dat300_comp1_final

September 24, 2020

[1]:
```
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```

[14]:
```
# import modules
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import os
import seaborn as sb
import tensorflow
import tensorflow_addons as tfa
from sklearn.metrics import mean_absolute_error, r2_score
from sklearn.tree import DecisionTreeRegressor
from sklearn.feature_selection import SelectFromModel
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.model_selection import (
    cross_val_score,
    GridSearchCV,
    train_test_split,
)
from sklearn.preprocessing import StandardScaler, MinMaxScaler
from itertools import compress
from sklearn.pipeline import make_pipeline
from sklearn.linear_model import ElasticNet
from scipy import stats
from tensorflow.keras.models import Sequential
from tensorflow.keras.layers import Dense, Flatten, Dropout, BatchNormalization
from tensorflow.keras.optimizers import Adam
from tensorflow.keras.losses import Huber
```

[3]:
```
# coefficient of determination (R^2) for regression
def r_square(y_true, y_pred):
    from tensorflow.keras import backend as K

    SS_res = K.sum(K.square(y_true - y_pred))
    SS_tot = K.sum(K.square(y_true - K.mean(y_true)))
    return 1 - SS_res / (SS_tot + K.epsilon())
```

```
def r_square_loss(y_true, y_pred):
    from tensorflow.keras import backend as K

    SS_res = K.sum(K.square(y_true - y_pred))
    SS_tot = K.sum(K.square(y_true - K.mean(y_true)))
    return 1 - (1 - SS_res / (SS_tot + K.epsilon()))
```

[4]:
```
# load data
x_train = pd.read_csv("./dat300-h2020-ca1/X_train.csv")
x_test = pd.read_csv("./dat300-h2020-ca1/X_test.csv")
y_train = pd.read_csv("./dat300-h2020-ca1/y_train.csv")
```

[5]:
```
# x_train inspection
x_train.describe()
```

[5]:

	Cement (component 1)(kg in a m^3 mixture)	Blast Furnace Slag (component 2)(kg in a m^3 mixture)	Fly Ash (component 3)(kg in a m^3 mixture)
count	618.000000	618.00000	618.000000
mean	279.573220	73.95966	54.507945
std	106.241869	85.24380	63.763533
min	102.000000	0.00000	0.000000
25%	190.085000	0.00000	0.000000
50%	272.700000	22.00000	0.000000
75%	350.000000	143.00000	117.540000
max	540.000000	316.10000	200.100000

```
       Water  (component 4)(kg in a m^3 mixture)  \
count                                  618.000000
mean                                   181.851537
std                                     20.947062
min                                    121.750000
25%                                    165.865000
50%                                    185.000000
75%                                    192.000000
max                                    246.900000

       Superplasticizer (component 5)(kg in a m^3 mixture)  \
count                                          618.000000
mean                                             6.047505
std                                              5.910278
min                                              0.000000
25%                                              0.000000
50%                                              6.275000
75%                                             10.000000
max                                             32.200000

       Coarse Aggregate  (component 6)(kg in a m^3 mixture)  \
count                                          618.000000
mean                                           974.788350
std                                             75.538967
min                                            801.000000
25%                                            932.000000
50%                                            968.000000
75%                                           1028.400000
max                                           1134.300000

       Fine Aggregate (component 7)(kg in a m^3 mixture)   Age (day)
count                                          618.000000  618.000000
mean                                           770.756197   45.991909
std                                             80.024256   64.971643
min                                            594.000000    1.000000
25%                                            721.375000    7.000000
50%                                            778.450000   28.000000
75%                                            822.000000   56.000000
max                                            992.600000  365.000000
```

[6]:
```
# x_test inspection
x_test.describe()
```

[6]:
```
       Cement (component 1)(kg in a m^3 mixture)  \
count                                  412.000000
mean                                   283.554248
std                                    101.931109
```

```
min                                    102.000000
25%                                    202.000000
50%                                    275.035000
75%                                    355.225000
max                                    540.000000

       Blast Furnace Slag (component 2)(kg in a m^3 mixture)  \
count                                          412.000000
mean                                            73.799223
std                                             87.913388
min                                              0.000000
25%                                              0.000000
50%                                             22.000000
75%                                            142.575000
max                                            359.400000

       Fly Ash (component 3)(kg in a m^3 mixture)  \
count                                    412.000000
mean                                      53.705922
std                                       64.418958
min                                        0.000000
25%                                        0.000000
50%                                        0.000000
75%                                      118.310000
max                                      194.900000

       Water  (component 4)(kg in a m^3 mixture)  \
count                                  412.000000
mean                                   181.138592
std                                     21.972857
min                                    121.750000
25%                                    164.022500
50%                                    185.700000
75%                                    193.000000
max                                    247.000000

