

80 value variable AP Distribution 30 20 10 ΑT variable In []: # MeTHOD FOR REMOVING OUTLIERS # Method 1: Z-Score z_scores = (df - df.mean()) / df.std() threshold = 2 # Set the z-score threshold for outlier detection df_no_outliers = df[(z_scores < threshold).all(axis=1)]</pre> # Method 2: Percentiles or IQR q1 = df.quantile(0.25)q3 = df.quantile(0.75)iqr = q3 - q1 $lower_bound = q1 - 1.5 * iqr$ upper_bound = q3 + 1.5 * iqrdf_no_outliers = df[((df > lower_bound) & (df < upper_bound)).all(axis=1)]</pre> In [42]: # Let's use the Percentiles or IQR Method q1 = df1.quantile(0.25)q3 = df1.quantile(0.75)iqr = q3 - q1 $lower_bound = q1 - 1.5 * iqr$ upper_bound = q3 + 1.5 * iqr# save it in new dataframe df2 = df1[((df1 > lower_bound) & (df1 < upper_bound)).all(axis=1)]</pre> print(f'shape of df1: {df1.shape}') print(f'shape of df2: {df2.shape}') shape of df1: (47840, 5) shape of df2: (47340, 5) As we see that we loss abot 500 data point represented as outliers In [44]: plt.style.use('fivethirtyeight') plt.figure(figsize=(15, 10)) for i, col in enumerate(df2.columns): plt.subplot(2, 3, i+1)sns.boxplot(df2[col],color='y',width=0.2,dodge=True,linewidth=2.5).set_title(col) plt.tight_layout() sns.set(font_scale=1.1) sns.despine() plt.show() AT AP 10 20 1005 1015 1020 1025 ΑT AP RH PE 90 100 420 430 440 450 460 470 480 5. ML Models 5.1 Prepare data for ML models 5.1.1 Split data Splitting the data into training, validation, and test sets is an essential step in machine learning model development. The purpose of this split is to evaluate and fine-tune the model's performance on unseen data. Here's a common approach to splitting the data: • Training set: This is the largest portion of the data used for training the machine learning model. It is used to establish the patterns and relationships between the input features and the target variable. Typically, we use 60% of the data is allocated to the training set. • Validation set: The validation set is used to fine-tune the model's hyperparameters and evaluate its performance during the training process. It helps in selecting the best-performing model based on the validation metrics. Typically, we use 20% of the data is allocated to the validation set. Test set: The test set is used to assess the final performance of the trained model on unseen data. It provides an unbiased evaluation of the model's generalization ability. The test set should only be used once, after the model is completely trained and tuned. Typically, we use 20% of the data is allocated to the test set. In [45]: DF_PATH = "train.pkl" DF_PATH1 = "test.pkl" In [48]: train = pd.read_pickle(DF_PATH) test = pd.read_pickle(DF_PATH1) print(f' train set represent 80% of data: {train.shape}') print(f' test set represent 20% of data: {test.shape}') train set represent 80% of data: (37872, 5) test set represent 20% of data: (9468, 5) In [47]: train.head(10) Out[47]: ΑT AP RH PE **5444** 6.75 39.40 1011.28 90.84 483.77 **44734** 10.08 41.16 1023.14 96.03 469.17 **39601** 14.32 44.60 1013.85 68.13 466.36 **2928** 19.04 51.86 1018.05 79.01 458.64 **29411** 29.17 67.45 1014.10 46.85 435.08 **24090** 25.69 59.54 1004.05 81.69 439.06 **42640** 30.22 74.90 1003.57 67.15 434.17 **32239** 10.40 40.43 1025.46 75.09 492.09 **34189** 24.13 73.18 1012.62 91.52 436.22 **43860** 18.26 69.94 1004.10 97.39 443.59 In [49]: # remove target feature X = train.drop('PE',axis=1) y = train['PE'] Split 80% of data into train set 60% and validation set 20% In [50]: from sklearn.model_selection import train_test_split from sklearn.preprocessing import StandardScaler In [51]: # split train data into train set and validation set X_train, X_val, y_train, y_val = train_test_split(X, y, test_size=0.2, random_state=42) print(f'--> X_train: {X_train.shape}') print(f'--> X_val: {X_val.shape}') print(f'--> y_train: {y_train.shape}') print(f'--> y_val: {y_val.shape}') --> X_train: (30297, 4) --> X_val: (7575, 4) --> y_train: (30297,) --> y_val: (7575,) 5.1.2 Feature Scaling Feature scaling is a data preprocessing technique used in machine learning to bring all features of the dataset onto a similar scale. It aims to standardize or normalize the features, ensuring that no single feature dominates the learning algorithm due to its larger magnitude. Standardization (Z-score normalization): This method scales the features to have zero mean and unit variance. Each feature is transformed by subtracting the mean of the feature and dividing by its standard deviation. Standardization preserves the shape of the distribution and works well when the data does not have outliers. it is usually a good idea to perform feature scaling to help your model converge faster. This is especially true if your input features have widely different ranges of values. You will only use x for this first model but it's good to practice feature scaling now so you can apply it later. For that, you will use the StandardScaler class from scikit-learn. This computes the z-score of your inputs. the z-score is given by the equation: $z = \frac{x - \mu}{\sigma}$ where μ is the mean of the feature values and σ is the standard deviation. The importance of feature scaling in machine learning cannot be overstated, as it directly impacts the performance and convergence of many algorithms. Here are some key reasons why feature scaling is crucial: • Improves Convergence: Many machine learning algorithms rely on optimization techniques that aim to minimize a loss function during training. Feature scaling helps the optimization process converge faster, as features on similar scales allow the algorithm to reach the optimal solution more efficiently. • Equalizes Feature Influence: When features have different scales, those with larger magnitudes can dominate the learning process. By scaling the features, each one contributes more equally to the model's training, avoiding biased results. Avoids Numerical Instabilities: Some algorithms, such as gradient descent-based methods, may encounter numerical instabilities when dealing with large differences in feature scales. Feature scaling helps to stabilize the computations and avoids overflow/underflow issues. • Improves Model Performance: Scaling can lead to improved model performance, especially in algorithms sensitive to

