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# APPENDICES

## Appendix – A

### (Python program for artificial neural network to validate the model)

```
# Quintessential libraries for pre-processing and preparing the data
import numpy as np
import pandas as pd

# Visualization libraries for plotting data
import matplotlib.pyplot as plt
import seaborn as sns                #advanced plotting that works on matplotlib
from mpl_toolkits import mplot3d     #3d plotting

# Learning algorithms libraries
from sklearn.linear_model import LinearRegression, Ridge, Lasso
from sklearn.tree import DecisionTreeRegressor
from sklearn.ensemble import RandomForestRegressor, GradientBoostingRegressor
import tensorflow.keras as tf
from scikeras.wrappers import KerasRegressor
import xgboost as xgbo

# Miscellanious libraries
from sklearn.model_selection import train_test_split, cross_val_score, KFold, GridSearchCV     # For
 splitting training and test data
from sklearn.metrics import mean_squared_error, r2_score                    # For optimization metrics
from google.colab import files                                  # For downloading  processed data & g
raphs


def importTestData(url):
  ''' This function loads data from a CSV file
      into a Pandas Dataframe'''
  df = pd.read_csv(url)
  print(df.head())        # Visualizing the 1st N rows of the DataFrame (N= 5 default, can be changed)
```

```
  print(df.shape)          # Prints the dimensions of the DataFrame (rows* columns)
  print(df.columns)        # Prints the names of columns of the DataFrame
  print(df.describe())     # Prints statistical data of each column of the DataFrame
  print(df.isnull().sum())  # Prints how many rows have Null/ Empty String/ NaN values for each colu
mn of the DataFrame
  return df


def creating_training_and_test_datasets(df, target_var, target_var_scaled, list_of_all_y_vars):

  # Creating dataframe for independent variables (variables whose values will be used for predicting d
ependent variable)
  X = df.drop(list_of_all_y_vars, axis = 1)
  print(X.head())

  # Creating dependent variable matrix (variable which is to be predicted)
  baseY = df[target_var]                    # base matrix or rather tuple created
  baseY = baseY.to_numpy()
  print(baseY.shape)                        # to_numpy creates array with no 2nd dimension
  scaledY = df[target_var_scaled].to_numpy()      # scaled matrix
  return X, baseY, scaledY

def creating_training_and_test_datasets(df, target_var, target_var_scaled, list_of_all_y_vars):


  # Creating dataframe for independent variables (variables whose values will be used for predicting dependent
variable)
  X = df.drop(list_of_all_y_vars, axis = 1)
  print(X.head())


  # Creating dependent variable matrix (variable which is to be predicted)
  baseY = df[target_var]                    # base matrix or rather tuple created
  baseY = baseY.to_numpy()
  print(baseY.shape)                        # to_numpy creates array with no 2nd dimension
  scaledY = df[target_var_scaled].to_numpy()      # scaled matrix
  return X, baseY, scaledY


X_train_std  = X_train.copy()
X_test_std  = X_test.copy()
for col in X_train:
  X_train_std[col] = (X_train[col] - np.mean(X_train[col]))/(np.std(X_train[col]))
  X_test_std[col] = (X_test[col] - np.mean(X_train[col]))/(np.std(X_train[col]))
```

```
y_train_std  = y_train.copy()
y_test_std  = y_test.copy()
y_train_std = (y_train - np.mean(y_train))/(np.std(y_train))
y_test_std = (y_test - np.mean(y_train))/(np.std(y_train))

def annModel(units = 20, learning_rate = 0.001):
  ann = tf.models.Sequential()
  ann.add(tf.layers.Dense(units = units, input_dim = 3, kernel_initializer='normal', activation = 'softmax'))
  ann.add(tf.layers.Dense(units=1))
  optimizer = tf.optimizers.Adam(learning_rate= learning_rate)
  ann.compile(optimizer=optimizer,loss="mean_squared_error", metrics=['mean_squared_error'])
  return ann

ef modelHyperparamaterTuning(name, model, trainX, trainY, pGrid =None ):

  # Provision for hyperparameter tuning
  if name == 'ANN':
    callback = tf.callbacks.EarlyStopping(monitor='loss', min_delta = 0.0000001, patience=100)
    model = KerasRegressor(model = model, units = 20, learning_rate = 0.001, epochs = 1500, batch_size = 40,
verbose = 0, callbacks = [callback])
  grid_search = GridSearchCV(estimator = model, param_grid = pGrid, cv=5,
                       scoring=['neg_root_mean_squared_error','r2'], refit='r2',
                       return_train_score=True)
  grid_result = grid_search.fit(trainX, trainY)
  print(grid_search.best_params_, grid_search.best_score_)

  means = zip(grid_result.cv_results_['mean_test_r2'],grid_result.cv_results_['mean_test_neg_root_mean_squar
ed_error'])
  stds = zip(grid_result.cv_results_['std_test_r2'], grid_result.cv_results_['std_test_neg_root_mean_squared_erro
r'])
  params = grid_result.cv_results_['params']
  for mean, stdev, param in zip(means, stds, params):
    print(mean[0], stdev[0], mean[1], stdev[1], param)

ef postHyperParameterTuningModelLearning(name, model, trainX, testX,trainY, testY,pGrid =None, standardi
zed =False, **kwargs ):
```

```
  if name =='ANN':
    callback = tf.callbacks.EarlyStopping(monitor='loss', min_delta = 0.0000001, patience=100)
    model = KerasRegressor(model = model, units = 15, learning_rate = 0.075, epochs = 2000, batch_size = 40,
verbose = 0, callbacks = [callback])
    # model = KerasRegressor(model = model, units = 15, learning_rate = 0.075, epochs = 2000, batch_size = 40
, verbose = 0, callbacks = [callback])

  # Cross validation
  results = cross_val_score(estimator= model, X= trainX, y = trainY, cv = KFold(n_splits=4))
  print(name, results.mean(), results.std())

  # Model training
  model.fit(trainX, trainY,**kwargs)
  # Model predicted values based on learning
  y_pred_train = model.predict(trainX)
  y_pred_test = model.predict(testX)

  # Performance review
  mse_train = mean_squared_error(trainY, y_pred_train)
  mse_test = mean_squared_error(testY, y_pred_test)
  r2_train = r2_score(trainY, y_pred_train)
  r2_test = r2_score(testY, y_pred_test)

  if max(testY) > 1 and name != 'ANN':
    mse_train = mse_train/(10**12)
    mse_test = mse_test/(10**12)

  if standardized:
    y_pred_train = (y_pred_train*np.std(y_train) + np.mean(y_train)).ravel()
    y_pred_test = (y_pred_test*np.std(y_train) + np.mean(y_train)).ravel()

print(name, mse_test, mse_train, r2_train, r2_test)
    # w = model.get_weights()
    # ann_viz(ann, title="ANN", view = True, filename="network")

  # Preparing Results file
```

```
  # models_arr.append(name)
  # mse_train_arr.append(mse_train)
  # mse_test_arr.append(mse_test)
  # r2_train_arr.append(r2_train)
  # r2_test_arr.append(r2_test)
  # train_arr.append(y_pred_train)
  # test_arr.append(y_pred_test)
  # r2_test_mean_arr.append(results.mean())
  # r2_test_std_arr.append(results.std())

r = np.arange(len(models_arr))
width = 0.4

plt.bar(r, mse_train_arr, color = 'b', width = width, edgecolor = 'black', label='MSE train')
plt.bar(r + width, mse_test_arr, color = 'g', width = width, edgecolor = 'black', label='MSE test')

plt.xlabel("Models")
plt.ylabel("MSE values")

# plt.grid(linestyle='--')
plt.xticks(r + width/2, models_arr)
plt.legend()
z=plt.gca().xaxis
for item in z.get_ticklabels():
    item.set_rotation(50)

plt.show()

r = np.arange(len(models_arr))
width = 0.4

# Add lower limit of 0.6 with 0.05 ticks
plt.bar(r, r2_train_arr, color = 'b', width = width, edgecolor = 'black', label='R2 train')
plt.bar(r + width, r2_test_arr, color = 'g', width = width, edgecolor = 'black', label='R2 test')

plt.xlabel("Models")
plt.ylabel("R2 values")
```

```
# plt.grid(linestyle='--')
# plt.rcParams["figure.figsize"] = (6,6)
plt.xticks(r + width/2, models_arr)
plt.ylim([0.6,1])
plt.legend(bbox_to_anchor=(0.15, -0.2))
z=plt.gca().xaxis
for item in z.get_ticklabels():
    item.set_rotation(50)

plt.savefig(f"Model_r2.png", bbox_inches='tight')
files.download(f"Model_r2.png")
plt.show()

name_arr = models_arr.copy()
name_arr.insert(0,'Composition')
name_arr.insert(1,'Load (N)')
name_arr.insert(2,'Sliding distance(m)')
name_arr.insert(3,'Observed wear')
name_arr.insert(4,'Observed wear(*10^-6)')
train_df = pd.DataFrame(np.transpose(train_arr), columns = name_arr)
test_df = pd.DataFrame(np.transpose(test_arr), columns = name_arr)
pred_data = pd.concat([train_df, test_df])

print(pred_data.shape)
```