       Superplasticizer (component 5)(kg in a m^3 mixture)  \
count                                          412.000000
mean                                             6.436522
std                                              6.066806
min                                              0.000000
25%                                              0.000000
50%                                              6.435000
75%                                             10.910000
max                                             32.200000

       Coarse Aggregate  (component 6)(kg in a m^3 mixture)  \
```

```
count                                                412.000000
mean                                                 970.113956
std                                                   80.974799
min                                                  801.000000
25%                                                  932.000000
50%                                                  966.500000
75%                                                 1034.750000
max                                                 1145.000000

       Fine Aggregate (component 7)(kg in a m^3 mixture)   Age (day)
count                                          412.000000  412.000000
mean                                           777.812913   45.167476
std                                             80.312789   60.441229
min                                            594.000000    3.000000
25%                                            746.025000   14.000000
50%                                            780.100000   28.000000
75%                                            830.750000   56.000000
max                                            992.600000  365.000000
```

[7]:
```
# y_train inspection
y_train.describe()
```

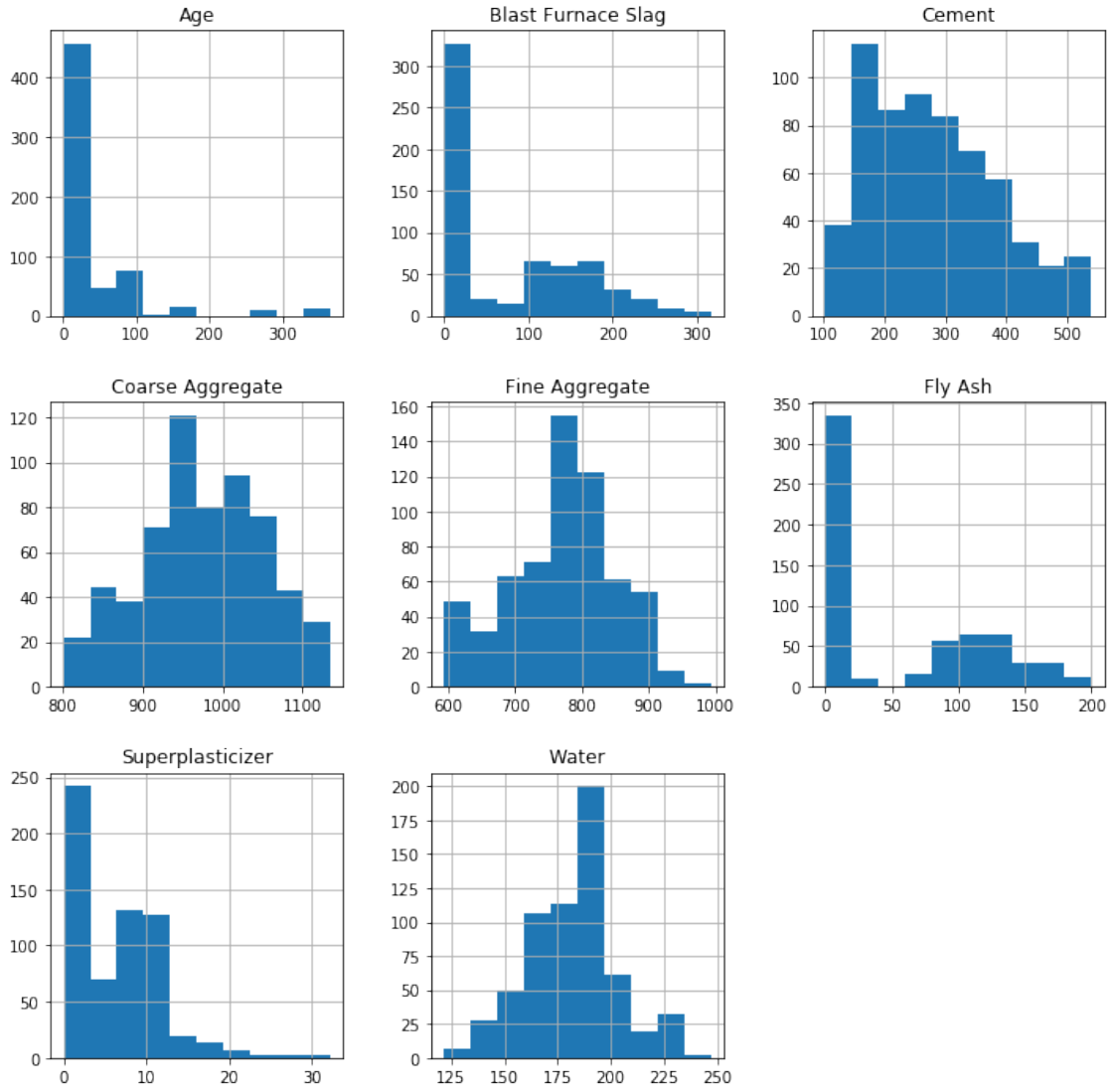
[7]:
```
       Concrete compressive strength(MPa, megapascals)
count                                       618.000000
mean                                         35.379932
std                                          16.276264
min                                           4.782206
25%                                          23.849492
50%                                          34.266957
75%                                          44.520204
max                                          81.751169
```

[8]:
```
# check for NaN
print(f"Number of NaN in x_train: {sum(x_train.isnull().sum())}")
print(f"Number of NaN in y_train: {sum(y_train.isnull().sum())}")
print(f"Number of NaN in x_test: {sum(x_test.isnull().sum())}")
```