ΑT

ΑT RH

RH

RH

100

RH Distribution

See the outliers in data Distribution

30

PE

460

1000 1005 1010 1015 1020 1025 1030 1035

10

feature scales, such as support vector machines, K-nearest neighbors, and neural networks. • Interpretability: Scaling can improve the interpretability of the model, as the model coefficients represent the relative importance of the features when they are on the same scale. • Regularization: In regularization techniques like L1 or L2 regularization, feature scaling ensures that the regularization term applies uniformly to all features, leading to fairer regularization penalties. • Consistent Preprocessing: Feature scaling provides a consistent preprocessing step, which can be essential when comparing different models or applying the same model to new data. print(f"Temperature Max, Min pre normalization for X_val: {X_val['AT'].max()}, {X_val['AT'].min()}") Temperature Max, Min pre normalization for X_train: 37.11, 1.81 Temperature Max, Min pre normalization for X_val: 37.11, 1.81 scaler = StandardScaler() X_train_scaled = scaler.fit_transform(X_train) X_val_scaled = scaler.transform(X_val) print(f" Temperature Max post normalization for X_train: {np.max(X_train_scaled[:,0])}") print(f" Temperature Min post normalization for X_train: {np.min(X_train_scaled[:,0])}") Temperature Max post normalization for X_train: 2.334411080307789 Temperature Min post normalization for X_train: -2.4163464525398117 Import libraries import numpy as np import pandas as pd import matplotlib.pyplot as plt import seaborn as sns from sklearn.linear_model import LinearRegression from sklearn.tree import DecisionTreeRegressor from sklearn.ensemble import RandomForestRegressor from lightgbm import LGBMRegressor from xgboost import XGBRegressor from sklearn import svm from sklearn.model_selection import train_test_split from sklearn.preprocessing import StandardScaler from sklearn.metrics import mean_absolute_error, mean_squared_error, make_scorer import tensorflow as tf from tensorflow.keras.models import Sequential from tensorflow.keras.layers import Dense from tensorflow.keras.activations import relu,linear from tensorflow.keras.losses import MeanSquaredError from tensorflow.keras.optimizers import Adam

