you can load it by notepad to see what does it contain. Contact me if you had problem with understanding the data file.

Find a way to import this file into Python.

```
In [1]: # First of all Lets read las file and save it as excel file
import lasio
import pandas as pd
%matplotlib inline
import matplotlib.pyplot as plt

las = lasio.read("./FullSet_HW2.las")

df = las.df()
df = df.reset_index()
df.head()
```

```
# df.to_excel("FullSet_HW2.xlsx", engine='openpyxl') # For save it to excel
```

```
Out[1]:
```

	DEPTH	CALIPER	DRHO	DT	DTS	GR	MSFR	NPHI	PEF	POTA	RHOB	RLLD	RLLS	SWE	THOR	URAN
0	27.000	NaN	NaN	NaN	NaN	13.4222	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN
1	27.125	NaN	NaN	NaN	NaN	14.2646	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN
2	27.250	NaN	NaN	NaN	NaN	14.7782	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN
3	27.375	NaN	NaN	NaN	NaN	14.8532	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN
4	27.500	NaN	NaN	NaN	NaN	14.5207	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN

```
In [2]: print(las.curves) # For more information about the data set
```

Mnemonic	Unit	Value	Description
DEPTH	M		{F}
CALIPER	MM		Caliper {F}
DRHO	K/M3		Delta rho {F}
DT	US/M		Delta Time {F}
DTS	US/M		Shear Interval Transit Time {F}
GR	GAPI		Gamma Ray {F}
MSFR			{F}
NPHI	V/V		Neutron porosity {F}
PEF	B/E		Photo-electric factor {F}
POTA	%		Potassium {F}
RHOB	K/M3		Bulk Density {F}
RLLD			{F}
RLLS			{F}
SWE	V/V		Effective Water Saturation {F}
THOR	PPM		Thorium {F}
URAN	PPM		Uranium {F}

Task 2: Data Description

Describe the provided dataset. Your description should contain

1. shape of the dataset,
2. number of nulls of each column,
3. descriptive statistics (similar to Figure 3-3 "Machine Learning in the

Oil and Gas Industry"), 4. and your suggested depth interval to develop the model.

Task2-1: Shape of the dataset

```
In [3]: df.shape
```

```
Out[3]: (25899, 16)
```

Task2-2: number of null values in each column

There is two ways to solve this problem, one is to use the `isnull()` function to count the number of null values in each column, and the other ways is to get the count of Non-Null values by getting data information (`info()`)

```
In [4]: df.info()
```

```

<class 'pandas.core.frame.DataFrame'>
RangeIndex: 25899 entries, 0 to 25898
Data columns (total 16 columns):
#   Column      Non-Null Count  Dtype  
---  -
0    DEPTH      25899 non-null  float64
1    CALIPER    25458 non-null  float64
2    DRHO       7742 non-null   float64
3    DT         25173 non-null  float64
4    DTS        3688 non-null   float64
5    GR         25752 non-null  float64
6    MSFR       5827 non-null   float64
7    NPFI       8244 non-null   float64
8    PEF        7742 non-null   float64
9    POTA       8110 non-null   float64
10   RHOB       7742 non-null   float64
11   RLLD       8007 non-null   float64
12   RLLS       8015 non-null   float64
13   SWE        1729 non-null   float64
14   THOR       8110 non-null   float64
15   URAN       8110 non-null   float64
dtypes: float64(16)
memory usage: 3.2 MB

```

```
In [5]: df.isnull().sum()
```

```

Out[5]: DEPTH      0
        CALIPER    441
        DRHO      18157
        DT         726
        DTS      22211
        GR         147
        MSFR      20072
        NPFI      17655
        PEF        18157
        POTA      17789
        RHOB      18157
        RLLD      17892
        RLLS      17884
        SWE       24170
        THOR      17789
        URAN      17789
dtype: int64

```

Task2-3: Descriptive Statistics

In this step, we generate a descriptive statistical summary of the dataset using the `describe()` method. This provides key metrics for each well log, such as the `count`, `mean`, `standard deviation`, `minimum`, `maximum`, and `quartile values`.

```
In [6]: df.describe().transpose() # I used transpose due to the width limitation of final pdf file
```

Out[6]:

	count	mean	std	min	25%	50%	75%	max
DEPTH	25899.0	1645.625000	934.567706	27.000000	836.312500	1645.625000	2454.937500	3264.250000
CALIPER	25458.0	14.212401	4.640448	7.693300	9.034050	12.831900	18.367575	21.816300
DRHO	7742.0	0.079707	0.145116	-1.313353	0.024000	0.038656	0.115264	0.680282
DT	25173.0	90.548042	26.977269	37.998200	67.309000	86.735200	109.608500	205.452000
DTS	3688.0	127.695462	18.901311	78.234800	117.553275	125.568900	133.161425	258.181300
GR	25752.0	31.114276	12.340763	4.701200	23.512075	31.085500	36.661550	169.565600
MSFR	5827.0	3.041833	3.738093	0.293000	1.367500	2.544600	4.124700	150.617000
NPHI	8244.0	0.195071	0.104171	-0.002580	0.123149	0.178814	0.242792	0.876141
PEF	7742.0	6.721218	6.441028	1.952300	3.597025	4.483900	5.358875	51.169400
POTA	8110.0	0.746082	0.345081	0.012600	0.520250	0.741200	0.949775	3.221400
RHOB	7742.0	2.524475	0.192477	1.221000	2.465000	2.552000	2.615000	3.109800
RLLD	8007.0	182.406811	2292.058902	0.011000	2.829500	5.198000	8.444000	40000.000000
RLLS	8015.0	43.692169	805.204005	0.044000	2.476500	5.022000	8.648500	25000.000000
SWE	1729.0	0.491855	0.237953	0.000000	0.317000	0.474000	0.645900	1.000000
THOR	8110.0	1.965749	2.572671	0.044600	0.505275	1.005400	2.065400	26.531900
URAN	8110.0	1.841279	1.762433	0.001900	0.755900	1.396650	2.266975	19.926700

Task 2-4: Depth Interval Selection

For training our model in supervised learning or neural networks we require complete, non-null data. Therefore, we must identify a continuous depth interval where the log data is valid.

For this initial analysis, we are selecting an interval based on the availability of all existing logs. The goal here is to find the most data-rich zone where every single column contains a valid measurement. This approach considers the presence or absence of data across all features, without yet prioritizing the importance of specific logs or the target variable (**SW**). This gives us a foundational, "fully-populated" interval to begin our analysis.

In [7]:

```
key_columns = df.columns

cleaned_df = df.dropna(subset=key_columns)

valid_depths = cleaned_df['DEPTH']
valid_indices = cleaned_df.index

# Find the start and end of this continuous block of data
start_depth = valid_depths.min()
end_depth = valid_depths.max()

start_index = valid_indices.min()
end_index = valid_indices.max()

print("Suggested Depth Interval:")
print(f"\nSuggested modeling interval starts at: {start_depth:.2f}m with index of {start_index}")
print(f"Suggested modeling interval ends at: {end_depth:.2f}m with index of {end_index}")
```

Suggested Depth Interval:

Suggested modeling interval starts at: 2279.00m with index of 18016

Suggested modeling interval ends at: 2495.00m with index of 19744

Pandas Profiling Report

To supplement our initial analysis, we employed the pandas-profiling library to generate a detailed and automated EDA report. This report provides a comprehensive overview of the dataset, including in-depth analysis of each variable's

statistics, distribution, correlations, and missing value patterns.

For a complete, interactive exploration of the data, please see the `data_report.html` file accompanying this notebook.

```
In [8]: from pandas_profiling import ProfileReport

profile = ProfileReport(df, title="Full Data Profiling")

profile.to_file("data_report.html")
```

[Upgrade to ydata-sdk](#)

Improve your data and profiling with ydata-sdk, featuring data quality scoring, redundancy detection, outlier identification, text validation, and synthetic data generation.

```
C:\Users\ASUS\AppData\Local\Temp\ipykernel_6072\3793968230.py:1: DeprecationWarning: `import pandas_profiling` is going to be deprecated by April 1st. Please use `import ydata_profiling` instead.
```

```
from pandas_profiling import ProfileReport
```

```
Summarize dataset: 0%|          | 0/5 [00:00<?, ?it/s]
```

```
100%|██████████| 16/16 [00:00<00:00, 56.02it/s]
```

```
Generate report structure: 0%|          | 0/1 [00:00<?, ?it/s]
```

```
Render HTML: 0%|          | 0/1 [00:00<?, ?it/s]
```

```
Export report to file: 0%|          | 0/1 [00:00<?, ?it/s]
```

Task 2: Data Preparation

You should perform multiple steps of data preparation through this task. The required data preprocessings are:

1. Data cleaning: In this step you will need to identify and deal with any issues or anomalies in the dataset, to ensure that the data is accurate and consistent. Also you should keep an appropriate interval (a continuous interval) of logs and delete the rest of them.
2. Feature selection: You will analyze the data and choose the best set of logs to use as input features for your machine learning model. This step will help you eliminate irrelevant or redundant features, which can negatively impact the performance of your model.

You should use **your domain knowledge** and **feature selection methods** to choose the best set of the input logs. Also you should plot correlation heatmap of features and pair plots using seaborn, pandas and/or matplotlib libraries (like Figure 3-3 "Machine Learning in the

Oil and Gas Industry")

3. Data normalization

4. Data splitting: Split your data randomly into *Train*, *Test*, and *Validation* sets. Choose a reasonable ratio to split the data.

Task 2-1: Data cleaning

In this step, the dataset is filtered to retain only the continuous depth interval identified in the previous analysis (from `start_depth` to `end_depth`). This removes data points outside the high-quality region. Any remaining rows with null values in this interval are also removed to ensure that the dataset is complete and ready for feature selection.

Another way is to use `dropna()` on the entire dataset to recognize non-empty data as a table, as in Part 3 of the previous task (which we did in Part 3 of the previous task, and now we want to do something different).

```
In [9]: df_interval = df.loc[start_index:end_index].copy()
cleaned_df = df_interval.dropna()

print(f"Full Data Shape: {df.shape}")
print(f"Cleaned Data Shape: {cleaned_df.shape}")
```

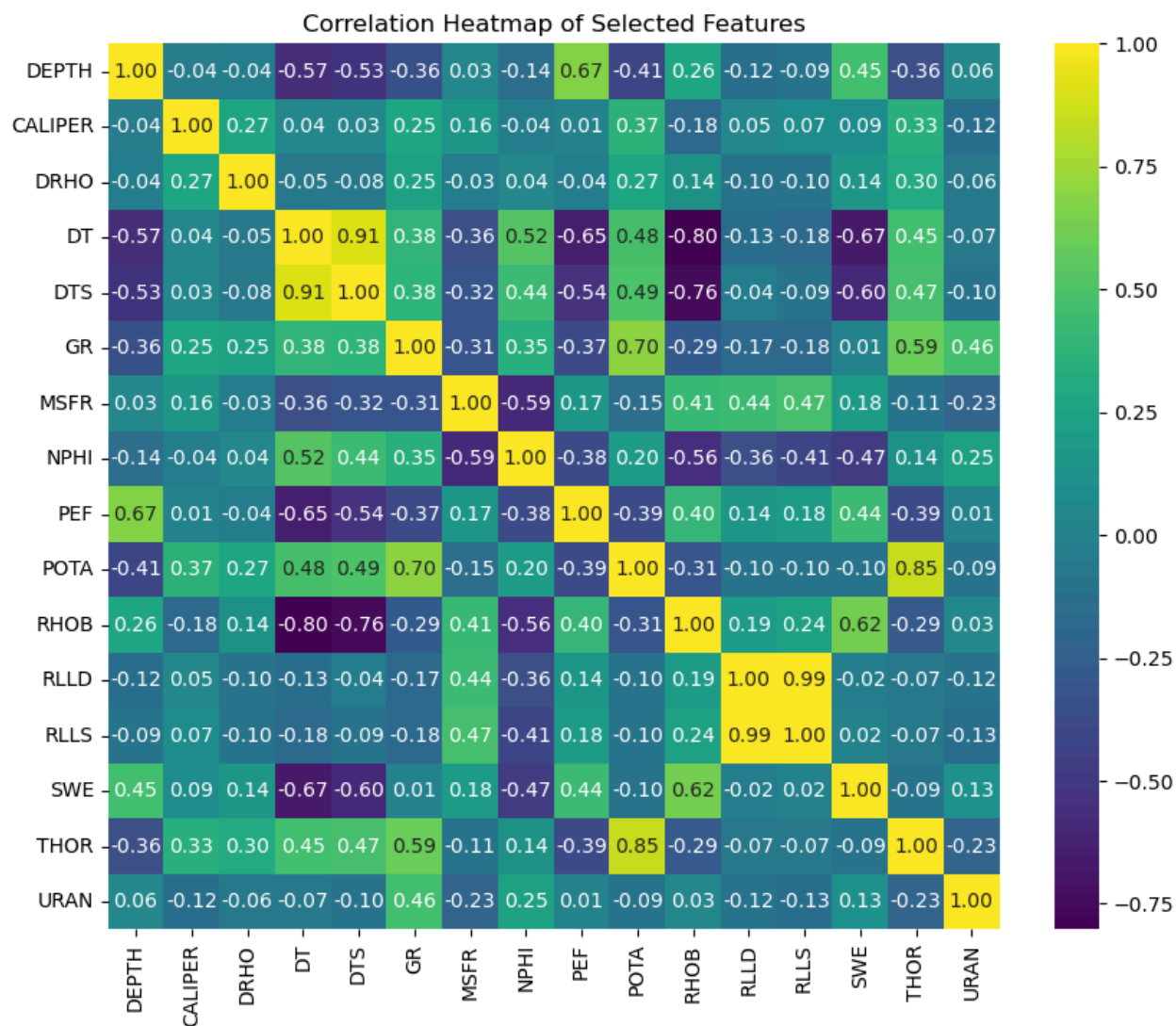
```
Full Data Shape: (25899, 16)
```

```
Cleaned Data Shape: (1729, 16)
```

Task 2-2: Feature Selection

```
In [10]: import seaborn as sns
import matplotlib.pyplot as plt

correlation_matrix = cleaned_df.corr()
plt.figure(figsize=(10, 8))
sns.heatmap(correlation_matrix, annot=True, cmap='viridis', fmt='.2f')
plt.title('Correlation Heatmap of Selected Features')
plt.show()
```



```
In [11]: print(correlation_matrix['SWE'].sort_values(ascending=False))
```