```
Number of NaN in x_train: 0
Number of NaN in y_train: 0
Number of NaN in x_test: 0
```

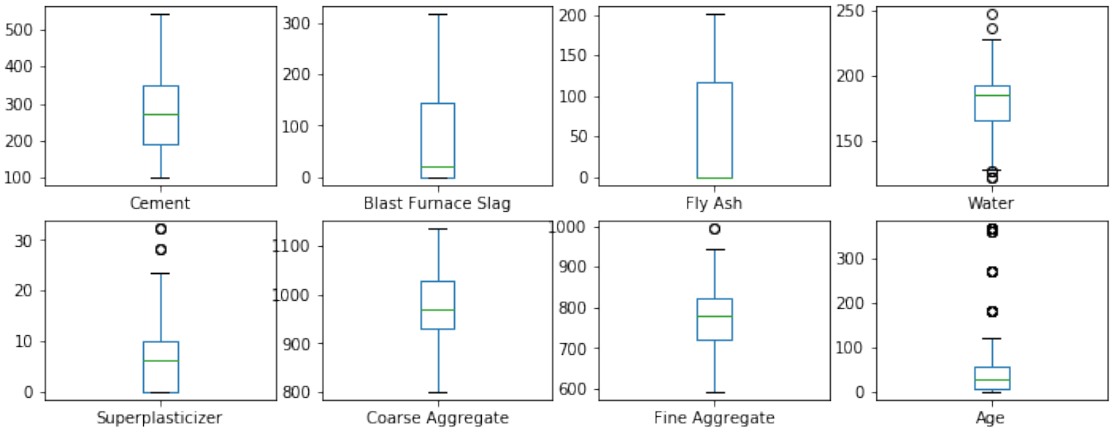
[9]:
```
# x_train histogram
# we remove units to prevent titles from merging
# to see units, look at earlier cells
columns = [
    "Cement",
    "Blast Furnace Slag",
```