In [81]: print(f"Temperature Max, Min pre normalization for X_train: {X_train['AT'].max()}, {X_train['AT'].min()}") In [52]: # scale In [88]: import numpy as np In [126... # import libraries import logging logging.getLogger("tensorflow").setLevel(logging.ERROR) tf.keras.backend.set_floatx('float64') tf.autograph.set_verbosity(0) We use framework optimization GridSearchCV to get best value of it's hyperparameter in seperate notebook you can check the full work in Github 5.2 Linear Regression In [91]: RMSE_DIC = {} In [92]: linear_model = LinearRegression() # fit on train data model_fit = linear_model.fit(X_train_scaled,y_train) # predict on train data prediction = model_fit.predict(X_val_scaled) In [93]: def RMSE(y,y_hat): return np.sqrt(mean_squared_error(y,y_hat)) In [94]: print(f"RMSE: {RMSE(y_val,prediction)}") print(f"MAE: {mean_absolute_error(y_val,prediction)}") RMSE: 4.562937139838695 MAE: 3.637839123894593 In [95]: RMSE_DIC["LinearRegression"] = 4.5629 5.3 DecisionTreeRegressor In [96]: # Create the Decision Tree Regressor decision_tree_model = DecisionTreeRegressor(min_samples_split = 2, $max_depth = 64$, random_state = 42).fit(X_train_scaled,y_train) In [97]: print(f"RMSE Of DecisionTreeRegressor: {RMSE(y_val, decision_tree_model.predict(X_val_scaled)):.4f}") print(f"MAE: {mean_absolute_error(y_val, decision_tree_model.predict(X_val_scaled)):.4f}") RMSE Of DecisionTreeRegressor: 0.4593 MAE: 0.0452 In [98]: RMSE_DIC["DecisionTreeRegressor"] = 0.4593 5.4 RandomForestRegressor # Create the RandomForestRegressor RandomForest_model = RandomForestRegressor(min_samples_split = 2, $max_depth = 64$, random_state = 42).fit(X_train_scaled,y_train) In [100... print(f"RMSE Of RandomForestRegressor: {RMSE(y_val, RandomForest_model.predict(X_val_scaled)):.4f}") print(f"MAE of RandomForestRegressor: {mean_absolute_error(y_val, RandomForest_model.predict(X_val_scaled)):.4f}") RMSE Of RandomForestRegressor: 0.6732 MAE of RandomForestRegressor: 0.2985 In [101... RMSE_DIC["RandomForestRegressor"] = 0.6732 5.5 LGBMRegressor In [104... | lgb_clf = LGBMRegressor(class_weight = 'balanced', learning_rate = 0.9, $max_depth = 20$, $n_{estimators} = 700$, random_state = 42, lgb_clf.fit(X_train_scaled, y_train, eval_set = [(X_train_scaled, y_train),(X_val_scaled, y_val)], early_stopping_rounds = 300, verbose=0, eval_metric='rmse' Out[104]: LGBMRegressor(class_weight='balanced', learning_rate=0.9, max_depth=20, n_estimators=700, random_state=42) In [105... RMSE_DIC["LGBMRegressor"] = 0.5692 5.6 XGBRegressor In [107... xgb_rg = XGBRegressor(learning_rate = 0.1, $max_depth = 70$, $n_{estimators} = 500$,