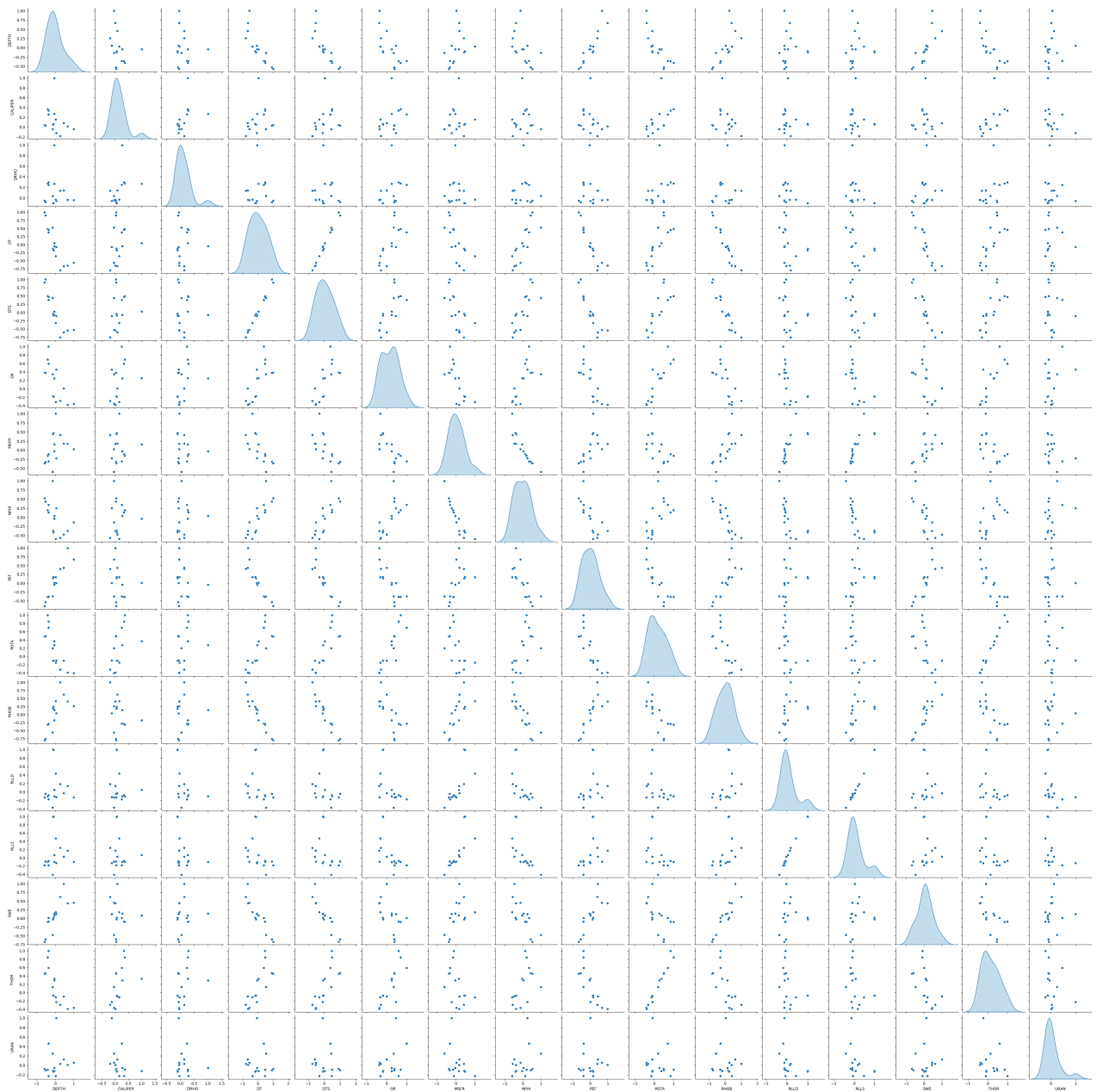
```
SWE      1.000000
RHOB     0.623229
DEPTH    0.454973
PEF       0.435940
MSFR     0.182287
DRHO     0.141433
URAN     0.125743
CALIPER  0.085070
RLLS     0.024209
GR        0.009662
RLLD     -0.024621
THOR     -0.089208
POTA     -0.100132
NPHI     -0.470558
DTS      -0.603210
DT       -0.673495
Name: SWE, dtype: float64
```

So based on the correlation heatmap analysis, a new subset of features was selected for the model. The columns `DRHO`, `DTS`, `GR`, `MSFR`, `POTA`, `RLLS`, `THOR`, `URAN`, and `CALIPER` were dropped for the following reasons:

- Low Correlation with Target: These logs showed a very weak linear correlation with our target variable, `SW`. Including them would likely add noise rather than predictive value.
- Redundancy: Some of the dropped features were highly correlated with other input features, making them redundant.

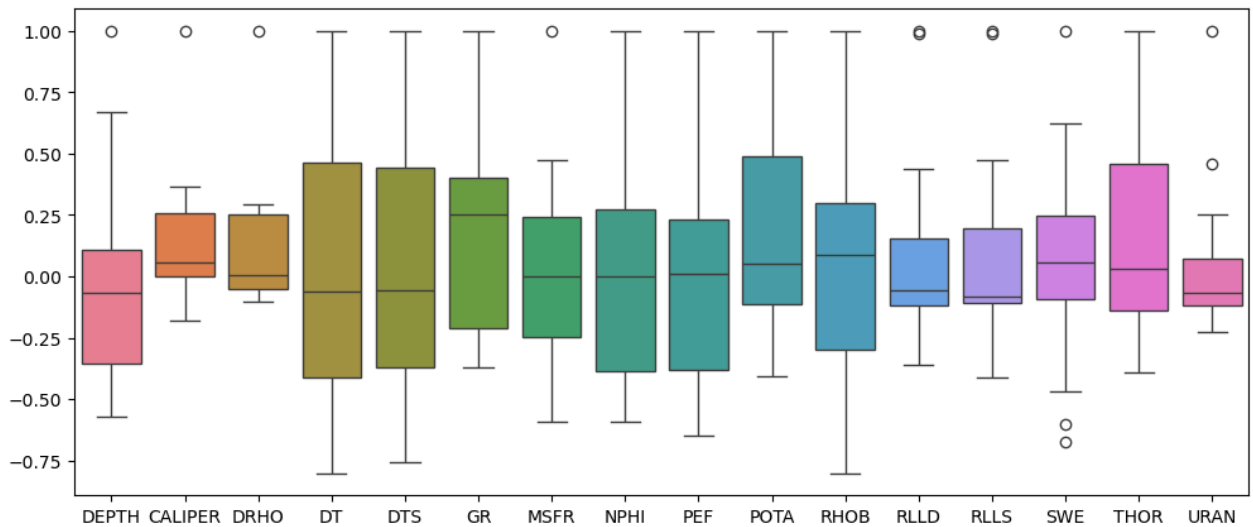
By removing these columns, we create a more focused and simpler model that relies on the most impactful features, which can improve performance and reduce the risk of overfitting.

```
In [12]: sns.pairplot(cleaned_df.corr() , diag_kind='kde')
plt.show()
```



Now lets see the boxplot for outliers existant

```
In [13]: plt.figure(figsize = (12, 5))
sns.boxplot(cleaned_df.corr())
plt.show()
```

Based on the above boxplot we can see there are many outliers that can affect our prediction and training process, so we have to remove them from our dataset

```
In [14]: def remove_outliers(df):

    cleaned_df = pd.DataFrame(columns = df.columns)

    for col in df.columns:

        Q1 = df[col].quantile(0.25)
        Q3 = df[col].quantile(0.75)
        IQR = Q3 - Q1

        lower_bound = Q1 - 1.5*IQR
        upper_bound = Q3 + 1.5*IQR

        col_cleaned = df[(df[col] >= lower_bound) & (df[col] <= upper_bound)][col]

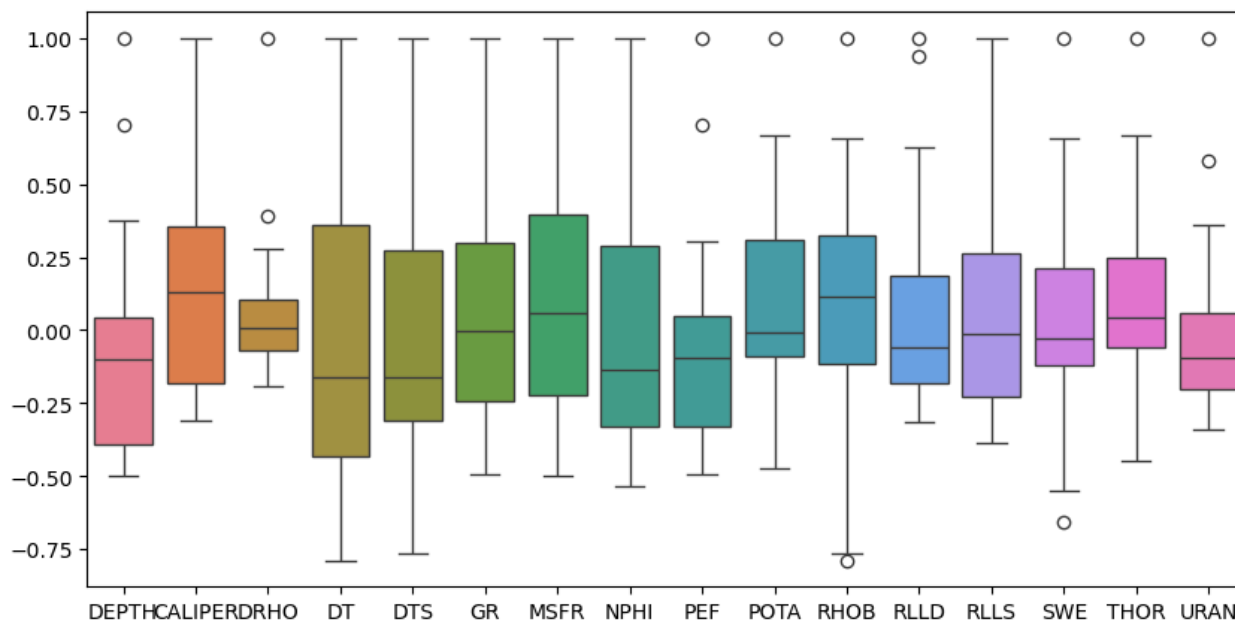
        cleaned_df[col] = col_cleaned
    return cleaned_df

cleaned_df = remove_outliers(cleaned_df)
```

```
In [15]: print(cleaned_df.isnull().sum())
cleaned_df.dropna(inplace=True)
```

```
DEPTH      0
CALIPER    153
DRHO       142
DT         90
DTS        95
GR         100
MSFR       53
NPHI       23
PEF         6
POTA       153
RHOB       15
RLLD       152
RLLS       152
SWE        0
THOR       153
URAN       96
dtype: int64
```

```
In [16]: plt.figure(figsize = (10 , 5))
sns.boxplot(cleaned_df.corr())
plt.show()
```



Before Normalization we should split our data to train, test, validation and the normalize them, so we do Data splitting before normalization

Task 2-3: Data splitting

Firs lets select our features and remove the features we dont need.

```
In [17]: selected_data = cleaned_df.drop(columns=["DRHO" , "DTS" , "GR" , "MSFR" , "POTA" , "RLLS" , "THOR" , "URAN"]
selected_data.describe()
```

```
Out[17]:
```

	DEPTH	DT	NPHI	PEF	RHOB	RLLD	SWE
count	1066.000000	1066.000000	1066.000000	1066.000000	1066.000000	1066.000000	1066.000000
mean	2398.152908	68.234893	0.190980	3.709300	2.542235	5.653699	0.483124
std	60.737737	8.408757	0.048319	0.797805	0.133942	3.532724	0.210770
min	2279.500000	50.878300	0.053319	2.104200	2.108000	0.944000	0.079500
25%	2349.906250	62.889475	0.159483	3.169600	2.449250	2.686750	0.321750
50%	2401.187500	67.492550	0.189737	3.532750	2.539000	4.840000	0.460650
75%	2455.343750	72.778450	0.221353	4.404750	2.632750	7.812250	0.625875
max	2495.000000	98.033800	0.319646	5.644100	2.867000	18.018000	1.000000

This figure provides a side-by-side visualization of the selected features used as input for the model. Each subplot displays a single well log on the horizontal axis plotted against valid Depth on the shared vertical axis. This layout allows for a comprehensive visual inspection and comparison of the data along the wellbore.

```
In [18]: data_to_plot = selected_data

columns_to_plot = data_to_plot.columns[1:]

num_plots = len(columns_to_plot)

fig, axs = plt.subplots(1, num_plots, figsize=(num_plots * 4, 12), sharey=True)

fig.suptitle('Selected Features vs. Depth', fontsize=20, y=1.02)

for i, col_name in enumerate(columns_to_plot):
    ax = axs[i]
```

```

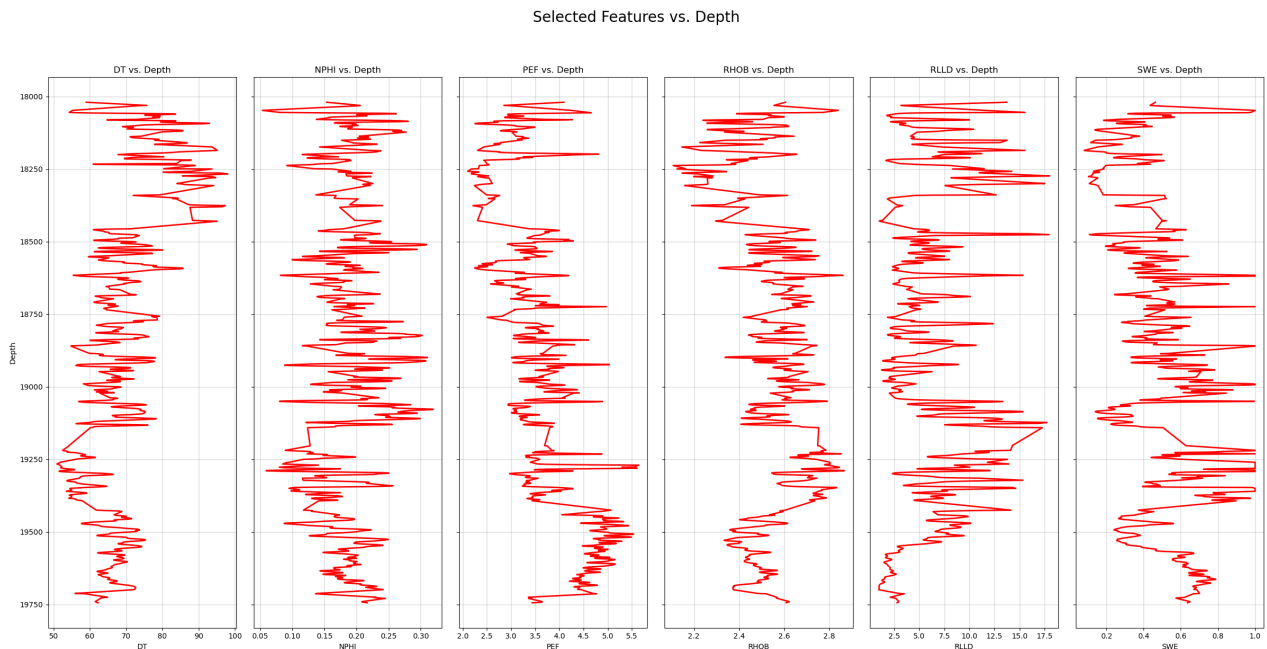
ax.plot(data_to_plot[col_name], data_to_plot.index, linewidth=2, color='red')
ax.set_xlabel(col_name)
ax.set_title(f'{col_name} vs. Depth')
ax.grid(True, alpha=0.5)

axs[0].set_ylabel('Depth')
axs[0].invert_yaxis()

plt.tight_layout(rect=[0, 0, 1, 0.98])

plt.show()

```



The data is first partitioned into training (70%), validation (15%), and test (15%) sets using `train_test_split`. The test set is held out to provide an unbiased final evaluation of the model. The validation set is used to monitor performance during training.

This is a standard and widely accepted convention in machine learning that provides a strong balance between model training and evaluation.