```
    "Fly Ash",
    "Water",
    "Superplasticizer",
    "Coarse Aggregate",
    "Fine Aggregate",
    "Age",
]
x_train_no_unit = pd.DataFrame(x_train.values, columns=columns)
x_train_hist = x_train_no_unit.hist(figsize=(12, 12))
```



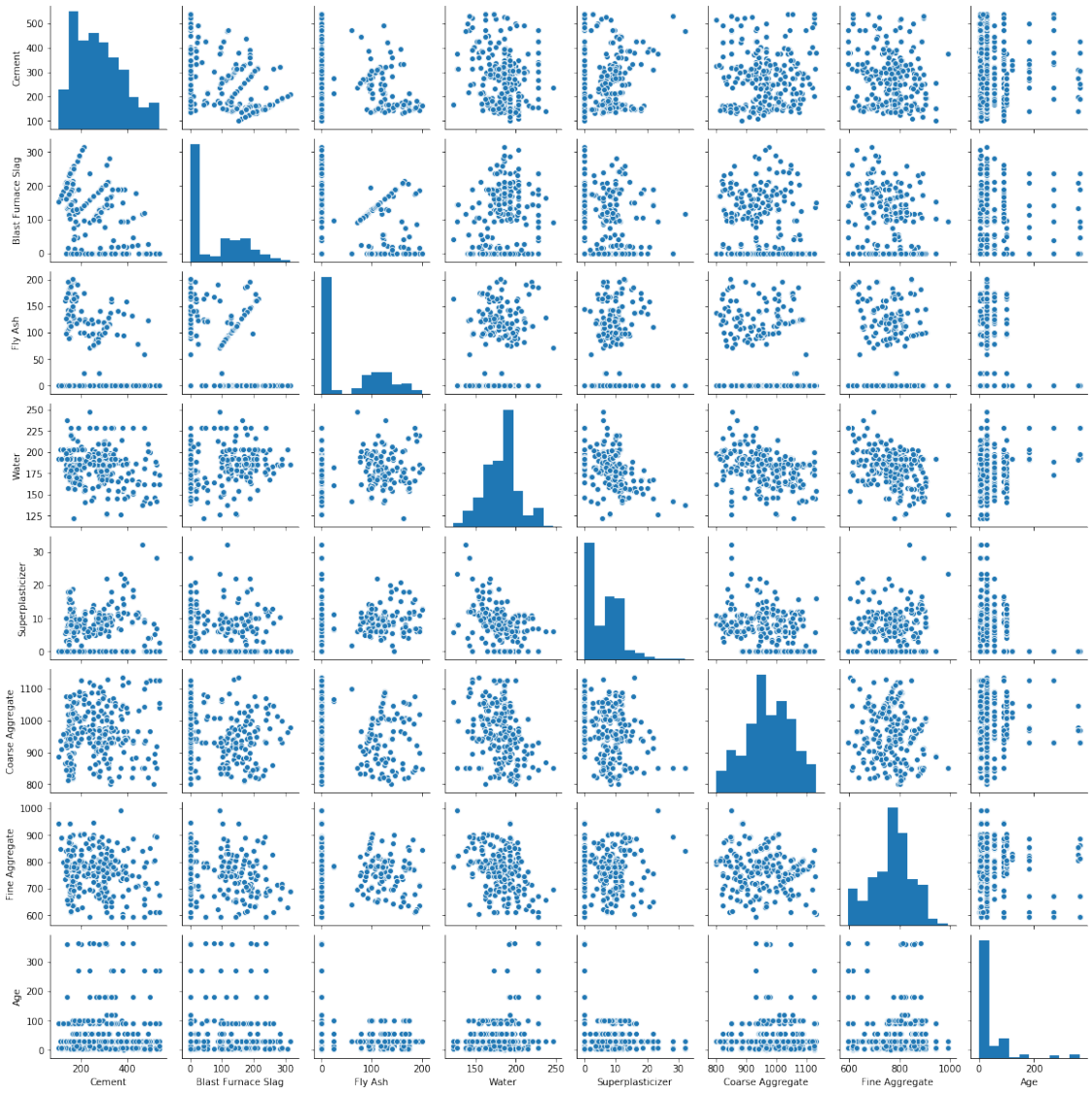
[10]:
```
# boxplot
x_train_box = x_train_no_unit.plot(
    kind="box",
```

```
    subplots=True,
    figsize=(12, 12),
    layout=(5, 4),
    sharex=False,
    sharey=False,
)
```



We can see that there are some outliers in some of the columns, we might want to remove those.

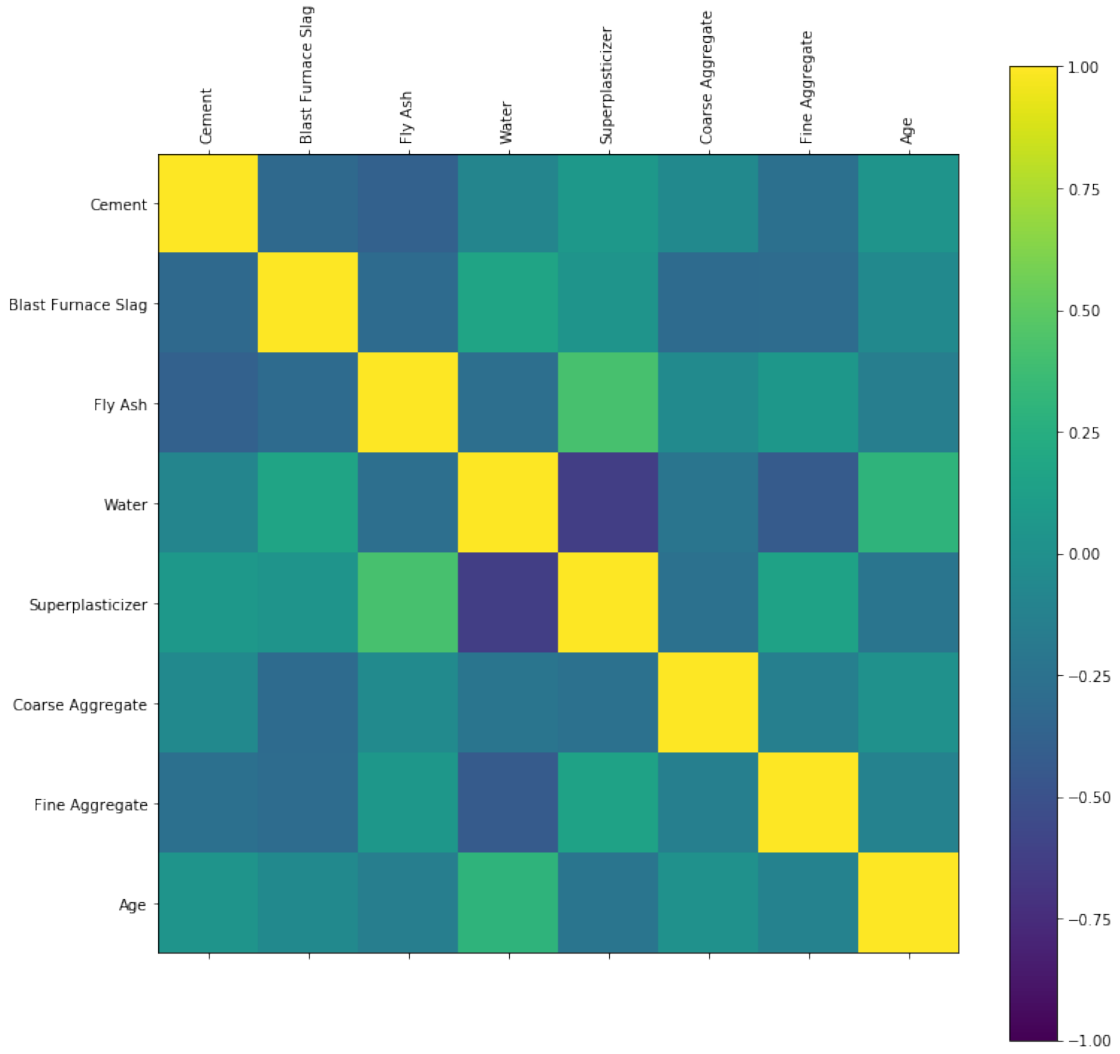
[11]:
```
# pairplot, if you right click and choose view image you can zoom into the␣
 ↪different columns.
sns = sb.pairplot(x_train_no_unit, height=2.0)
```



[10]:
```
# correlation plot
feature_names = list(x_train_no_unit)
correlations = x_train_no_unit.corr()
fig = plt.figure(figsize=(12, 12))
ax = fig.add_subplot(111)
cax = ax.matshow(correlations, vmin=-1, vmax=1)
fig.colorbar(cax)
ticks = np.arange(0, len(feature_names), 1)
ax.set_xticks(ticks)
ax.set_yticks(ticks)
ax.set_yticklabels(feature_names)
ax.set_xticklabels(feature_names, rotation=90)
```