 $random_state = 42,$ xgb_rg.fit(X_train_scaled, y_train, eval_set = [(X_val_scaled, y_val)], early_stopping_rounds = 300, verbose=0, eval_metric=['rmse','mae'] Out[107]: XGBRegressor(base_score=None, booster=None, callbacks=None, colsample_bylevel=None, colsample_bynode=None, colsample_bytree=None, early_stopping_rounds=None, enable_categorical=False, eval_metric=None, feature_types=None, gamma=None, gpu_id=None, grow_policy=None, importance_type=None, interaction_constraints=None, learning_rate=0.1, max_bin=None, max_cat_threshold=None, max_cat_to_onehot=None, max_delta_step=None, max_depth=70, max_leaves=None, min_child_weight=None, missing=nan, monotone_constraints=None, n_estimators=500, n_jobs=None, num_parallel_tree=None, predictor=None, random_state=42, ...) In [109... RMSE_DIC["XGBRegressor"] = 0.3080 **5.7 SVM** In [110... regr = svm.SVR() # fit regr.fit(X_train_scaled, y_train) # predict y_hat = regr.predict(X_val_scaled) print(f"RMSE: {RMSE(y_val, y_hat)}") print(f"MAE: {mean_absolute_error(y_val, y_hat)}") RMSE: 4.101138865225424 MAE: 3.0602853705365365 In [111... | RMSE_DIC['SVM'] = 4.1011 5.8 Ensembles Voting In [112... from sklearn.ensemble import VotingRegressor voting_rg = VotingRegressor(estimators = [('Dt',decision_tree_model), ('rf',RandomForest_model), ('lgb',lgb_clf), ('xgb',xgb_rg),]) voting_rg.fit(X_train_scaled, y_train) Out[112]: VotingRegressor(estimators=[('Dt', DecisionTreeRegressor(max_depth=64, random_state=42)), ('rf', RandomForestRegressor(max_depth=64, random_state=42)), ('lgb', LGBMRegressor(class_weight='balanced', learning_rate=0.9, max_depth=20, n_estimators=700, random_state=42)), ('xgb', XGBRegressor(base_score=None, booster=None, callbacks=None, colsample_bylevel=None, colsam... gamma=None, gpu_id=None, grow_policy=None, importance_type=None, interaction_constraints=None, learning_rate=0.1, max_bin=None, max_cat_threshold=None, max_cat_to_onehot=None, max_delta_step=None, max_depth=70, max_leaves=None, min_child_weight=None, missing=nan, monotone_constraints=None, n estimators=500, n_jobs=None, num_parallel_tree=None, predictor=None, random_state=42, ...))]) In [113... print(f"RMSE Of stacking: {RMSE(y_val, voting_rg.predict(X_val_scaled)):.4f}") print(f"MAE of stacking: {mean_absolute_error(y_val, voting_rg.predict(X_val_scaled)):.4f}") RMSE Of stacking: 0.3823 MAE of stacking: 0.1372 In [114... RMSE_DIC['Stacking'] = 0.3823 In [115... RMSE_DIC Out[115]: {'LinearRegression': 4.5629, 'DecisionTreeRegressor': 0.4593, 'RandomForestRegressor': 0.6732, 'LGBMRegressor': 0.5692, 'XGBRegressor': 0.308, 'SVM': 4.1011, 'Stacking': 0.3823} In such cases, the ensemble might not bring significant improvements as we see that XGBRegressor has better score. • It's important to note that the performance of ensemble models can vary depending on the specific dataset and problem. In [125... import plotly.express as px # Example data $x = list(RMSE_DIC.keys())$ y = list(RMSE_DIC.values()) # Create the bar plot fig = px.bar(x=x, y=y, title='RMSE FOR MODELS', color = x, labels={'x': 'Models Name', 'y': 'RMSE'}, width=1000, height=400) # Display the plot fig.show()

5.9 artificial neural network

regression, and pattern recognition.

hidden

layer

"multilayer perceptron"

Temperatur

Pressure

Humidity

Vacuum

5.9.1 Cost function for regularized linear regression

The difference is the regularization term, $\frac{\lambda}{2m}\sum_{j=0}^{n-1}w_j^2$

parameter b is not regularized. This is standard practice.

Where each iteration performs simultaneous updates on w_j for all j.

What changes with regularization is computing the gradients.

• m is the number of training examples in the data set

• $f_{\mathbf{w},b}(x^{(i)})$ is the model's prediction, while $y^{(i)}$ is the target

The gradient calculation for linear regression

• For a linear regression model

The term which adds regularization is $\frac{\lambda}{m}w_j$.

 $f_{\mathbf{w},b}(x) = \mathbf{w} \cdot \mathbf{x} + b$

problems.

5.9.2 Gradient descent with regularization

where:

the form:

The equation for the cost function regularized linear regression is:

Input layer

layer

outputs.

It is a computational model inspired by the structure and functioning of biological neural networks, such as the human brain. An ANN consists of interconnected artificial neurons, or nodes, organized in layers. Each node receives input

The basic building block of an ANN is the artificial neuron, also known as a perceptron. It takes multiple inputs, applies weights to each input, sums them up, and passes the sum through an activation function to produce an output. The activation function introduces non-linearities and allows the network to learn complex relationships between inputs and

ANNs are capable of learning from data through a process called training. During training, the network adjusts the weights of its connections based on a specified learning algorithm and a set of training examples. This process enables the network to approximate or learn patterns, make predictions, and perform various tasks, including classification,

Multiple hidden layers

neural network architecture

Hidden layer

FIGURE 4: Structure of artificial neural network (ANN) [34].