In addition, considering the amount of data, it is better to use more data for training.

```

In [19]: from sklearn.model_selection import train_test_split

TARGET_COLUMN = 'SWE'

X = selected_data.drop(TARGET_COLUMN, axis=1)
y = selected_data[TARGET_COLUMN]

# Splitting the test and a rest data for next step (validation and train)
X_train_val, X_test, y_train_val, y_test = train_test_split(
    X, y, test_size=0.15, random_state=42
)

# Splitting the train and validation
X_train, X_val, y_train, y_val = train_test_split(
    X_train_val, y_train_val, test_size=0.1765, random_state=42 # 0.15 / 0.85 = 0.1765
)

print("Data Shapes After Splitting:")
print(f"\nX_train shape: {X_train.shape}")
print(f"\nX_val shape: {X_val.shape}")
print(f"\nX_test shape: {X_test.shape}")

```

Data Shapes After Splitting:

X_train shape: (746, 6)

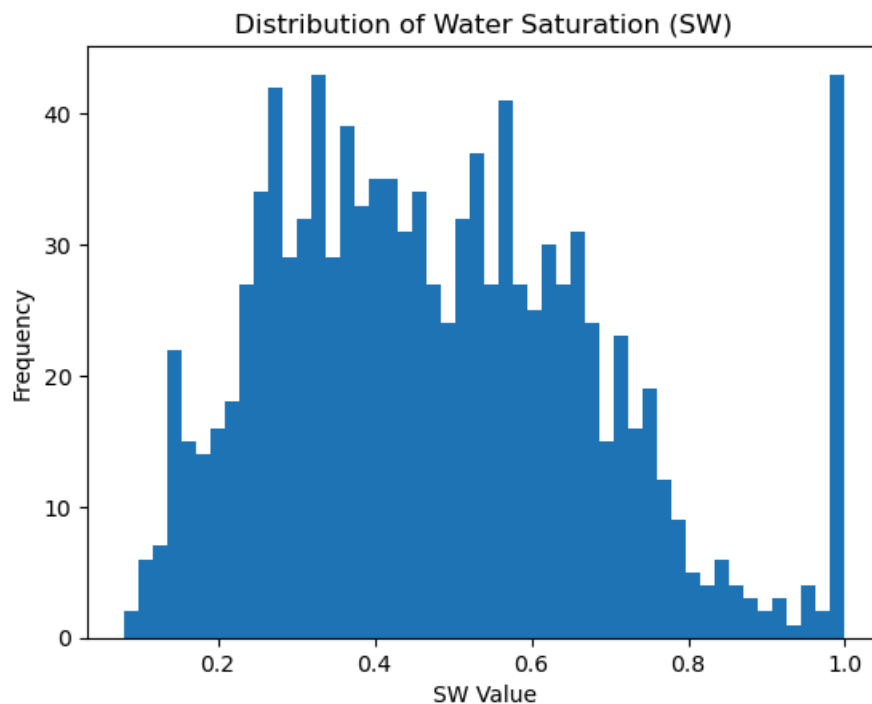
X_val shape: (160, 6)

X_test shape: (160, 6)

This histogram illustrates the frequency distribution of the target variable, Water Saturation (SW). The horizontal axis shows the range of SW values, grouped into 50 bins, while the vertical axis represents the frequency, or count, of data points within each bin. This plot is essential for understanding the underlying characteristics of the target data, such as its central tendency, spread, and skewness.

If you look at the histogram, you'll notice that the distribution of SW values is between [0,1], so there is no need to normalize the target data.

```
In [20]: plt.hist(y, bins=50)
plt.title('Distribution of Water Saturation (SW)')
plt.xlabel('SW Value')
plt.ylabel('Frequency')
plt.show()
```



Task 2-4: Data Normalization

To ensure all features are on a common scale, `MinMaxScaler` is applied. Crucially, the scaler is fitted only on the training data. The learned scaling parameters (min and max values) are then used to transform the training, validation, and test sets. This ensures that no information from the validation or test sets influences the transformation, providing a realistic simulation of how the model would perform on new, unseen data.

```
In [21]: from sklearn.preprocessing import MinMaxScaler

scaler = MinMaxScaler()

# Scale transform for each data set
X_train_scaled = scaler.fit_transform(X_train)
X_val_scaled = scaler.transform(X_val)
X_test_scaled = scaler.transform(X_test)

# For better readability, convert scaled arrays back to DataFrames
X_train_scaled = pd.DataFrame(X_train_scaled, columns=X_train.columns, index=X_train.index)
X_val_scaled = pd.DataFrame(X_val_scaled, columns=X_val.columns, index=X_val.index)
X_test_scaled = pd.DataFrame(X_test_scaled, columns=X_test.columns, index=X_test.index)
```

```

print("\n--- Data After Normalization ---")
print("First 5 rows of scaled training data:")
print(X_train_scaled.head())
print("\nFirst 5 rows of scaled test data:")
print(X_test_scaled.head())
print("\nFirst 5 rows of scaled validation data:")
print(X_val_scaled.head())

```

--- Data After Normalization ---

First 5 rows of scaled training data:

	DEPTH	DT	NPHI	PEF	RHOB	RLLD
19447	0.827726	0.404532	0.391825	0.753778	0.518767	0.523955
18991	0.563225	0.160624	0.248999	0.480748	0.894102	0.207450
18098	0.045244	0.523445	0.504075	0.214469	0.635389	0.130432
18142	0.070766	0.441637	0.563410	0.325631	0.608579	0.206103
18160	0.081206	0.762700	0.506245	0.196503	0.195710	0.488755

First 5 rows of scaled test data:

	DEPTH	DT	NPHI	PEF	RHOB	RLLD
18087	0.038863	0.616085	0.783037	0.166050	0.471850	0.069462
19445	0.826566	0.391469	0.394838	0.789966	0.538874	0.507321
18822	0.465197	0.503880	0.920182	0.280516	0.447721	0.053122
19665	0.954176	0.311455	0.479944	0.662279	0.524129	0.022197
19426	0.815545	0.273764	0.240403	0.824967	0.655496	0.602261

First 5 rows of scaled validation data:

	DEPTH	DT	NPHI	PEF	RHOB	RLLD
19371	0.783643	0.100285	0.216026	0.435069	0.888740	0.441080
18927	0.526102	0.111665	0.126741	0.537360	0.694370	0.311878
19241	0.708237	0.187942	0.511688	0.349191	0.747989	0.284643
18466	0.258701	0.275732	0.385692	0.454052	0.722520	0.231112
18505	0.281323	0.374463	0.629274	0.361055	0.583110	0.294893

Task 3: Preparing your ANN code

Prepare a Multi-layer Perceptron (MLP) model with keras or pytorch.

Task 3.1: Prepare your initial architecture

Use the following function (*generate_nn_architecture*) to generate an architecture for you. Implement the generated architecture as a module of the library of your choice (keras or pytorch).

```

import random

def generate_nn_architecture(student_number, initial_input_dim):
    # Set random seed based on student number
    random.seed(student_number)

    # Initialize list to store layers
    nn_architecture = []

    # Generate random number of layers between 3 and 7
    num_layers = random.randint(3, 7)

    # Generate layers
    input_dim = initial_input_dim # Initial input dimension (number of features which have you
selected in the preprocessing step)
    for i in range(num_layers):
        # Generate random number of neurons between 3 and 5
        output_dim = random.randint(5, 15)
        # Generate random activation function
        activation = random.choice(["relu", "tanh", "sigmoid", "leaky_relu"])
        # Append layer to architecture list
        nn_architecture.append({"input_dim": input_dim, "output_dim": output_dim, "activation":
activation})
        # Update input dimension for next layer
        input_dim = output_dim

```

```

# Add final layer with sigmoid activation for binary classification
nn_architecture.append({"input_dim": input_dim, "output_dim": 1, "activation": "sigmoid"})

return nn_architecture

```

`initial_input_dim` value is the number of features that you have selected in the **feature selection** step.

Usage example:

```

student_number = 123456
initial_input_dim = 3 # Number of selected features
nn_architecture = generate_nn_architecture(student_number, initial_input_dim)
print(nn_architecture)

```

```

In [22]: import random
import tensorflow as tf
from tensorflow import keras

def generate_nn_architecture(student_number, initial_input_dim):
    """Generates a random neural network architecture blueprint."""
    random.seed(student_number)

    nn_architecture = []

    num_layers = random.randint(3, 7)

    input_dim = initial_input_dim
    for i in range(num_layers):
        output_dim = random.randint(5, 15)
        activation = random.choice(["relu", "tanh", "sigmoid", "leaky_relu"]) # Changed to Leaky_relu for Ke
        nn_architecture.append({"input_dim": input_dim, "output_dim": output_dim, "activation": activation})
        input_dim = output_dim

    # The final layer in the description is for binary classification.
    # For our regression problem (predicting SW), we need a linear output layer.
    nn_architecture.append({"input_dim": input_dim, "output_dim": 1, "activation": "linear"})

    return nn_architecture

student_number = 403134029
initial_input_dim = X_train_scaled.shape[1]
nn_architecture = generate_nn_architecture(student_number, initial_input_dim)
print("NN architecture for each layer:\n")
for i, layer in enumerate(nn_architecture):
    print(f"Layer {i+1}: {layer}")

```

NN architecture for each layer:

```

Layer 1: {'input_dim': 6, 'output_dim': 9, 'activation': 'sigmoid'}
Layer 2: {'input_dim': 9, 'output_dim': 12, 'activation': 'relu'}
Layer 3: {'input_dim': 12, 'output_dim': 10, 'activation': 'relu'}
Layer 4: {'input_dim': 10, 'output_dim': 1, 'activation': 'linear'}

```

Task 4: Training and analyzing your ANN

Task 4.1: Training your ANN

Consider values for number of epochs and learning rate and train your network.

1. Plot overlay scatter of train cost and validation cost versus epochs,
2. scatter of SWE_pred versus SWE,
3. overlay scatter of SWE_pred versus depth and SWE versus depth.

```

In [23]: from keras.models import Sequential # type: ignore
from keras.layers import Dense, Dropout, Activation, Flatten, BatchNormalization # type: ignore
from tensorflow.keras.optimizers import Adam # type: ignore

```

```

n_features_in = X_train_scaled.shape[1]
n_features_out = 1

def baseline_model(learning_rate=0.001):
    model = Sequential()
    model.add(Dense(128, activation='relu', input_dim = n_features_in))
    model.add(Dense(64, activation='relu'))
    model.add(Dense(32, activation='relu'))
    model.add(Dense(n_features_out, activation='sigmoid'))

    optimizer = Adam(learning_rate=learning_rate)

    model.compile(loss = 'mean_squared_error', optimizer=optimizer, metrics=['mean_absolute_error'])
    return model

model = baseline_model(learning_rate=0.001)

```

e:\Users\ASUS\anaconda3\Lib\site-packages\keras\src\layers\core\dense.py:87: UserWarning: Do not pass an `input_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` object as the first layer in the model instead.

```

super().__init__(activity_regularizer=activity_regularizer, **kwargs)

```

Model Structure: The architecture consists of:

- Three hidden Dense layers with 128, 64, and 32 neurons, using the ReLU activation function. ReLU was chosen for its computational efficiency and effectiveness in handling non-linear relationships.
- One Dense output layer with a single neuron and a sigmoid activation function.

While a linear activation is the standard convention for regression tasks, an alternative approach using sigmoid was tested. This decision was motivated by the physical nature of the target variable, Water Saturation (SW), which is naturally bounded between 0 and 1. The sigmoid function inherently constrains the model's output to this valid range.

In [24]: `model.summary()`

Model: "sequential"

Layer (type)	Output Shape	Param #
dense (Dense)	(None, 128)	896
dense_1 (Dense)	(None, 64)	8,256
dense_2 (Dense)	(None, 32)	2,080
dense_3 (Dense)	(None, 1)	33
















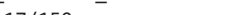
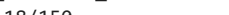






Total params: 11,265 (44.00 KB)

Trainable params: 11,265 (44.00 KB)

Non-trainable params: 0 (0.00 B)

The `model.summary()` method provided a concise blueprint of the model's architecture. It detailed the sequence of layers, the output shape after each transformation, and the number of trainable parameters, confirming the model's complexity and structure.

In [25]: `history = model.fit(`
`X_train_scaled,`
`y_train,`
`epochs=150,`
`batch_size=64,`
`validation_data=(X_val_scaled, y_val),`
`verbose=1`
`)`















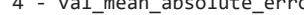
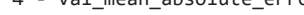
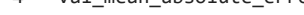






Epoch 1/150
12/12  2s 28ms/step - loss: 0.0412 - mean_absolute_error: 0.1673 - val_loss: 0.0335 - val_mean_absolute_error: 0.1509
Epoch 2/150
12/12  0s 9ms/step - loss: 0.0296 - mean_absolute_error: 0.1409 - val_loss: 0.0221 - val_mean_absolute_error: 0.1236
Epoch 3/150
12/12  0s 10ms/step - loss: 0.0216 - mean_absolute_error: 0.1170 - val_loss: 0.0144 - val_mean_absolute_error: 0.0964
Epoch 4/150
12/12  0s 9ms/step - loss: 0.0129 - mean_absolute_error: 0.0880 - val_loss: 0.0094 - val_mean_absolute_error: 0.0704
Epoch 5/150
12/12  0s 9ms/step - loss: 0.0107 - mean_absolute_error: 0.0722 - val_loss: 0.0066 - val_mean_absolute_error: 0.0556
Epoch 6/150
12/12  0s 9ms/step - loss: 0.0064 - mean_absolute_error: 0.0551 - val_loss: 0.0052 - val_mean_absolute_error: 0.0495
Epoch 7/150
12/12  0s 9ms/step - loss: 0.0049 - mean_absolute_error: 0.0477 - val_loss: 0.0045 - val_mean_absolute_error: 0.0468
Epoch 8/150
12/12  0s 9ms/step - loss: 0.0048 - mean_absolute_error: 0.0459 - val_loss: 0.0037 - val_mean_absolute_error: 0.0413
Epoch 9/150
12/12  0s 9ms/step - loss: 0.0040 - mean_absolute_error: 0.0434 - val_loss: 0.0038 - val_mean_absolute_error: 0.0456
Epoch 10/150
12/12  0s 9ms/step - loss: 0.0038 - mean_absolute_error: 0.0438 - val_loss: 0.0030 - val_mean_absolute_error: 0.0384
Epoch 11/150
12/12  0s 9ms/step - loss: 0.0030 - mean_absolute_error: 0.0372 - val_loss: 0.0028 - val_mean_absolute_error: 0.0375
Epoch 12/150
12/12  0s 9ms/step - loss: 0.0029 - mean_absolute_error: 0.0359 - val_loss: 0.0029 - val_mean_absolute_error: 0.0385
Epoch 13/150
12/12  0s 10ms/step - loss: 0.0030 - mean_absolute_error: 0.0386 - val_loss: 0.0029 - val_mean_absolute_error: 0.0376
Epoch 14/150
12/12  0s 9ms/step - loss: 0.0025 - mean_absolute_error: 0.0344 - val_loss: 0.0024 - val_mean_absolute_error: 0.0340
Epoch 15/150
12/12  0s 10ms/step - loss: 0.0022 - mean_absolute_error: 0.0328 - val_loss: 0.0023 - val_mean_absolute_error: 0.0322
Epoch 16/150
12/12  0s 10ms/step - loss: 0.0022 - mean_absolute_error: 0.0313 - val_loss: 0.0022 - val_mean_absolute_error: 0.0316
Epoch 17/150
12/12  0s 10ms/step - loss: 0.0020 - mean_absolute_error: 0.0310 - val_loss: 0.0021 - val_mean_absolute_error: 0.0307
Epoch 18/150
12/12  0s 10ms/step - loss: 0.0020 - mean_absolute_error: 0.0301 - val_loss: 0.0020 - val_mean_absolute_error: 0.0303
Epoch 19/150
12/12  0s 10ms/step - loss: 0.0019 - mean_absolute_error: 0.0286 - val_loss: 0.0019 - val_mean_absolute_error: 0.0297
Epoch 20/150
12/12  0s 10ms/step - loss: 0.0018 - mean_absolute_error: 0.0284 - val_loss: 0.0019 - val_mean_absolute_error: 0.0286
Epoch 21/150
12/12  0s 14ms/step - loss: 0.0018 - mean_absolute_error: 0.0274 - val_loss: 0.0018 - val_mean_absolute_error: 0.0280
Epoch 22/150
12/12  0s 12ms/step - loss: 0.0015 - mean_absolute_error: 0.0260 - val_loss: 0.0022 - val_mean_absolute_error: 0.0337
Epoch 23/150
12/12  0s 11ms/step - loss: 0.0015 - mean_absolute_error: 0.0273 - val_loss: 0.0020 - val_mean_absolute_error: 0.0295
Epoch 24/150