## APPENDIX – B

## (List of Publications)

### International SCI/SCIE Journal Publications

1. **V Kumar,** A Mishra, A Mohan, S Mohan. *Fabrication of stircast ZA/$ZrB_2$ reinforced in-situ composites*. Mater. Res. Express 6(2019) 126555. DOI:10.1088/2053-1591/ab53f2.
2. **V Kumar**, G Gautam, A Mohan, S Mohan. *Tribology of insitu Zn-Al/$ZrB_2$ Composites in Reciprocating Motion*. International Journal of Metal casting (2022). DOI:10.1007/s40962-022-00764-2.
3. **V Kumar**, AK Yadav, G Gautam, A Mohan, S Mohan. *Influence of insitu formed $ZrB_2$ reinforcement on dry sliding tribological behavior of ZA based metal matrix composites*. International Journal of Metal casting (2022). DOI: 10.1007/s40962-022-00806-9.
4. **V Kumar**, G Gautam, A Singh, V Singh, S Mohan[1], A Mohan. *Tribological Behaviour Of ZA/$ZrB_2$ Insitu Composites Using Response Surface Methodology And Artificial Neural Network.* Surface topography Metrology and properties (2022). DOI: 10.1088/2051-672X/ac9426.
5. **V Kumar**, Ankit, G Gautam, A Mohan, S Mohan. *Correlating Surface Topography of Relaxed Layer to Wear and Friction***.** Tribology transactions (2022)(Under review).