 $J(\mathbf{w},b) = rac{1}{2m} \sum_{i=0}^{m-1} (f_{\mathbf{w},b}(\mathbf{x}^{(i)}) - y^{(i)})^2 + rac{\lambda}{2m} \sum_{i=0}^{n-1} w_j^2$

 $f_{\mathbf{w},b}(\mathbf{x}^{(i)}) = \mathbf{w} \cdot \mathbf{x}^{(i)} + b$

 $J(\mathbf{w},b) = rac{1}{2m} \sum_{i=0}^{m-1} (f_{\mathbf{w},b}(\mathbf{x}^{(i)}) - y^{(i)})^2$

 $w_j = w_j - lpha rac{\partial J(\mathbf{w}, b)}{\partial w_j}$ for $\mathbf{j} := 0...$ n-1

 $rac{\partial J(\mathbf{w},b)}{\partial w_i} = rac{1}{m} \sum_{i=0}^{m-1} (f_{\mathbf{w},b}(\mathbf{x}^{(i)}) - y^{(i)}) x_j^{(i)} + rac{\lambda}{m} w_j$

 $rac{\partial J(\mathbf{w},b)}{\partial b} = rac{1}{m} \sum_{i=0}^{m-1} (f_{\mathbf{w},b}(\mathbf{x}^{(i)}) - y^{(i)})$

The same model selection process can also be used when choosing between different neural network architectures.

we 'll loop over some different architectures below and evaluate RMSE on each one to get best architecture for our

12 units

16 units

12 units

5.9.3 model selection process from different neural network architectures

Including this term encourages gradient descent to minimize the size of the parameters. Note, in this example, the

The basic algorithm for running gradient descent does not change with regularization, it is:

repeat until convergence: {

 $b = b - lpha rac{\partial J(\mathbf{w}, b)}{\partial b}$

Compare this to the cost function without regularization (which we implemented in a previous work above), which is of

hidden

layer

Power

prediction

(1)

(2)

(1)

(2)

(3)

Output layer

hidden

layer

signals, performs a computation, and produces an output signal that may serve as input for other nodes.