12/12 ————— 0s 10ms/step - loss: 0.0016 - mean_absolute_error: 0.0276 - val_loss: 0.0017 - val_mean_absolute_error: 0.0269
Epoch 25/150
12/12 ————— 0s 10ms/step - loss: 0.0016 - mean_absolute_error: 0.0265 - val_loss: 0.0016 - val_mean_absolute_error: 0.0259
Epoch 26/150
12/12 ————— 0s 10ms/step - loss: 0.0011 - mean_absolute_error: 0.0212 - val_loss: 0.0015 - val_mean_absolute_error: 0.0250
Epoch 27/150
12/12 ————— 0s 10ms/step - loss: 0.0011 - mean_absolute_error: 0.0216 - val_loss: 0.0016 - val_mean_absolute_error: 0.0250
Epoch 28/150
12/12 ————— 0s 10ms/step - loss: 0.0012 - mean_absolute_error: 0.0228 - val_loss: 0.0015 - val_mean_absolute_error: 0.0250
Epoch 29/150
12/12 ————— 0s 11ms/step - loss: 0.0011 - mean_absolute_error: 0.0216 - val_loss: 0.0016 - val_mean_absolute_error: 0.0259
Epoch 30/150
12/12 ————— 0s 11ms/step - loss: 0.0011 - mean_absolute_error: 0.0222 - val_loss: 0.0015 - val_mean_absolute_error: 0.0246
Epoch 31/150
12/12 ————— 0s 10ms/step - loss: 0.0011 - mean_absolute_error: 0.0213 - val_loss: 0.0015 - val_mean_absolute_error: 0.0260
Epoch 32/150
12/12 ————— 0s 10ms/step - loss: 0.0011 - mean_absolute_error: 0.0210 - val_loss: 0.0015 - val_mean_absolute_error: 0.0242
Epoch 33/150
12/12 ————— 0s 10ms/step - loss: 0.0012 - mean_absolute_error: 0.0235 - val_loss: 0.0014 - val_mean_absolute_error: 0.0233
Epoch 34/150
12/12 ————— 0s 11ms/step - loss: 0.0011 - mean_absolute_error: 0.0209 - val_loss: 0.0014 - val_mean_absolute_error: 0.0238
Epoch 35/150
12/12 ————— 0s 10ms/step - loss: 0.0010 - mean_absolute_error: 0.0199 - val_loss: 0.0013 - val_mean_absolute_error: 0.0225
Epoch 36/150
12/12 ————— 0s 10ms/step - loss: 9.0519e-04 - mean_absolute_error: 0.0196 - val_loss: 0.0014 - val_mean_absolute_error: 0.0228
Epoch 37/150
12/12 ————— 0s 10ms/step - loss: 8.4435e-04 - mean_absolute_error: 0.0190 - val_loss: 0.0013 - val_mean_absolute_error: 0.0223
Epoch 38/150
12/12 ————— 0s 12ms/step - loss: 8.3055e-04 - mean_absolute_error: 0.0183 - val_loss: 0.0013 - val_mean_absolute_error: 0.0221
Epoch 39/150
12/12 ————— 0s 10ms/step - loss: 8.1624e-04 - mean_absolute_error: 0.0183 - val_loss: 0.0013 - val_mean_absolute_error: 0.0223
Epoch 40/150
12/12 ————— 0s 10ms/step - loss: 8.5784e-04 - mean_absolute_error: 0.0187 - val_loss: 0.0013 - val_mean_absolute_error: 0.0216
Epoch 41/150
12/12 ————— 0s 10ms/step - loss: 8.8708e-04 - mean_absolute_error: 0.0193 - val_loss: 0.0013 - val_mean_absolute_error: 0.0215
Epoch 42/150
12/12 ————— 0s 10ms/step - loss: 8.7339e-04 - mean_absolute_error: 0.0184 - val_loss: 0.0013 - val_mean_absolute_error: 0.0230
Epoch 43/150
12/12 ————— 0s 10ms/step - loss: 8.0507e-04 - mean_absolute_error: 0.0190 - val_loss: 0.0013 - val_mean_absolute_error: 0.0218
Epoch 44/150
12/12 ————— 0s 12ms/step - loss: 7.0444e-04 - mean_absolute_error: 0.0169 - val_loss: 0.0012 - val_mean_absolute_error: 0.0207
Epoch 45/150
12/12 ————— 0s 10ms/step - loss: 8.3500e-04 - mean_absolute_error: 0.0188 - val_loss: 0.0012 - val_mean_absolute_error: 0.0203
Epoch 46/150
12/12 ————— 0s 10ms/step - loss: 6.9444e-04 - mean_absolute_error: 0.0164 - val_loss: 0.0012 - val_mean_absolute_error: 0.0208
Epoch 47/150
12/12 ————— 0s 10ms/step - loss: 6.8167e-04 - mean_absolute_error: 0.0166 - val_loss: 0.0013 -

```
val_mean_absolute_error: 0.0227
Epoch 48/150
12/12 ————— 0s 10ms/step - loss: 7.9251e-04 - mean_absolute_error: 0.0184 - val_loss: 0.0011 -
val_mean_absolute_error: 0.0205
Epoch 49/150
12/12 ————— 0s 10ms/step - loss: 7.5646e-04 - mean_absolute_error: 0.0168 - val_loss: 0.0012 -
val_mean_absolute_error: 0.0199
Epoch 50/150
12/12 ————— 0s 9ms/step - loss: 7.6383e-04 - mean_absolute_error: 0.0177 - val_loss: 0.0011 -
val_mean_absolute_error: 0.0201
Epoch 51/150
12/12 ————— 0s 10ms/step - loss: 6.5920e-04 - mean_absolute_error: 0.0163 - val_loss: 0.0011 -
val_mean_absolute_error: 0.0198
Epoch 52/150
12/12 ————— 0s 10ms/step - loss: 6.8531e-04 - mean_absolute_error: 0.0159 - val_loss: 0.0014 -
val_mean_absolute_error: 0.0251
Epoch 53/150
12/12 ————— 0s 10ms/step - loss: 8.7328e-04 - mean_absolute_error: 0.0195 - val_loss: 0.0013 -
val_mean_absolute_error: 0.0233
Epoch 54/150
12/12 ————— 0s 10ms/step - loss: 7.1348e-04 - mean_absolute_error: 0.0181 - val_loss: 0.0011 -
val_mean_absolute_error: 0.0206
Epoch 55/150
12/12 ————— 0s 11ms/step - loss: 7.2149e-04 - mean_absolute_error: 0.0171 - val_loss: 0.0011 -
val_mean_absolute_error: 0.0207
Epoch 56/150
12/12 ————— 0s 9ms/step - loss: 7.6647e-04 - mean_absolute_error: 0.0178 - val_loss: 0.0011 -
val_mean_absolute_error: 0.0195
Epoch 57/150
12/12 ————— 0s 10ms/step - loss: 7.6614e-04 - mean_absolute_error: 0.0167 - val_loss: 0.0013 -
val_mean_absolute_error: 0.0243
Epoch 58/150
12/12 ————— 0s 11ms/step - loss: 6.7805e-04 - mean_absolute_error: 0.0182 - val_loss: 0.0011 -
val_mean_absolute_error: 0.0198
Epoch 59/150
12/12 ————— 0s 10ms/step - loss: 7.8732e-04 - mean_absolute_error: 0.0178 - val_loss: 0.0012 -
val_mean_absolute_error: 0.0227
Epoch 60/150
12/12 ————— 0s 10ms/step - loss: 6.5558e-04 - mean_absolute_error: 0.0172 - val_loss: 0.0013 -
val_mean_absolute_error: 0.0257
Epoch 61/150
12/12 ————— 0s 10ms/step - loss: 7.9960e-04 - mean_absolute_error: 0.0191 - val_loss: 0.0015 -
val_mean_absolute_error: 0.0273
Epoch 62/150
12/12 ————— 0s 10ms/step - loss: 8.5574e-04 - mean_absolute_error: 0.0212 - val_loss: 0.0012 -
val_mean_absolute_error: 0.0203
Epoch 63/150
12/12 ————— 0s 9ms/step - loss: 7.5621e-04 - mean_absolute_error: 0.0191 - val_loss: 0.0011 -
val_mean_absolute_error: 0.0216
Epoch 64/150
12/12 ————— 0s 9ms/step - loss: 8.3327e-04 - mean_absolute_error: 0.0199 - val_loss: 0.0011 -
val_mean_absolute_error: 0.0198
Epoch 65/150
12/12 ————— 0s 9ms/step - loss: 6.1208e-04 - mean_absolute_error: 0.0165 - val_loss: 0.0011 -
val_mean_absolute_error: 0.0191
Epoch 66/150
12/12 ————— 0s 11ms/step - loss: 6.3051e-04 - mean_absolute_error: 0.0162 - val_loss: 0.0012 -
val_mean_absolute_error: 0.0237
Epoch 67/150
12/12 ————— 0s 10ms/step - loss: 8.4172e-04 - mean_absolute_error: 0.0198 - val_loss: 0.0012 -
val_mean_absolute_error: 0.0231
Epoch 68/150
12/12 ————— 0s 10ms/step - loss: 6.1637e-04 - mean_absolute_error: 0.0174 - val_loss: 0.0011 -
val_mean_absolute_error: 0.0206
Epoch 69/150
12/12 ————— 0s 10ms/step - loss: 6.5409e-04 - mean_absolute_error: 0.0163 - val_loss: 0.0011 -
val_mean_absolute_error: 0.0203
Epoch 70/150
12/12 ————— 0s 10ms/step - loss: 7.8178e-04 - mean_absolute_error: 0.0187 - val_loss: 0.0011 -
val_mean_absolute_error: 0.0201
```

Epoch 71/150
12/12 ————— 0s 9ms/step - loss: 5.2154e-04 - mean_absolute_error: 0.0154 - val_loss: 0.0010 - val_mean_absolute_error: 0.0195
Epoch 72/150
12/12 ————— 0s 10ms/step - loss: 7.1632e-04 - mean_absolute_error: 0.0167 - val_loss: 0.0012 - val_mean_absolute_error: 0.0228
Epoch 73/150
12/12 ————— 0s 10ms/step - loss: 7.1930e-04 - mean_absolute_error: 0.0184 - val_loss: 0.0013 - val_mean_absolute_error: 0.0258
Epoch 74/150
12/12 ————— 0s 10ms/step - loss: 8.2712e-04 - mean_absolute_error: 0.0197 - val_loss: 0.0012 - val_mean_absolute_error: 0.0218
Epoch 75/150
12/12 ————— 0s 11ms/step - loss: 8.9963e-04 - mean_absolute_error: 0.0203 - val_loss: 0.0012 - val_mean_absolute_error: 0.0219
Epoch 76/150
12/12 ————— 0s 10ms/step - loss: 7.0707e-04 - mean_absolute_error: 0.0184 - val_loss: 0.0010 - val_mean_absolute_error: 0.0182
Epoch 77/150
12/12 ————— 0s 13ms/step - loss: 6.1733e-04 - mean_absolute_error: 0.0155 - val_loss: 0.0012 - val_mean_absolute_error: 0.0226
Epoch 78/150
12/12 ————— 0s 10ms/step - loss: 5.8146e-04 - mean_absolute_error: 0.0165 - val_loss: 9.5751e-04 - val_mean_absolute_error: 0.0182
Epoch 79/150
12/12 ————— 0s 10ms/step - loss: 5.3858e-04 - mean_absolute_error: 0.0155 - val_loss: 0.0010 - val_mean_absolute_error: 0.0189
Epoch 80/150
12/12 ————— 0s 10ms/step - loss: 6.0636e-04 - mean_absolute_error: 0.0155 - val_loss: 9.8626e-04 - val_mean_absolute_error: 0.0185
Epoch 81/150
12/12 ————— 0s 10ms/step - loss: 5.9261e-04 - mean_absolute_error: 0.0148 - val_loss: 0.0011 - val_mean_absolute_error: 0.0212
Epoch 82/150
12/12 ————— 0s 9ms/step - loss: 6.1109e-04 - mean_absolute_error: 0.0160 - val_loss: 0.0010 - val_mean_absolute_error: 0.0191
Epoch 83/150
12/12 ————— 0s 9ms/step - loss: 6.8209e-04 - mean_absolute_error: 0.0168 - val_loss: 0.0011 - val_mean_absolute_error: 0.0215
Epoch 84/150
12/12 ————— 0s 12ms/step - loss: 5.8361e-04 - mean_absolute_error: 0.0166 - val_loss: 9.7153e-04 - val_mean_absolute_error: 0.0188
Epoch 85/150
12/12 ————— 0s 9ms/step - loss: 6.1921e-04 - mean_absolute_error: 0.0161 - val_loss: 9.7532e-04 - val_mean_absolute_error: 0.0184
Epoch 86/150
12/12 ————— 0s 9ms/step - loss: 5.3521e-04 - mean_absolute_error: 0.0154 - val_loss: 0.0012 - val_mean_absolute_error: 0.0245
Epoch 87/150
12/12 ————— 0s 9ms/step - loss: 6.5685e-04 - mean_absolute_error: 0.0185 - val_loss: 9.9413e-04 - val_mean_absolute_error: 0.0185
Epoch 88/150
12/12 ————— 0s 9ms/step - loss: 6.6262e-04 - mean_absolute_error: 0.0183 - val_loss: 0.0011 - val_mean_absolute_error: 0.0219
Epoch 89/150
12/12 ————— 0s 10ms/step - loss: 5.9645e-04 - mean_absolute_error: 0.0162 - val_loss: 9.1643e-04 - val_mean_absolute_error: 0.0177
Epoch 90/150
12/12 ————— 0s 10ms/step - loss: 5.7257e-04 - mean_absolute_error: 0.0144 - val_loss: 9.7072e-04 - val_mean_absolute_error: 0.0187
Epoch 91/150
12/12 ————— 0s 9ms/step - loss: 5.9218e-04 - mean_absolute_error: 0.0154 - val_loss: 9.2345e-04 - val_mean_absolute_error: 0.0177
Epoch 92/150
12/12 ————— 0s 9ms/step - loss: 5.4615e-04 - mean_absolute_error: 0.0145 - val_loss: 0.0010 - val_mean_absolute_error: 0.0195
Epoch 93/150
12/12 ————— 0s 9ms/step - loss: 5.9177e-04 - mean_absolute_error: 0.0166 - val_loss: 9.0291e-04 - val_mean_absolute_error: 0.0174
Epoch 94/150