```
# comment the two lines below if you are using matplotlib >= 3.1.2, <= 3.1.0
bottom, top = ax.get_ylim()
ax.set_ylim(bottom + 0.5, top - 0.5)

plt.show()
```



[22]:
```
# remove outliers (this was not used in our best results)
Q1 = x_train.quantile(0.25)
Q3 = x_train.quantile(0.75)
IQR = Q3-Q1
mask = ((x_train < (Q1 - 1.5 * IQR)) | (x_train > (Q3 + 1.5 * IQR))).any(axis=1)
print("Observations BEFORE removing outliers:", x_train.shape[0])
x_train = x_train[~mask]
y_train = y_train[~mask]
```

```
# X = X.values
# _test = x_test.values
print("Observations AFTER removing outliers:", x_train.shape[0])
```

```
Observations BEFORE removing outliers: 618
Observations AFTER removing outliers: 569
```

[11]:
```
# find feature importance using DecisionTreeRegressor and transform data (not␣
 ↪used)
regr = DecisionTreeRegressor(criterion="mae", random_state=0)
selector = SelectFromModel(regr)
selector.fit(x_train, y_train)
x_train_trans = selector.transform(x_train)
x_test_trans = selector.transform(x_test)
```

[12]:
```
# print out the features that were kept by the DecisionTreeRegressor
filt = selector.get_support()
column_names = list(x_train_no_unit)
chosen_columns = list(compress(column_names, filt))
print(chosen_columns)
```

```
['Cement', 'Age']
```

[12]:
```
# StandardScaler
scaler = StandardScaler()
x_train = scaler.fit_transform(x_train)
x_test = scaler.transform(x_test)
```

[ ]:
```
# MinMaxScaler (not used in best results)
scaler = MinMaxScaler((0,1))
x_train = scaler.fit_transform(x_train)
x_test = scaler.transform(x_test)
```

[13]:
```
# use GridSearchCV to find optimal hyperparameters for GradientBoostingRegressor
regr = GradientBoostingRegressor()
parameters = {
    "learning_rate": [0.0001, 0.001, 0.01, 0.1, 0.2, 0.3],
    "n_estimators": [100, 500, 1000, 2000, 5000, 10000],
}
search = GridSearchCV(
    regr, param_grid=parameters, scoring="r2", cv=5, n_jobs=-1, verbose=1
)
search.fit(x_train, y_train)
```