<pre>kernel_regularizer = tf.keras.regularizers.12(0.1), name = 'L4', input_shape=(4,)), Dense(units = 64, activation='relu', kernel_regularizer = tf.keras.regularizers.12(0.1), name = 'L44'), Dense(units = 1, name = 'L444')], [Dense(units = 125, activation='relu', kernel_regularizer = tf.keras.regularizers.12(0.1), name = 'L5', input_shape=(4,)),</pre>	
<pre>Dense(units = 64, activation='relu',</pre>	
<pre>Dense(units = 125, activation='relu',</pre>	
<pre>kernel_regularizer = tf.keras.regularizers.12(0.1), name = 'L7', input_shape=(4,)), Dense(units = 164, activation='relu', kernel_regularizer = tf.keras.regularizers.12(0.1), name = 'L77'), Dense(units = 125, activation='relu', kernel_regularizer = tf.keras.regularizers.12(0.1), name = 'L777'), Dense(units = 64, activation='relu',</pre>	
<pre>kernel_regularizer = tf.keras.regularizers.l2(0.1), name = 'L7777'), Dense(units = 1, name = 'L77777')], [Dense(units = 300, activation='relu', kernel_regularizer = tf.keras.regularizers.l2(0.1), name = 'L8', input_shape=(4,)), Dense(units = 200, activation='relu',</pre>	
<pre>kernel_regularizer = tf.keras.regularizers.l2(0.1), name = 'L88'), Dense(units = 164, activation='relu', kernel_regularizer = tf.keras.regularizers.l2(0.1), name = 'L888'), Dense(units = 125, activation='relu', kernel_regularizer = tf.keras.regularizers.l2(0.1), name = 'L8888'), Dense(units = 64, activation='relu', kernel_regularizer = tf.keras.regularizers.l2(0.1), name = 'L88888'), Dense(units = 1, name = 'L888888')],</pre>	
<pre># Add more Layer configurations as desired] best_model = None best_loss = float('inf') # Loop over each Layer architecture and train/evaluate the model for architecture in layer_architectures: model = tf.keras.Sequential(architecture) # Compile the model model.compile(optimizer= Adam(learning_rate=0.01), loss= MeanSquaredError()) # Fit the model</pre>	
<pre>model.fit(X_train_scaled, y_train, epochs=50, verbose=0) # Predict y_pred = model.predict(X_val_scaled) loss = RMSE(y_val, y_pred) print(f"Architecture: {architecture}") print(f"Loss: {loss:.4f}") # Track the best model based on the lowest loss if loss < best_loss: best_loss = loss best_model = model</pre>	
<pre>print(f'< best_loss: {best_loss}') print(f'< best_model: {best_model}') 237/237 [====================================</pre>	
bject at 0x0000017ECB228FA0>] Loss: 4.1791 237/237 [====================================	se o
Loss: 4.3159 237/237 [====================================	
237/237 [====================================	
Architecture: [<keras.layers.core.dense.dense 0x0000017e845224c0="" at="" object="">, <keras.layers.core.dense.dense 0x0000017e84522940="" at="" object="">, <keras.layers.core.dense.dense 0x0000017e845229a0="" at="" object="">] Loss: 4.4496 237/237 [====================================</keras.layers.core.dense.dense></keras.layers.core.dense.dense></keras.layers.core.dense.dense>	cor se o cor
237/237 [====================================	cor
As we see that more simple our architecture without regularization more the score we get, however, we more complex model we should use regularization parameter. Neural network is better with using more complex data so here we see that it's not that good for our data here as we get onlt 4.17 score compared to XGBRegressor it's not that good, so using Neural network here is not sufficient In [132 RMSE_DIC["ANN"] = 4.1791	
Result In [136 RMSE_DIC Out[136]: {'LinearRegression': 4.5629,	
'RandomForestRegressor': 0.6732, 'LGBMRegressor': 0.5692, 'XGBRegressor': 0.308, 'SVM': 4.1011, 'Stacking': 0.3823, 'ANN': 4.1791} In [135 import plotly.express as px # Example data	
<pre>x = list(RMSE_DIC.keys()) y = list(RMSE_DIC.values()) # Create the bar plot fig = px.bar(x=x, y=y, title='RMSE FOR MODELS',</pre>	
<pre>fig.show()</pre>	
RMSE FOR MODELS color LinearRegression DecisionTreeRegressor	
RandomForestRegressor LGBMRegressor XGBRegressor SVM Stacking ANN	
LinearRegression LinearRegression LGBMRegressor LGBMRegressor ANN Stacking ANN	
6.Deployment In []:	

In [131... # set seed for reproducibility
tf.random.set_seed(1234)

layer_architectures = [

Define a list of layer architectures to try

Dense(units = 1, name = 'L11')],

Dense(units = 1, name = 'L22222')],

Dense(units = 1, name = 'L9999')],

[Dense(units = 65, activation='relu',

name = 'L2', input_shape=(4,)),
Dense(units = 1, name = 'L22')],

[Dense(units = 65, activation='relu',

Dense(units = 25, activation='relu',

Dense(units = 1, name = 'L999')],

[Dense(units = 125, activation='relu',

Dense(units = 65, activation='relu',

Dense(units = 1, name = 'L333')],

[Dense(units = 65, activation='relu',

name = L33'),

name = 'L3', input_shape=(4,)),

name = 'L9', input_shape=(4,)),

[Dense(units = 40, activation='relu', name = 'L1', input_shape=(4,)),

kernel_regularizer = tf.keras.regularizers.l2(0.1),

kernel_regularizer = tf.keras.regularizers.l2(0.1),

kernel_regularizer = tf.keras.regularizers.l2(0.1),

kernel_regularizer = tf.keras.regularizers.l2(0.1),

kernel_regularizer = tf.keras.regularizers.12(0.1), name = 'L99'),

[Dense(units = 65, activation='relu', name = 'L2222', input_shape=(4,)),

[Dense(units = 65, activation='relu', name = 'L999999', input_shape=(4,)),
Dense(units = 25, activation='relu', name = 'L999999'),