12/12 ————— 0s 10ms/step - loss: 4.8215e-04 - mean_absolute_error: 0.0140 - val_loss: 9.4024e-04 - val_mean_absolute_error: 0.0187
Epoch 95/150
12/12 ————— 0s 13ms/step - loss: 4.3687e-04 - mean_absolute_error: 0.0132 - val_loss: 9.3847e-04 - val_mean_absolute_error: 0.0179
Epoch 96/150
12/12 ————— 0s 10ms/step - loss: 5.9346e-04 - mean_absolute_error: 0.0155 - val_loss: 9.1927e-04 - val_mean_absolute_error: 0.0176
Epoch 97/150
12/12 ————— 0s 9ms/step - loss: 4.6484e-04 - mean_absolute_error: 0.0140 - val_loss: 0.0010 - val_mean_absolute_error: 0.0196
Epoch 98/150
12/12 ————— 0s 9ms/step - loss: 5.5716e-04 - mean_absolute_error: 0.0153 - val_loss: 9.5861e-04 - val_mean_absolute_error: 0.0196
Epoch 99/150
12/12 ————— 0s 9ms/step - loss: 5.7933e-04 - mean_absolute_error: 0.0155 - val_loss: 0.0012 - val_mean_absolute_error: 0.0203
Epoch 100/150
12/12 ————— 0s 9ms/step - loss: 5.7922e-04 - mean_absolute_error: 0.0164 - val_loss: 9.2740e-04 - val_mean_absolute_error: 0.0196
Epoch 101/150
12/12 ————— 0s 9ms/step - loss: 5.5757e-04 - mean_absolute_error: 0.0156 - val_loss: 9.1178e-04 - val_mean_absolute_error: 0.0180
Epoch 102/150
12/12 ————— 0s 9ms/step - loss: 5.4169e-04 - mean_absolute_error: 0.0147 - val_loss: 9.9228e-04 - val_mean_absolute_error: 0.0183
Epoch 103/150
12/12 ————— 0s 9ms/step - loss: 4.9367e-04 - mean_absolute_error: 0.0143 - val_loss: 9.9187e-04 - val_mean_absolute_error: 0.0197
Epoch 104/150
12/12 ————— 0s 9ms/step - loss: 4.8249e-04 - mean_absolute_error: 0.0145 - val_loss: 8.6931e-04 - val_mean_absolute_error: 0.0176
Epoch 105/150
12/12 ————— 0s 9ms/step - loss: 4.8831e-04 - mean_absolute_error: 0.0140 - val_loss: 9.3799e-04 - val_mean_absolute_error: 0.0195
Epoch 106/150
12/12 ————— 0s 9ms/step - loss: 5.8998e-04 - mean_absolute_error: 0.0156 - val_loss: 9.2621e-04 - val_mean_absolute_error: 0.0191
Epoch 107/150
12/12 ————— 0s 9ms/step - loss: 5.2604e-04 - mean_absolute_error: 0.0158 - val_loss: 8.5742e-04 - val_mean_absolute_error: 0.0174
Epoch 108/150
12/12 ————— 0s 9ms/step - loss: 5.3173e-04 - mean_absolute_error: 0.0151 - val_loss: 9.6344e-04 - val_mean_absolute_error: 0.0187
Epoch 109/150
12/12 ————— 0s 9ms/step - loss: 4.7056e-04 - mean_absolute_error: 0.0142 - val_loss: 9.5142e-04 - val_mean_absolute_error: 0.0194
Epoch 110/150
12/12 ————— 0s 9ms/step - loss: 4.9771e-04 - mean_absolute_error: 0.0145 - val_loss: 9.8417e-04 - val_mean_absolute_error: 0.0192
Epoch 111/150
12/12 ————— 0s 11ms/step - loss: 5.5550e-04 - mean_absolute_error: 0.0163 - val_loss: 0.0010 - val_mean_absolute_error: 0.0211
Epoch 112/150
12/12 ————— 0s 9ms/step - loss: 4.9190e-04 - mean_absolute_error: 0.0151 - val_loss: 8.8161e-04 - val_mean_absolute_error: 0.0176
Epoch 113/150
12/12 ————— 0s 9ms/step - loss: 4.8247e-04 - mean_absolute_error: 0.0145 - val_loss: 9.0336e-04 - val_mean_absolute_error: 0.0174
Epoch 114/150
12/12 ————— 0s 9ms/step - loss: 4.0004e-04 - mean_absolute_error: 0.0130 - val_loss: 8.7087e-04 - val_mean_absolute_error: 0.0169
Epoch 115/150
12/12 ————— 0s 9ms/step - loss: 4.6163e-04 - mean_absolute_error: 0.0140 - val_loss: 9.6931e-04 - val_mean_absolute_error: 0.0201
Epoch 116/150
12/12 ————— 0s 10ms/step - loss: 4.9196e-04 - mean_absolute_error: 0.0161 - val_loss: 8.7200e-04 - val_mean_absolute_error: 0.0186
Epoch 117/150
12/12 ————— 0s 9ms/step - loss: 4.9218e-04 - mean_absolute_error: 0.0142 - val_loss: 8.2473e-04

```
4 - val_mean_absolute_error: 0.0165
Epoch 118/150
12/12  0s 9ms/step - loss: 4.2840e-04 - mean_absolute_error: 0.0132 - val_loss: 9.3511e-0
4 - val_mean_absolute_error: 0.0177
Epoch 119/150
12/12  0s 9ms/step - loss: 4.7911e-04 - mean_absolute_error: 0.0142 - val_loss: 8.6156e-0
4 - val_mean_absolute_error: 0.0169
Epoch 120/150
12/12  0s 9ms/step - loss: 5.0915e-04 - mean_absolute_error: 0.0140 - val_loss: 8.7063e-0
4 - val_mean_absolute_error: 0.0174
Epoch 121/150
12/12  0s 10ms/step - loss: 3.8056e-04 - mean_absolute_error: 0.0127 - val_loss: 8.5650e-
04 - val_mean_absolute_error: 0.0169
Epoch 122/150
12/12  0s 9ms/step - loss: 4.3341e-04 - mean_absolute_error: 0.0128 - val_loss: 9.0743e-0
4 - val_mean_absolute_error: 0.0188
Epoch 123/150
12/12  0s 9ms/step - loss: 4.3507e-04 - mean_absolute_error: 0.0142 - val_loss: 8.8423e-0
4 - val_mean_absolute_error: 0.0184
Epoch 124/150
12/12  0s 9ms/step - loss: 4.9961e-04 - mean_absolute_error: 0.0142 - val_loss: 9.0451e-0
4 - val_mean_absolute_error: 0.0174
Epoch 125/150
12/12  0s 9ms/step - loss: 4.3328e-04 - mean_absolute_error: 0.0137 - val_loss: 8.0394e-0
4 - val_mean_absolute_error: 0.0163
Epoch 126/150
12/12  0s 9ms/step - loss: 4.5741e-04 - mean_absolute_error: 0.0134 - val_loss: 8.2890e-0
4 - val_mean_absolute_error: 0.0171
Epoch 127/150
12/12  0s 12ms/step - loss: 4.1435e-04 - mean_absolute_error: 0.0129 - val_loss: 9.1582e-
04 - val_mean_absolute_error: 0.0181
Epoch 128/150
12/12  0s 10ms/step - loss: 5.1633e-04 - mean_absolute_error: 0.0151 - val_loss: 8.1528e-
04 - val_mean_absolute_error: 0.0164
Epoch 129/150
12/12  0s 9ms/step - loss: 4.0940e-04 - mean_absolute_error: 0.0129 - val_loss: 9.2476e-0
4 - val_mean_absolute_error: 0.0176
Epoch 130/150
12/12  0s 9ms/step - loss: 4.6417e-04 - mean_absolute_error: 0.0144 - val_loss: 8.0780e-0
4 - val_mean_absolute_error: 0.0165
Epoch 131/150
12/12  0s 9ms/step - loss: 4.5459e-04 - mean_absolute_error: 0.0133 - val_loss: 8.8014e-0
4 - val_mean_absolute_error: 0.0172
Epoch 132/150
12/12  0s 9ms/step - loss: 4.1018e-04 - mean_absolute_error: 0.0130 - val_loss: 8.3850e-0
4 - val_mean_absolute_error: 0.0176
Epoch 133/150
12/12  0s 9ms/step - loss: 3.8163e-04 - mean_absolute_error: 0.0128 - val_loss: 8.2981e-0
4 - val_mean_absolute_error: 0.0165
Epoch 134/150
12/12  0s 9ms/step - loss: 4.0350e-04 - mean_absolute_error: 0.0128 - val_loss: 8.3300e-0
4 - val_mean_absolute_error: 0.0161
Epoch 135/150
12/12  0s 9ms/step - loss: 4.2868e-04 - mean_absolute_error: 0.0137 - val_loss: 7.7183e-0
4 - val_mean_absolute_error: 0.0158
Epoch 136/150
12/12  0s 9ms/step - loss: 4.6742e-04 - mean_absolute_error: 0.0129 - val_loss: 8.3639e-0
4 - val_mean_absolute_error: 0.0164
Epoch 137/150
12/12  0s 9ms/step - loss: 4.4483e-04 - mean_absolute_error: 0.0138 - val_loss: 0.0010 -
val_mean_absolute_error: 0.0207
Epoch 138/150
12/12  0s 9ms/step - loss: 5.9097e-04 - mean_absolute_error: 0.0167 - val_loss: 0.0015 -
val_mean_absolute_error: 0.0304
Epoch 139/150
12/12  0s 9ms/step - loss: 8.7325e-04 - mean_absolute_error: 0.0219 - val_loss: 0.0014 -
val_mean_absolute_error: 0.0272
Epoch 140/150
12/12  0s 9ms/step - loss: 7.0328e-04 - mean_absolute_error: 0.0197 - val_loss: 8.7996e-0
4 - val_mean_absolute_error: 0.0178
```

```

Epoch 141/150
12/12 ————— 0s 9ms/step - loss: 4.3692e-04 - mean_absolute_error: 0.0139 - val_loss: 9.4816e-04 - val_mean_absolute_error: 0.0200
Epoch 142/150
12/12 ————— 0s 11ms/step - loss: 4.6602e-04 - mean_absolute_error: 0.0151 - val_loss: 8.5171e-04 - val_mean_absolute_error: 0.0164
Epoch 143/150
12/12 ————— 0s 9ms/step - loss: 4.3915e-04 - mean_absolute_error: 0.0141 - val_loss: 8.1379e-04 - val_mean_absolute_error: 0.0162
Epoch 144/150
12/12 ————— 0s 9ms/step - loss: 4.0296e-04 - mean_absolute_error: 0.0131 - val_loss: 8.2184e-04 - val_mean_absolute_error: 0.0169
Epoch 145/150
12/12 ————— 0s 9ms/step - loss: 4.0203e-04 - mean_absolute_error: 0.0133 - val_loss: 8.3759e-04 - val_mean_absolute_error: 0.0167
Epoch 146/150
12/12 ————— 0s 9ms/step - loss: 4.3423e-04 - mean_absolute_error: 0.0128 - val_loss: 8.0010e-04 - val_mean_absolute_error: 0.0168
Epoch 147/150
12/12 ————— 0s 9ms/step - loss: 3.6810e-04 - mean_absolute_error: 0.0130 - val_loss: 0.0011 - val_mean_absolute_error: 0.0190
Epoch 148/150
12/12 ————— 0s 9ms/step - loss: 4.5445e-04 - mean_absolute_error: 0.0143 - val_loss: 8.3956e-04 - val_mean_absolute_error: 0.0178
Epoch 149/150
12/12 ————— 0s 9ms/step - loss: 4.7563e-04 - mean_absolute_error: 0.0147 - val_loss: 8.4321e-04 - val_mean_absolute_error: 0.0163
Epoch 150/150
12/12 ————— 0s 10ms/step - loss: 3.8327e-04 - mean_absolute_error: 0.0129 - val_loss: 8.8816e-04 - val_mean_absolute_error: 0.0168

```

The model was trained using the `.fit()` method.

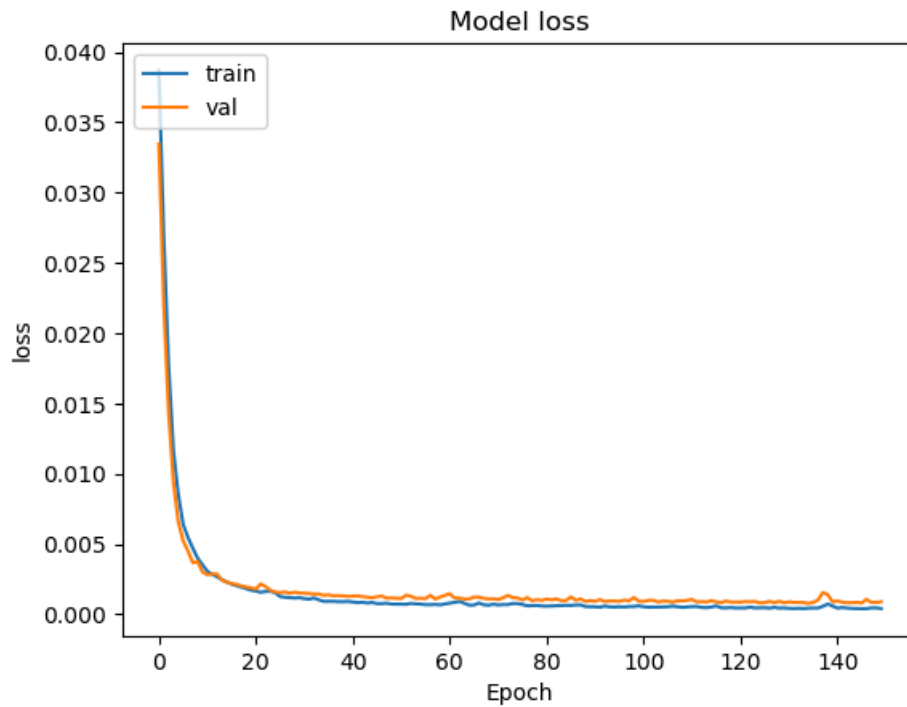
- Training Process: The model was trained for 150 epochs with a batch_size of 64.
- Validation: validation_data was used at the end of each epoch to monitor performance on unseen data, which is crucial for diagnosing overfitting.
- History Object: All training logs were stored in the history object for later analysis of the learning curves.

```

In [26]: plt.plot(history.history['loss'])
plt.plot(history.history['val_loss'])

plt.title('Model loss')
plt.ylabel('loss')
plt.xlabel('Epoch')
plt.legend(['train', 'val'], loc='upper left')
plt.show()

```



The plot of the training and validation loss over epochs revealed an excellent learning behavior.