```
Fitting 5 folds for each of 36 candidates, totalling 180 fits
[Parallel(n_jobs=-1)]: Using backend LokyBackend with 4 concurrent workers.
[Parallel(n_jobs=-1)]: Done  42 tasks      | elapsed:   12.6s
```

```
[Parallel(n_jobs=-1)]: Done 180 out of 180 | elapsed:  1.2min finished
C:\Users\hej\Miniconda3\envs\skola\lib\site-
packages\sklearn\ensemble\gradient_boosting.py:1450: DataConversionWarning: A
column-vector y was passed when a 1d array was expected. Please change the shape
of y to (n_samples, ), for example using ravel().
  y = column_or_1d(y, warn=True)
```

[13]:
```
GridSearchCV(cv=5, error_score='raise-deprecating',
             estimator=GradientBoostingRegressor(alpha=0.9,
                                                 criterion='friedman_mse',
                                                 init=None, learning_rate=0.1,
                                                 loss='ls', max_depth=3,
                                                 max_features=None,
                                                 max_leaf_nodes=None,
                                                 min_impurity_decrease=0.0,
                                                 min_impurity_split=None,
                                                 min_samples_leaf=1,
                                                 min_samples_split=2,
                                                 min_weight_fraction_leaf=0.0,
                                                 n_estimators=100,
                                                 n_iter_no_change=None,
                                                 presort='auto',
                                                 random_state=None,
                                                 subsample=1.0, tol=0.0001,
                                                 validation_fraction=0.1,
                                                 verbose=0, warm_start=False),
             iid='warn', n_jobs=-1,
             param_grid={'learning_rate': [0.0001, 0.001, 0.01, 0.1, 0.2, 0.3],
                         'n_estimators': [100, 500, 1000, 2000, 5000, 10000]},
             pre_dispatch='2*n_jobs', refit=True, return_train_score=False,
             scoring='r2', verbose=1)
```

[14]:
```
# show best score and the chosen hyperparameters for GradientBoostingRegressor
print("Best score:", search.best_score_)
print("Best parameters:",search.best_params_)
```

```
Best score: 0.9055826412051831
Best parameters: {'learning_rate': 0.01, 'n_estimators': 10000}
```

[15]:
```
# elasticNet pipeline
param_alpha = [0.00001, 0.0001, 0.001, 0.01, 0.5, 0.1, 1]
param_ratio = [0.01, 0.1, 0.25, 0.5, 0.75, 0.9, 1.0]
param_grid = [
    {"elasticnet__alpha": param_alpha, "elasticnet__l1_ratio": param_ratio}
]
elnet_pipe = make_pipeline(StandardScaler(), ElasticNet())
```

[16]:
```
# elasticNet gridsearch
elnet_search = GridSearchCV(
    estimator=elnet_pipe,
    param_grid=param_grid,
    scoring="r2",
    cv=5,
    n_jobs=-1,
    verbose=1,
)
```

[17]:
```
# fit elasticNet
elnet_search.fit(x_train, y_train)
```