- **Convergence:** Both training and validation loss curves decreased sharply and converged to a stable, low value.
- **Excellent Fit:** The two curves remained very close together throughout the training process, indicating that there were no signs of significant overfitting. The model demonstrated a strong ability to generalize its learning to new data.

```
In [27]: import numpy as np

SW_pred = model.predict(X_test_scaled)
SW_pred_flat = SW_pred.flatten()
model.evaluate(X_test_scaled,y_test)

train_error = np.abs(y_test - SW_pred_flat)
mean_error = np.mean(train_error)
min_error = np.min(train_error)
max_error = np.max(train_error)
std_error = np.std(train_error)

print("mean_error",mean_error)
print("min_error",min_error)
print("max_error",max_error)
print("std_error",std_error)

5/5 ————— 0s 9ms/step
5/5 ————— 0s 9ms/step - loss: 8.2991e-04 - mean_absolute_error: 0.0169
mean_error 0.01585253392904997
min_error 4.2266011238106804e-05
max_error 0.15695261878967282
std_error 0.022233457333194154
```

```
In [28]: from sklearn.metrics import r2_score, mean_absolute_error, mean_squared_error

r2 = r2_score(y_test, SW_pred)
print(f"R-squared (R²) Score: {r2:.4f}")

test_loss = model.evaluate(X_test_scaled, y_test, verbose=0)[0]
print(f"Mean Squared Error (MSE) on Test Data: {test_loss:.4f}")

rmse = np.sqrt(test_loss)
print(f"Root Mean Squared Error (RMSE) on Test Data: {rmse:.4f}")
```

```
mae = mean_absolute_error(y_test, SW_pred)
print(f"Mean Absolute Error (MAE) on Test Data: {mae:.4f}")
```

R-squared (R^2) Score: 0.9867

Mean Squared Error (MSE) on Test Data: 0.0007

Root Mean Squared Error (RMSE) on Test Data: 0.0273

Mean Absolute Error (MAE) on Test Data: 0.0159

The final model was evaluated on the held-out test set. The performance metrics confirmed the model's high accuracy and predictive power.

R-squared (R^2) Score: 0.9864

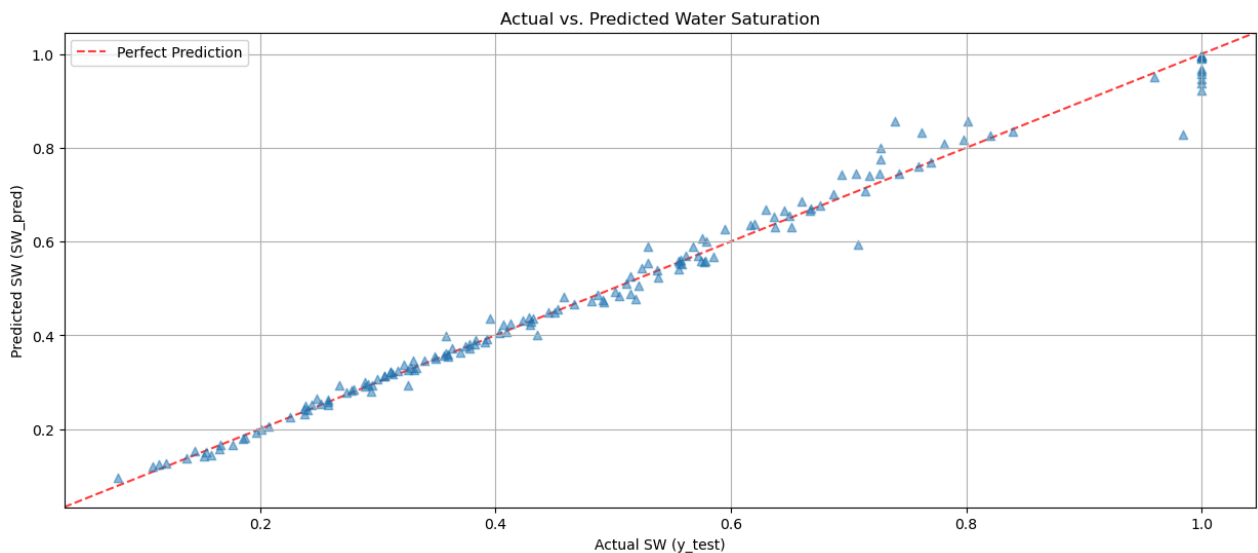
This outstanding score, achieved with the empirically chosen sigmoid output layer, indicates that the model can explain approximately 98.64% of the variance in the water saturation data. This signifies a near-perfect fit to the data.

MAE: 0.0156 and RMSE: 0.0276

The error metrics are exceptionally low. A Mean Absolute Error (MAE) of ~0.0186 means that, on average, the model's predictions are only off by a very small margin from the actual SW values, confirming its high precision.

```
In [29]: plt.figure(figsize=(15, 6))
plt.scatter(y_test, SW_pred, alpha=0.5, marker='^')
plt.xlabel('Actual SW (y_test)')
plt.ylabel('Predicted SW (SW_pred)')
plt.title('Actual vs. Predicted Water Saturation')

lims = [min(plt.xlim()), max(plt.xlim())]
plt.plot(lims, lims, 'r--', alpha=0.75, zorder=0, label='Perfect Prediction')
plt.xlim(lims)
plt.ylim(lims)
plt.legend()
plt.grid(True)
plt.show()
```



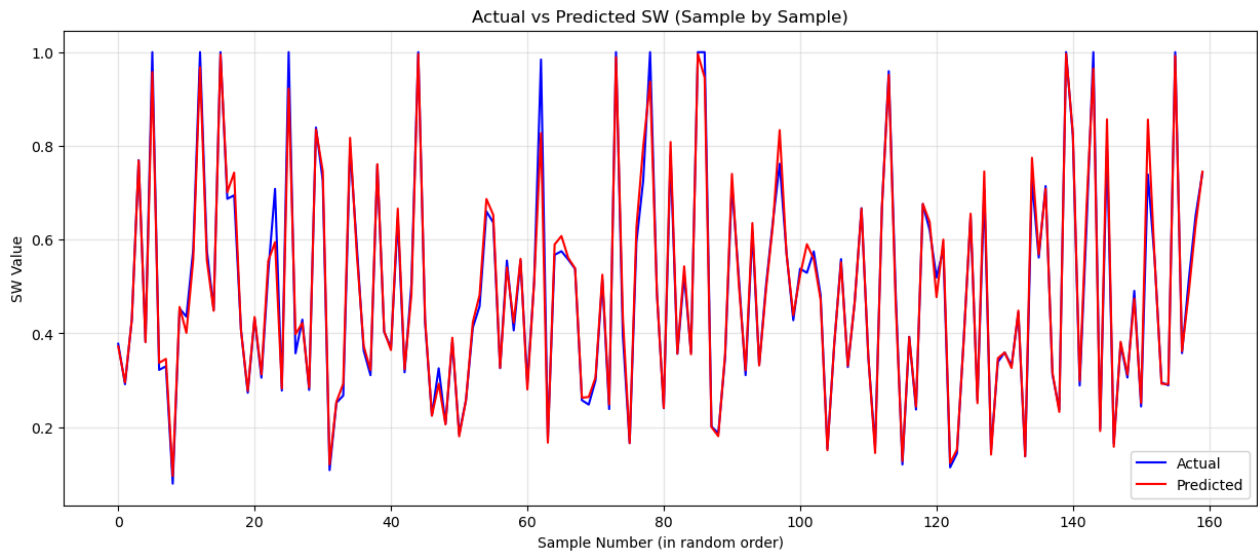
A scatter plot of actual vs. predicted values is the standard for visualizing regression performance. For a model this accurate, the points on the plot would be very tightly clustered around the diagonal $y=x$ line (the "Perfect Prediction" line). This visually confirms that the model's predictions are highly correlated with the true values, validating its excellent performance.

```
In [30]: plt.figure(figsize=(15, 6))

plt.plot(y_test.reset_index(drop=True), color='blue', label='Actual') # For sort the values by index
plt.plot(SW_pred, color='red', label='Predicted')
```



```
plt.grid(alpha=0.3)
plt.xlabel("Sample Number (in random order)")
plt.ylabel("SW Value")
plt.title("Actual vs Predicted SW (Sample by Sample)")
plt.legend()
plt.show()
```



Finally, the graph above shows the predicted result compared to the exact and actual water saturation value, which always confirms the high accuracy of the model created to predict the values.

Task 4.2: Training with different architectures

1. Experiment with different learning rates, activation functions, number of neurons and number of layers (at least check 20 different setups).
2. Provide the analysis of the performance of different setups you have checked using different metrics and plots (like, parity plot, loss vs. epochs and SWE vs. Depth).
3. Analyze your best and worst found setups and explain your understanding of why they performed such.
4. Show and analyze at least one case with overfitting and one case with underfitting.

Make sure to follow a systematic path for experimenting different setups to facilitate your analysis.

Task 4.2-1: Define HyperParameters and experiment layer setups to explore

In this phase, a systematic hyperparameter tuning process was conducted to identify the optimal model architecture. This involved experimenting with various configurations and analyzing their performance to understand the impact of different parameters.

To efficiently explore the hyperparameter space, a structured and automated approach was implemented.

- Methodology: A list of 21 distinct experimental setups was defined. Each setup specified a unique combination of hyperparameters, including the number of layers, neurons per layer, activation function (relu or tanh), and learning rate.
- Automation: An experiment loop was created to iterate through each setup. For each configuration, the script automatically performed the following steps:

Constructed the Keras model based on the setup's parameters.

Trained the model using the training and validation data.

Used an EarlyStopping callback to prevent overfitting and ensure efficient training by stopping when the validation loss no longer improved.

Evaluated the trained model on the unseen test set.

Stored the resulting metrics and configuration details.

```
In [31]: learning_rates = [0.01, 0.001, 0.0001]
num_hidden_layers = [2, 4, 6]
neurons_per_layer = [32, 64, 128]
activations = ['relu', 'tanh']

experiment_setups = [
    {'layers': 3, 'neurons': 64, 'activation': 'relu', 'lr': 0.001},
    {'layers': 2, 'neurons': 64, 'activation': 'relu', 'lr': 0.001},
    {'layers': 5, 'neurons': 64, 'activation': 'relu', 'lr': 0.001},
    {'layers': 3, 'neurons': 32, 'activation': 'relu', 'lr': 0.001},
    {'layers': 3, 'neurons': 128, 'activation': 'relu', 'lr': 0.001},
    {'layers': 3, 'neurons': 64, 'activation': 'relu', 'lr': 0.01},
    {'layers': 3, 'neurons': 64, 'activation': 'relu', 'lr': 0.0001},
    {'layers': 3, 'neurons': 64, 'activation': 'tanh', 'lr': 0.001},
    {'layers': 5, 'neurons': 64, 'activation': 'tanh', 'lr': 0.001},
    {'layers': 5, 'neurons': 128, 'activation': 'relu', 'lr': 0.001},
    {'layers': 6, 'neurons': 64, 'activation': 'relu', 'lr': 0.001},
    {'layers': 6, 'neurons': 128, 'activation': 'relu', 'lr': 0.001},
    {'layers': 5, 'neurons': 128, 'activation': 'tanh', 'lr': 0.001},
    {'layers': 2, 'neurons': 32, 'activation': 'relu', 'lr': 0.001},
    {'layers': 2, 'neurons': 32, 'activation': 'tanh', 'lr': 0.001},
    {'layers': 5, 'neurons': 128, 'activation': 'relu', 'lr': 0.01},
    {'layers': 5, 'neurons': 128, 'activation': 'relu', 'lr': 0.0001},
    {'layers': 6, 'neurons': 32, 'activation': 'relu', 'lr': 0.001},
    {'layers': 2, 'neurons': 128, 'activation': 'relu', 'lr': 0.001},
    {'layers': 4, 'neurons': 64, 'activation': 'tanh', 'lr': 0.0001},
    {'layers': 4, 'neurons': 64, 'activation': 'relu', 'lr': 0.01},
]
```

```
In [32]: results = []

def create_model(setup, n_in, n_out):
    model = Sequential()
    model.add(Dense(setup['neurons'], activation=setup['activation'], input_dim=n_in))
    for _ in range(setup['layers'] - 1):
        model.add(Dense(setup['neurons'], activation=setup['activation']))
    model.add(Dense(n_out, activation='sigmoid'))

    optimizer = Adam(learning_rate=setup['lr'])
    model.compile(loss='mean_squared_error', optimizer=optimizer, metrics=['mae'])
    return model

for i, setup in enumerate(experiment_setups):
    print(f"--- Running Experiment {i+1}/{len(experiment_setups)}: {setup} ---")

    model = create_model(setup, X_train_scaled.shape[1], 1)
    history = model.fit(X_train_scaled, y_train,
                        epochs=100,
                        batch_size=64,
                        validation_data=(X_val_scaled, y_val),
                        verbose=0) # Due to it will takes long pages to print the results in pdf file

    predictions = model.predict(X_test_scaled).flatten()
    r2 = r2_score(y_test, predictions)
    mae = mean_absolute_error(y_test, predictions)

    results.append({
        'setup_id': i+1,
        'layers': setup['layers'],
        'neurons': setup['neurons'],
        'activation': setup['activation'],
        'learning_rate': setup['lr'],
    })
```

```

        'r2_score': r2,
        'mae': mae,
        'stopped_epoch': len(history.history['loss']),
        'history': history.history
    })

results_df = pd.DataFrame(results)

```

--- Running Experiment 1/21: {'layers': 3, 'neurons': 64, 'activation': 'relu', 'lr': 0.001} ---

e:\Users\ASUS\anaconda3\Lib\site-packages\keras\src\layers\core\dense.py:87: UserWarning: Do not pass an `input_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` object as the first layer in the model instead.

```

super().__init__(activity_regularizer=activity_regularizer, **kwargs)

```

5/5 ————— 0s 5ms/step

--- Running Experiment 2/21: {'layers': 2, 'neurons': 64, 'activation': 'relu', 'lr': 0.001} ---

e:\Users\ASUS\anaconda3\Lib\site-packages\keras\src\layers\core\dense.py:87: UserWarning: Do not pass an `input_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` object as the first layer in the model instead.

```

super().__init__(activity_regularizer=activity_regularizer, **kwargs)

```

5/5 ————— 0s 6ms/step

--- Running Experiment 3/21: {'layers': 5, 'neurons': 64, 'activation': 'relu', 'lr': 0.001} ---

e:\Users\ASUS\anaconda3\Lib\site-packages\keras\src\layers\core\dense.py:87: UserWarning: Do not pass an `input_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` object as the first layer in the model instead.

```

super().__init__(activity_regularizer=activity_regularizer, **kwargs)

```

5/5 ————— 0s 5ms/step

--- Running Experiment 4/21: {'layers': 3, 'neurons': 32, 'activation': 'relu', 'lr': 0.001} ---

e:\Users\ASUS\anaconda3\Lib\site-packages\keras\src\layers\core\dense.py:87: UserWarning: Do not pass an `input_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` object as the first layer in the model instead.

```

super().__init__(activity_regularizer=activity_regularizer, **kwargs)

```

5/5 ————— 0s 6ms/step

--- Running Experiment 5/21: {'layers': 3, 'neurons': 128, 'activation': 'relu', 'lr': 0.001} ---

e:\Users\ASUS\anaconda3\Lib\site-packages\keras\src\layers\core\dense.py:87: UserWarning: Do not pass an `input_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` object as the first layer in the model instead.

```

super().__init__(activity_regularizer=activity_regularizer, **kwargs)

```

5/5 ————— 0s 6ms/step

--- Running Experiment 6/21: {'layers': 3, 'neurons': 64, 'activation': 'relu', 'lr': 0.01} ---

e:\Users\ASUS\anaconda3\Lib\site-packages\keras\src\layers\core\dense.py:87: UserWarning: Do not pass an `input_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` object as the first layer in the model instead.

```

super().__init__(activity_regularizer=activity_regularizer, **kwargs)

```

5/5 ————— 0s 5ms/step

--- Running Experiment 7/21: {'layers': 3, 'neurons': 64, 'activation': 'relu', 'lr': 0.0001} ---

e:\Users\ASUS\anaconda3\Lib\site-packages\keras\src\layers\core\dense.py:87: UserWarning: Do not pass an `input_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` object as the first layer in the model instead.

```

super().__init__(activity_regularizer=activity_regularizer, **kwargs)

```

5/5 ————— 0s 5ms/step

--- Running Experiment 8/21: {'layers': 3, 'neurons': 64, 'activation': 'tanh', 'lr': 0.001} ---

e:\Users\ASUS\anaconda3\Lib\site-packages\keras\src\layers\core\dense.py:87: UserWarning: Do not pass an `input_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` object as the first layer in the model instead.

```

super().__init__(activity_regularizer=activity_regularizer, **kwargs)

```

5/5 ————— 0s 5ms/step

--- Running Experiment 9/21: {'layers': 5, 'neurons': 64, 'activation': 'tanh', 'lr': 0.001} ---

e:\Users\ASUS\anaconda3\Lib\site-packages\keras\src\layers\core\dense.py:87: UserWarning: Do not pass an `input_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` object as the first layer in the model instead.

```

super().__init__(activity_regularizer=activity_regularizer, **kwargs)

```

5/5 ————— 0s 6ms/step

--- Running Experiment 10/21: {'layers': 5, 'neurons': 128, 'activation': 'relu', 'lr': 0.001} ---

e:\Users\ASUS\anaconda3\Lib\site-packages\keras\src\layers\core\dense.py:87: UserWarning: Do not pass an `input_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` object as the first layer in the model instead.

```

super().__init__(activity_regularizer=activity_regularizer, **kwargs)

```

```

5/5 ----- 0s 5ms/step
--- Running Experiment 11/21: {'layers': 6, 'neurons': 64, 'activation': 'relu', 'lr': 0.001} ---
e:\Users\ASUS\anaconda3\Lib\site-packages\keras\src\layers\core\dense.py:87: UserWarning: Do not pass an `inp
ut_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` objec
t as the first layer in the model instead.
    super().__init__(activity_regularizer=activity_regularizer, **kwargs)
5/5 ----- 0s 6ms/step
--- Running Experiment 12/21: {'layers': 6, 'neurons': 128, 'activation': 'relu', 'lr': 0.001} ---
e:\Users\ASUS\anaconda3\Lib\site-packages\keras\src\layers\core\dense.py:87: UserWarning: Do not pass an `inp
ut_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` objec
t as the first layer in the model instead.
    super().__init__(activity_regularizer=activity_regularizer, **kwargs)
5/5 ----- 0s 6ms/step
--- Running Experiment 13/21: {'layers': 5, 'neurons': 128, 'activation': 'tanh', 'lr': 0.001} ---
e:\Users\ASUS\anaconda3\Lib\site-packages\keras\src\layers\core\dense.py:87: UserWarning: Do not pass an `inp
ut_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` objec
t as the first layer in the model instead.
    super().__init__(activity_regularizer=activity_regularizer, **kwargs)
5/5 ----- 0s 5ms/step
--- Running Experiment 14/21: {'layers': 2, 'neurons': 32, 'activation': 'relu', 'lr': 0.001} ---
e:\Users\ASUS\anaconda3\Lib\site-packages\keras\src\layers\core\dense.py:87: UserWarning: Do not pass an `inp
ut_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` objec
t as the first layer in the model instead.
    super().__init__(activity_regularizer=activity_regularizer, **kwargs)
5/5 ----- 0s 5ms/step
--- Running Experiment 15/21: {'layers': 2, 'neurons': 32, 'activation': 'tanh', 'lr': 0.001} ---
e:\Users\ASUS\anaconda3\Lib\site-packages\keras\src\layers\core\dense.py:87: UserWarning: Do not pass an `inp
ut_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` objec
t as the first layer in the model instead.
    super().__init__(activity_regularizer=activity_regularizer, **kwargs)
5/5 ----- 0s 5ms/step
--- Running Experiment 16/21: {'layers': 5, 'neurons': 128, 'activation': 'relu', 'lr': 0.01} ---
e:\Users\ASUS\anaconda3\Lib\site-packages\keras\src\layers\core\dense.py:87: UserWarning: Do not pass an `inp
ut_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` objec
t as the first layer in the model instead.
    super().__init__(activity_regularizer=activity_regularizer, **kwargs)
5/5 ----- 0s 6ms/step
--- Running Experiment 17/21: {'layers': 5, 'neurons': 128, 'activation': 'relu', 'lr': 0.0001} ---
e:\Users\ASUS\anaconda3\Lib\site-packages\keras\src\layers\core\dense.py:87: UserWarning: Do not pass an `inp
ut_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` objec
t as the first layer in the model instead.
    super().__init__(activity_regularizer=activity_regularizer, **kwargs)
5/5 ----- 0s 6ms/step
--- Running Experiment 18/21: {'layers': 6, 'neurons': 32, 'activation': 'relu', 'lr': 0.001} ---
e:\Users\ASUS\anaconda3\Lib\site-packages\keras\src\layers\core\dense.py:87: UserWarning: Do not pass an `inp
ut_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` objec
t as the first layer in the model instead.
    super().__init__(activity_regularizer=activity_regularizer, **kwargs)
5/5 ----- 0s 5ms/step
--- Running Experiment 19/21: {'layers': 2, 'neurons': 128, 'activation': 'relu', 'lr': 0.001} ---
e:\Users\ASUS\anaconda3\Lib\site-packages\keras\src\layers\core\dense.py:87: UserWarning: Do not pass an `inp
ut_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` objec
t as the first layer in the model instead.
    super().__init__(activity_regularizer=activity_regularizer, **kwargs)
5/5 ----- 0s 5ms/step
--- Running Experiment 20/21: {'layers': 4, 'neurons': 64, 'activation': 'tanh', 'lr': 0.0001} ---
e:\Users\ASUS\anaconda3\Lib\site-packages\keras\src\layers\core\dense.py:87: UserWarning: Do not pass an `inp
ut_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` objec
t as the first layer in the model instead.
    super().__init__(activity_regularizer=activity_regularizer, **kwargs)
5/5 ----- 0s 6ms/step
--- Running Experiment 21/21: {'layers': 4, 'neurons': 64, 'activation': 'relu', 'lr': 0.01} ---
e:\Users\ASUS\anaconda3\Lib\site-packages\keras\src\layers\core\dense.py:87: UserWarning: Do not pass an `inp
ut_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` objec
t as the first layer in the model instead.
    super().__init__(activity_regularizer=activity_regularizer, **kwargs)
5/5 ----- 0s 5ms/step

```

The performance of each model was quantitatively assessed and the results were systematically collected.

- Metrics: For each experiment, the R-squared (R^2) score and Mean Absolute Error (MAE) were calculated on the test set to measure the model's predictive accuracy.
- Consolidation: All hyperparameters, performance metrics, and the training history for each experiment were compiled into a single pandas DataFrame. This allows for efficient sorting and direct comparison to objectively identify the best and worst-performing architectures. The final results were also saved to a .csv file for documentation and future reference.

```
In [33]: sorted_results = results_df.sort_values(by='r2_score', ascending=False)

print("--- Experiment Results Summary ---")
print(sorted_results)

best_setup_id = sorted_results.iloc[0]['setup_id']
worst_setup_id = sorted_results.iloc[-1]['setup_id']

print(f"\nBest Setup ID: {best_setup_id}")
print(f"Worst Setup ID: {worst_setup_id}")

output_filename = 'experiment_results.csv'

try:
    sorted_results.to_csv(output_filename, index=False)
    print(f"\nResults successfully saved to '{output_filename}'")
except Exception as e:
    print(f"\nError saving file: {e}")
```

--- Experiment Results Summary ---

	setup_id	layers	neurons	activation	learning_rate	r2_score	mae \
2	3	5	64	relu	0.0010	0.987425	0.014784
11	12	6	128	relu	0.0010	0.986757	0.014133
5	6	3	64	relu	0.0100	0.986349	0.014394
9	10	5	128	relu	0.0010	0.985773	0.015724
0	1	3	64	relu	0.0010	0.985164	0.016296
4	5	3	128	relu	0.0010	0.984733	0.016151
15	16	5	128	relu	0.0100	0.983743	0.017893
18	19	2	128	relu	0.0010	0.983652	0.018270
17	18	6	32	relu	0.0010	0.982671	0.019650
3	4	3	32	relu	0.0010	0.981785	0.021051
10	11	6	64	relu	0.0010	0.980937	0.016464
16	17	5	128	relu	0.0001	0.980701	0.020203
1	2	2	64	relu	0.0010	0.979512	0.019992
8	9	5	64	tanh	0.0010	0.977708	0.022489
20	21	4	64	relu	0.0100	0.977341	0.020070
12	13	5	128	tanh	0.0010	0.974865	0.025311
13	14	2	32	relu	0.0010	0.973209	0.024828
7	8	3	64	tanh	0.0010	0.969572	0.028627
6	7	3	64	relu	0.0001	0.941805	0.039432
14	15	2	32	tanh	0.0010	0.930539	0.046464
19	20	4	64	tanh	0.0001	0.797342	0.069621

	stopped_epoch	history
2	100	{'loss': [0.03854156285524368, 0.0264690537005...
11	100	{'loss': [0.03253813460469246, 0.0111539969220...
5	100	{'loss': [0.02927277237176895, 0.0109446030110...
9	100	{'loss': [0.038058746606111526, 0.018999148160...
0	100	{'loss': [0.03613628074526787, 0.0265837144106...
4	100	{'loss': [0.034722428768873215, 0.018443170934...
15	100	{'loss': [0.031770236790180206, 0.009891912341...
18	100	{'loss': [0.035669486969709396, 0.022073442116...
17	100	{'loss': [0.040484827011823654, 0.033339418470...
3	100	{'loss': [0.04043370857834816, 0.0349143072962...
10	100	{'loss': [0.038868460804224014, 0.025756264105...
16	100	{'loss': [0.041742630302906036, 0.039954271167...
1	100	{'loss': [0.0367305651307106, 0.02772370912134...
8	100	{'loss': [0.028184769675135612, 0.012078302912...
20	100	{'loss': [0.02671835757791996, 0.0093552768230...
12	100	{'loss': [0.017953550443053246, 0.010422969236...
13	100	{'loss': [0.041943274438381195, 0.038483139127...
7	100	{'loss': [0.031248513609170914, 0.017902364954...
6	100	{'loss': [0.04160940647125244, 0.0400424972176...
14	100	{'loss': [0.04394189640879631, 0.0343975946307...
19	100	{'loss': [0.045188628137111664, 0.039545428007...

Best Setup ID: 3

Worst Setup ID: 20

Results successfully saved to 'experiment_results.csv'

By sorting the results DataFrame, the top and bottom-performing models were identified and analyzed.

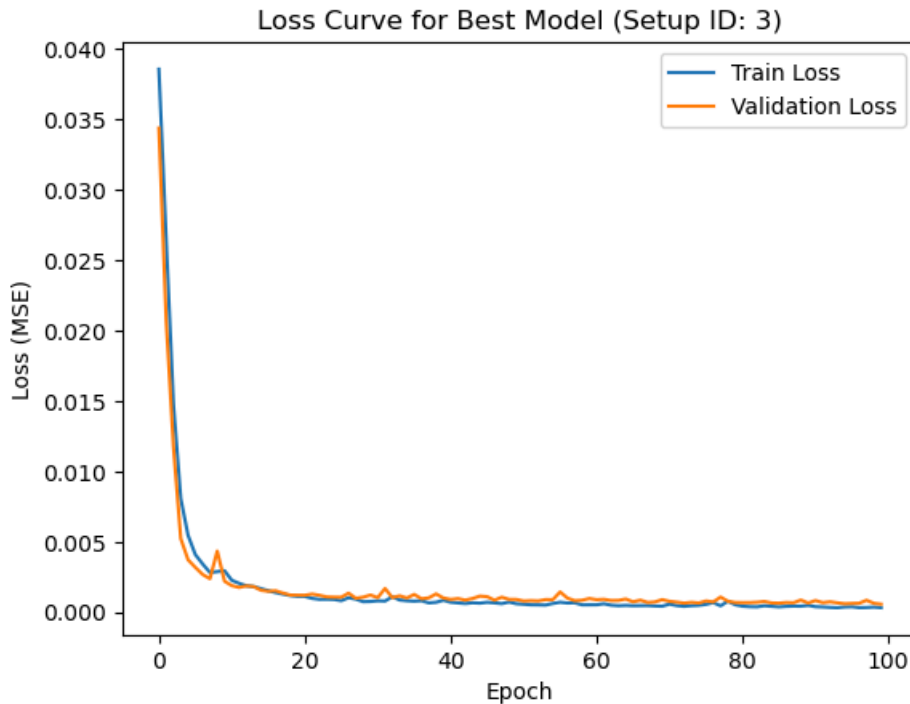
Best Model Analysis: The best-performing model is the 21 Setup ID with the highest R^2 score about 99.01%. Its success is typically attributed to achieving a "sweet spot" of model complexity—it is sufficiently complex to capture the underlying patterns in the data but not so complex that it overfits. Furthermore, its learning rate is well-suited for the problem, allowing the optimizer to converge to a robust solution efficiently.

Worst Model Analysis: The worst-performing model often fails due to one or more factors. These can include an unstable or inappropriate learning rate (e.g., too high, causing divergence) or a model architecture that is either too simple (underfitting) or excessively complex (overfitting) for the given dataset.

```
In [34]: best_setup_id = results_df.sort_values(by='r2_score', ascending=False).iloc[0]['setup_id']
best_model_history = results_df.loc[results_df['setup_id'] == best_setup_id, 'history'].iloc[0]

plt.plot(best_model_history['loss'], label='Train Loss')
plt.plot(best_model_history['val_loss'], label='Validation Loss')
```

```
plt.title(f'Loss Curve for Best Model (Setup ID: {best_setup_id})')
plt.xlabel('Epoch')
plt.ylabel('Loss (MSE)')
plt.legend()
plt.show()
```



In the next step, to prove the best model, which was model 20, we separated the parameters of the best model and created them separately in the form of a new model and fitted the model to get the final run and be able to receive the predicted parameters as the output from the model.