```
Fitting 5 folds for each of 49 candidates, totalling 245 fits

[Parallel(n_jobs=-1)]: Using backend LokyBackend with 4 concurrent workers.
[Parallel(n_jobs=-1)]: Done 190 tasks      | elapsed:    0.5s
[Parallel(n_jobs=-1)]: Done 245 out of 245 | elapsed:    0.7s finished
```

[17]:
```
GridSearchCV(cv=5, error_score='raise-deprecating',
             estimator=Pipeline(memory=None,
                                steps=[('standardscaler',
                                        StandardScaler(copy=True,
                                                       with_mean=True,
                                                       with_std=True)),
                                       ('elasticnet',
                                        ElasticNet(alpha=1.0, copy_X=True,
                                                   fit_intercept=True,
                                                   l1_ratio=0.5, max_iter=1000,
                                                   normalize=False,
                                                   positive=False,
                                                   precompute=False,
                                                   random_state=None,
                                                   selection='cyclic',
                                                   tol=0.0001,
                                                   warm_start=False))],
                                verbose=False),
             iid='warn', n_jobs=-1,
             param_grid=[{'elasticnet__alpha': [1e-05, 0.0001, 0.001, 0.01, 0.5,
                                                0.1, 1],
                          'elasticnet__l1_ratio': [0.01, 0.1, 0.25, 0.5, 0.75,
                                                   0.9, 1.0]}],
             pre_dispatch='2*n_jobs', refit=True, return_train_score=False,
             scoring='r2', verbose=1)
```

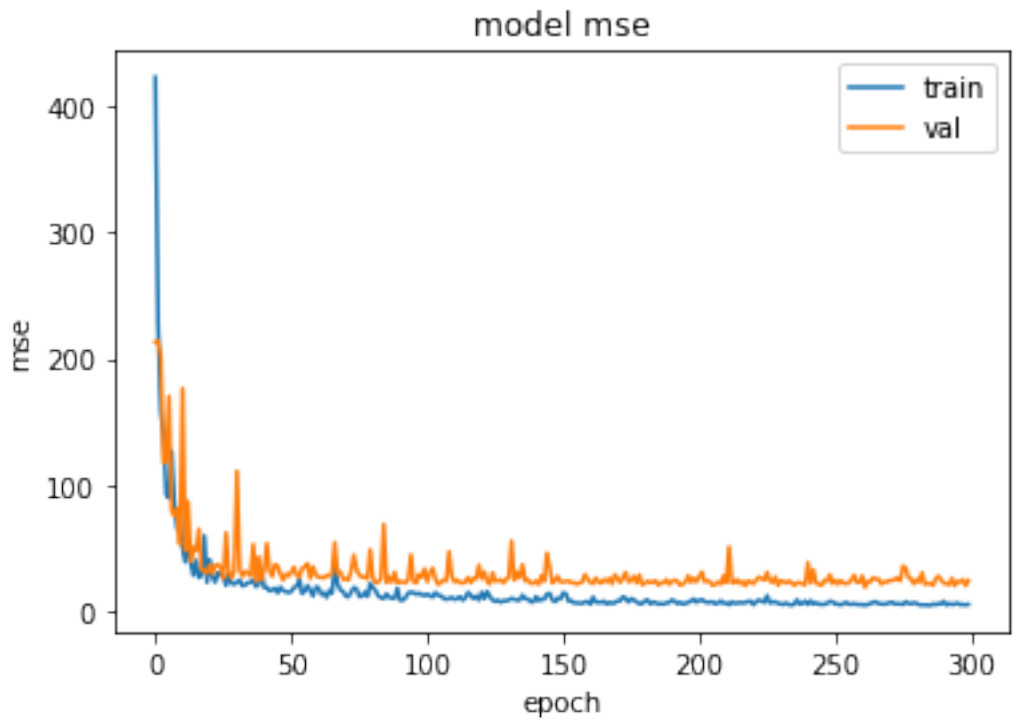
[18]:
```
# show best score and the chosen hyperparameters for elasticNet
print("Best score:", elnet_search.best_score_)
print("Best parameters:", elnet_search.best_params_)
```

```
Best score: 0.5675444140321406
Best parameters: {'elasticnet__alpha': 0.001, 'elasticnet__l1_ratio': 0.1}
```

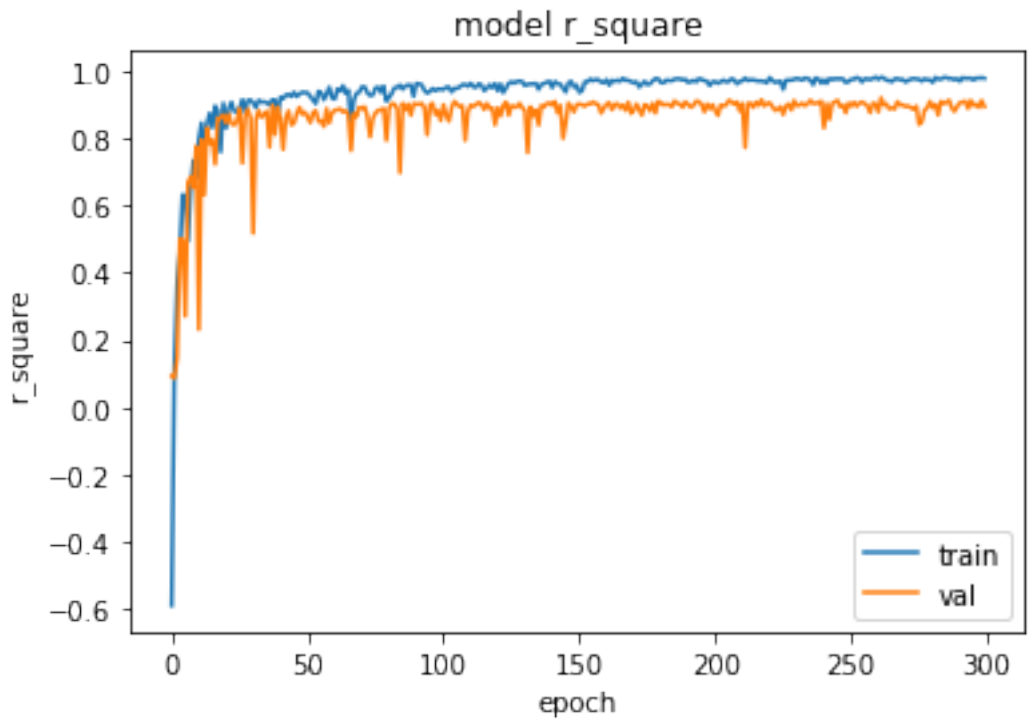
[17]:
```
# keras ANN
# we just tested different number of layers, nodes, optimizers and loss␣
 ↪functions
# we also tried removing features and outliers but that made the result worse
sample_vector_length = x_train.shape[1]
model = Sequential(
    [
        Dense(2000, activation="relu", input_shape=(sample_vector_length,)),
        Dense(2000, activation="relu"),
        Dense(2000, activation="relu"),
        Dense(1),
    ]
)
model.compile(
    optimizer=tensorflow.keras.optimizers.Nadam(),
    loss="mse",
    metrics=[r_square],
)
```

[18]:
```
# fit model
history = model.fit(
    x_train,
    y_train,
    epochs=300,
    validation_split=0.2,
    batch_size=25,
    verbose=0,
)
```

[19]:
```
# plot mse metric
epochs_from_end = 300
epoch_x_values = list(
    range(
        len(history.history["loss"]) - epochs_from_end,
        len(history.history["loss"]),
    )
)
plt.plot(epoch_x_values, history.history["loss"][-epochs_from_end:])
plt.plot(epoch_x_values, history.history["val_loss"][-epochs_from_end:])
plt.title("model mse")
plt.ylabel("mse")
plt.xlabel("epoch")
plt.legend(["train", "val"], loc="upper right")
plt.show()
```



[20]:
```
# plot r^2 metric
epochs_from_end = 300
epoch_x_values = list(
    range(
        len(history.history["r_square"]) - epochs_from_end,
        len(history.history["r_square"]),
    )
)
plt.plot(epoch_x_values, history.history["r_square"][-epochs_from_end:])
plt.plot(epoch_x_values, history.history["val_r_square"][-epochs_from_end:])
plt.title("model r_square")
plt.ylabel("r_square")
plt.xlabel("epoch")
plt.legend(["train", "val"], loc="lower right")
plt.show()
```



[21]:
```
# show some info about model and training to save for later reference
print("StandardScaler\n")
print(model.summary(), "\n")
print(history.params, "\n")
print(
    f"mean train loss last 10 epochs: {np.mean(history.history['loss'][-50:])}"
)
print(
    f"mean val loss last 10 epochs: {np.mean(history.history['val_loss'][-50:
 ↪])}"
)
print(
    f"mean train r^2 last 10 epochs: {np.mean(history.history['r_square'][-50:
 ↪])}"
)
print(
    f"mean val r^2 last 10 epochs: {np.mean(history.history['val_r_square'][-50:
 ↪])}"
)
```

```
StandardScaler

Model: "sequential_2"
_________________________________________________________________
```

```
Layer (type)                 Output Shape              Param #
=================================================================
dense_8 (Dense)              (None, 2000)              18000
_________________________________________________________________
dense_9 (Dense)              (None, 2000)              4002000
_________________________________________________________________
dense_10 (Dense)             (None, 2000)              4002000
_________________________________________________________________
dense_11 (Dense)             (None, 1)                 2001
=================================================================
Total params: 8,024,001
Trainable params: 8,024,001
Non-trainable params: 0
_________________________________________________________________
None

{'verbose': 0, 'epochs': 300, 'steps': 20}

mean train loss last 10 epochs: 6.364300756454468
mean val loss last 10 epochs: 24.777511138916015
mean train r^2 last 10 epochs: 0.9737379086017609
mean val r^2 last 10 epochs: 0.8936805200576782
```

[ ]:
```python
# train new model on all traindata
pred_model = Sequential(
    [
        Dense(2000, activation="relu", input_shape=(sample_vector_length,)),
        Dense(2000, activation="relu"),
        Dense(2000, activation="relu"),
        Dense(1),
    ]
)
pred_model.compile(
    optimizer=tensorflow.keras.optimizers.Nadam(),
    loss="mse",
    metrics=[r_square],
)
```

[ ]:
```python
pred_history = pred_model.fit(
    x_train, y_train, epochs=300, batch_size=25, verbose=1
)
```

[ ]:
```python
# make prediction on test data (not used in best result, might have overfitted?)
y_pred = pred_model.predict(x_test)
```

[22]:
```python
# make prediction on test data using first model
y_pred = model.predict(x_test)
```

[32]:
```
# create the csv file for upload to kaggle
dfscore = pd.DataFrame(y_pred)
ID = np.arange(0, len(dfscore), dtype=np.int64)
dfID = pd.DataFrame(ID)
dfscore.columns = ["Predicted"]
dfID.columns = ["Id"]
final_df = pd.concat([dfID, dfscore], axis=1)
final_df.to_csv("Julius&Markus_comp1_ver1.csv", sep=",", index=False)
```