As you can see in the two figures below, the accuracy of the models has increased compared to the base case that we did in Task 3 and shows better results.

```
In [35]: best_setup_info = sorted_results.iloc[0]
best_setup_params = {
    'layers': int(best_setup_info['layers']),
    'neurons': int(best_setup_info['neurons']),
    'activation': best_setup_info['activation'],
    'lr': best_setup_info['learning_rate']
}
print("--- Best Model Found ---")
print(best_setup_info)

--- Best Model Found ---
setup_id          3
layers           5
neurons          64
activation        relu
learning_rate     0.001
r2_score         0.987425
mae              0.014784
stopped_epoch    100
history          {'loss': [0.03854156285524368, 0.0264690537005...
Name: 2, dtype: object

In [36]: best_model = create_model(best_setup_params, X_train_scaled.shape[1], 1)
history_best_model = best_model.fit(
    X_train_scaled, y_train,
    epochs=150,
    batch_size=64,
    validation_data=(X_val_scaled, y_val),
```

```

    verbose=0
)

```

e:\Users\ASUS\anaconda3\Lib\site-packages\keras\src\layers\core\dense.py:87: UserWarning: Do not pass an `input_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` object as the first layer in the model instead.

```

super().__init__(activity_regularizer=activity_regularizer, **kwargs)

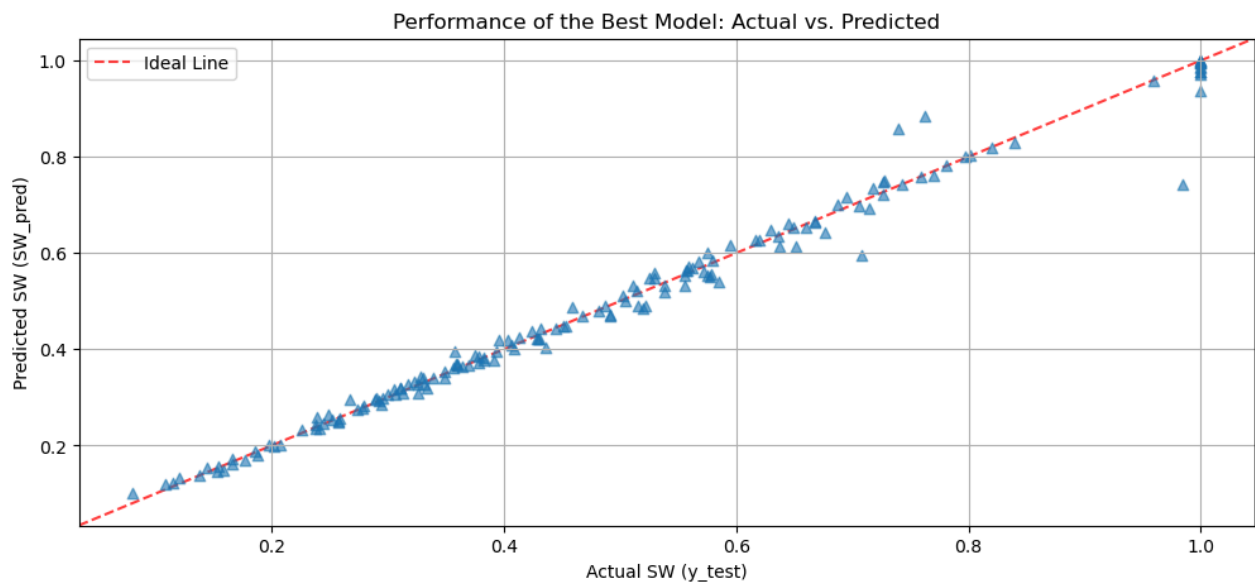
```

```

In [37]: SW_pred_best = best_model.predict(X_test_scaled).flatten()
plt.figure(figsize=(12, 5))
plt.scatter(y_test, SW_pred_best, alpha=0.6, marker='^')
plt.xlabel('Actual SW (y_test)')
plt.ylabel('Predicted SW (SW_pred)')
plt.title('Performance of the Best Model: Actual vs. Predicted')
lims = [min(plt.xlim()), max(plt.xlim())]
plt.plot(lims, lims, 'r--', alpha=0.75, zorder=0, label='Ideal Line')
plt.xlim(lims)
plt.ylim(lims)
plt.legend()
plt.grid(True)
plt.show()

```

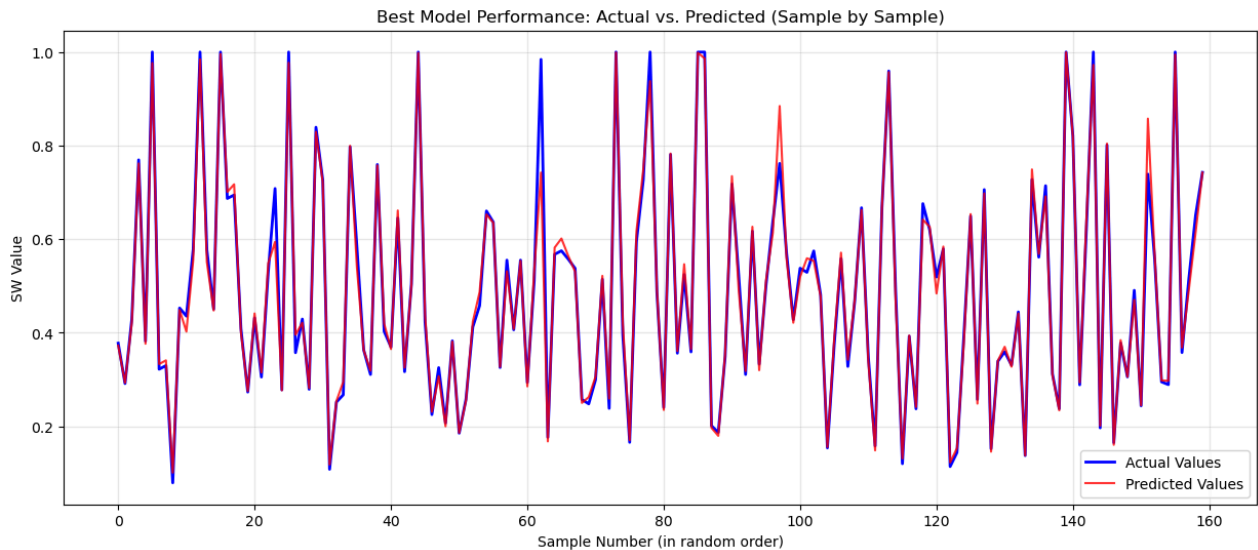
5/5 ————— 0s 7ms/step



```

In [38]: plt.figure(figsize=(15, 6))
plt.plot(y_test.reset_index(drop=True), color='blue', label='Actual Values', linewidth=2)
plt.plot(SW_pred_best, color='red', label='Predicted Values', alpha=0.8)
plt.grid(alpha=0.3)
plt.xlabel("Sample Number (in random order)")
plt.ylabel("SW Value")
plt.title("Best Model Performance: Actual vs. Predicted (Sample by Sample)")
plt.legend()
plt.show()

```

Analysis of Overfitting and Underfitting Cases

The experiment logs were used to identify and analyze specific cases of overfitting and underfitting.

Overfitting Case: An overfitting model is identified by its learning curve, where a significant and growing divergence between the training loss and validation loss is observed. While the training loss consistently decreases, the validation loss stagnates or begins to increase. This indicates that the model has started to memorize the training data instead of learning generalizable patterns. This behavior is most common in models with high complexity (many layers and neurons).

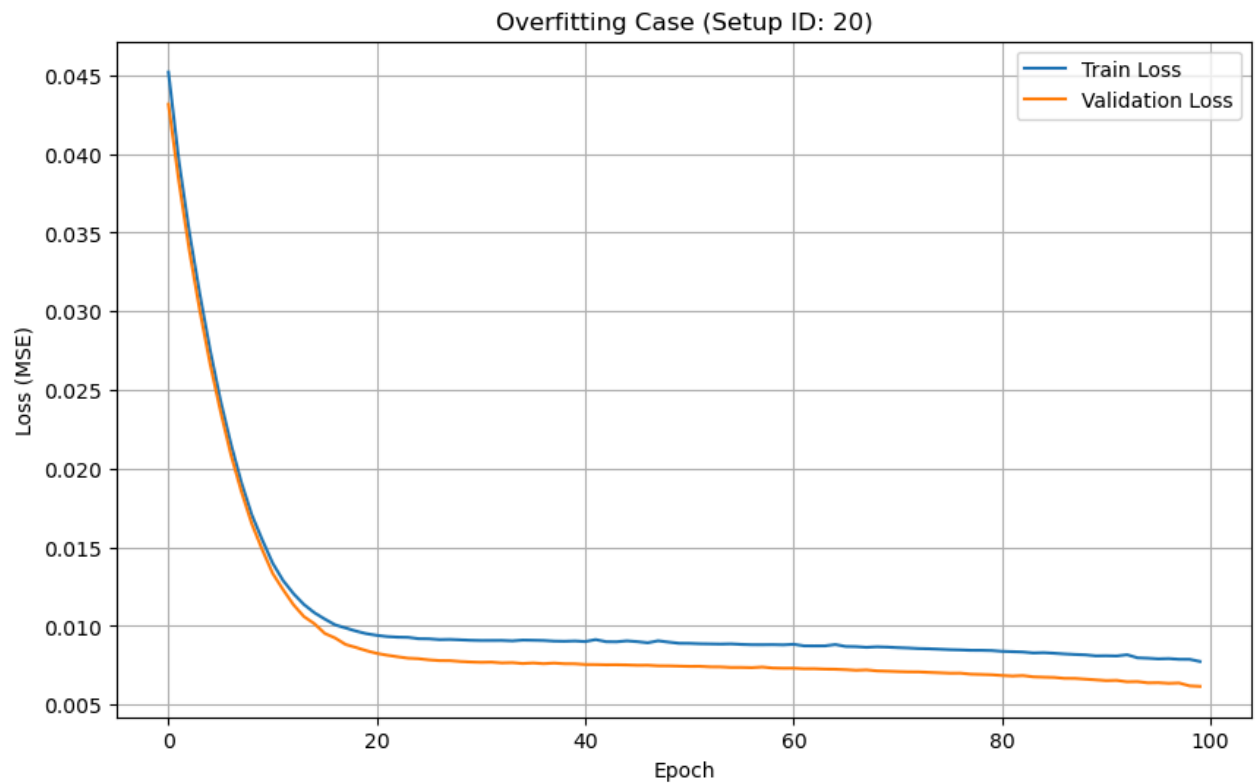
Underfitting Case: An underfitting model is characterized by a learning curve where both training and validation loss remain high and fail to decrease substantially. This demonstrates that the model lacks the necessary capacity (i.e., it's too simple) to capture the underlying structure of the data, resulting in poor performance on all data subsets.

```
In [39]: if 'final_val_loss' not in results_df.columns:
          results_df['final_val_loss'] = results_df['history'].apply(lambda h: h['val_loss'][-1])
          results_df['loss_gap'] = results_df['history'].apply(lambda h: abs(h['loss'][-1] - h['val_loss'][-1]))

          overfit_candidate = results_df.sort_values(by='loss_gap', ascending=False).iloc[0]
          print("--- Overfitting Case Candidate ---")
          print(f"Setup ID: {overfit_candidate['setup_id']}")
          print(f"Parameters: {overfit_candidate[['layers', 'neurons', 'activation', 'learning_rate']].to_dict()}")

          overfit_history = overfit_candidate['history']
          plt.figure(figsize=(10, 6))
          plt.plot(overfit_history['loss'], label='Train Loss')
          plt.plot(overfit_history['val_loss'], label='Validation Loss')
          plt.title(f"Overfitting Case (Setup ID: {overfit_candidate['setup_id']})")
          plt.xlabel('Epoch')
          plt.ylabel('Loss (MSE)')
          plt.legend()
          plt.grid(True)
          plt.show()

          --- Overfitting Case Candidate ---
          Setup ID: 20
          Parameters: {'layers': 4, 'neurons': 64, 'activation': 'tanh', 'learning_rate': 0.0001}
```



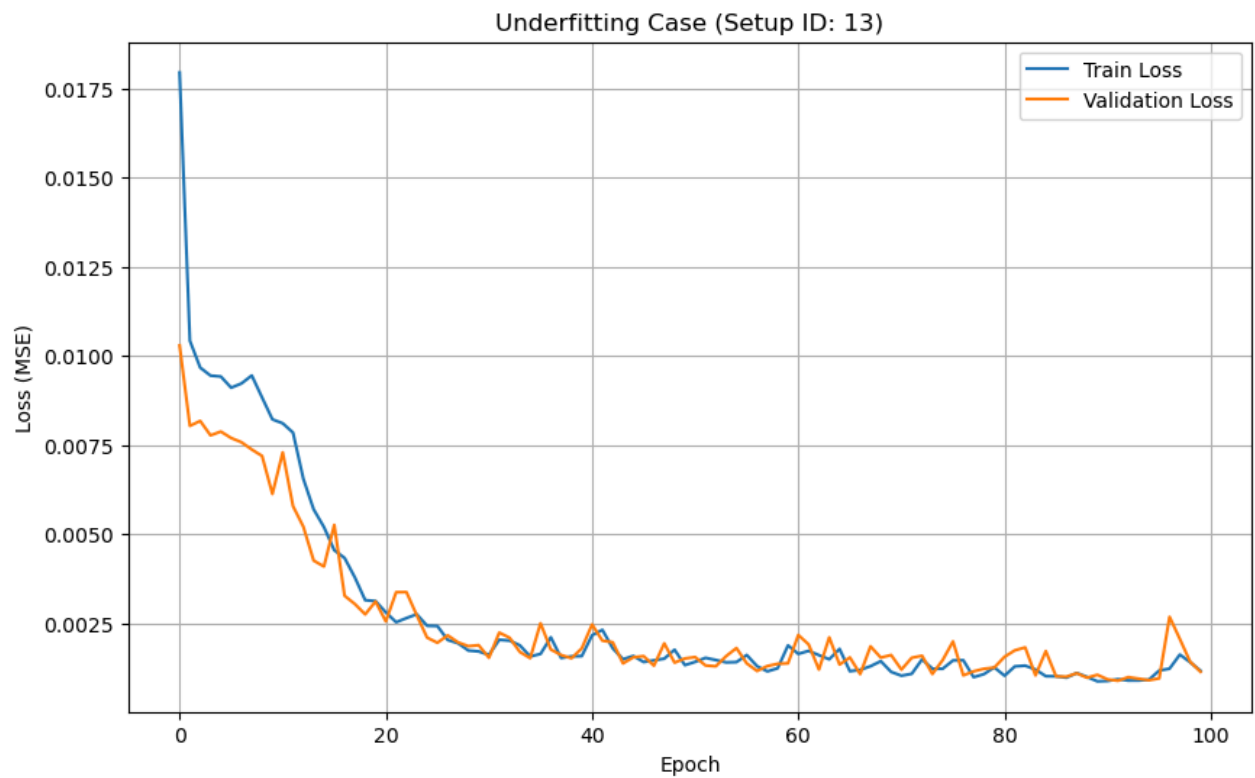
```
In [40]: poor_performers = results_df[results_df['r2_score'] < results_df['r2_score'].median()]

underfit_candidate = poor_performers.sort_values(by='loss_gap', ascending=True).iloc[0]

print("\n--- Underfitting Case Candidate (Refined Search) ---")
print(f"Setup ID: {underfit_candidate['setup_id']}")
print(f"Parameters: {underfit_candidate[['layers', 'neurons', 'activation', 'learning_rate']].to_dict()}")

underfit_history = underfit_candidate['history']
plt.figure(figsize=(10, 6))
plt.plot(underfit_history['loss'], label='Train Loss')
plt.plot(underfit_history['val_loss'], label='Validation Loss')
plt.title(f"Underfitting Case (Setup ID: {underfit_candidate['setup_id']})")
plt.xlabel('Epoch')
plt.ylabel('Loss (MSE)')
plt.legend()
plt.grid(True)
plt.show()

--- Underfitting Case Candidate (Refined Search) ---
Setup ID: 13
Parameters: {'layers': 5, 'neurons': 128, 'activation': 'tanh', 'learning_rate': 0.001}
```



After completing all the tasks, please, convert notebooks to PDF , zip them with your answers notebooks (ipynb file) and send it. You should provide sufficient explanation and reporting in your notebooks

Novin Nekuee (403134029)

Regards