Case Study 1: Superconductivity

Matt Farrow

May 11, 2022

1 Introduction

The data for this analysis comes from UCI's Machine Learning Repository and examines the relationship between superconductive materials and their respective critical temperatures. Superconductive materials have the unique ability of being able to have their electrical resistance disappear as their temperatures drops below a specific critical temperature.

The ovjective of this case study is to use linear regression with both L1 and L2 regularization to exame the ability to predict a superconductor's critical temperature. In addition, this analysis will attempt to determine which feature(s) lend the most importance to the prediction.

Unrelated to this analysis, my grandfather was an engineer on the Superconducting Super Collider here in Texas before it was shut down in 1993.

2 Methods

2.1 Data Examination

The initial data set is comprised of two separate files: `train.csv` and `unique_m.csv`. As a result of the files being able to matched row-by-row, they were combined into a single data set for the purposes of this analysis. The response variable `critical_temp` existed in both data sets; the variable was dropped from one of the data sets prior to joining. The new data set contains 21,263 observations and 168 variables including our response.

In understanding the data, there were no missing values and the data appeared to be in a proper format for proceeding with analysis. The exception to that was the `material` variable which contained 15,542 unique strings of data. This amount of unique data would not prove useful to a linear regression analysis, so `material` was dropped from the data set.

An examination of the response variable `critical_`temp as a histogram shows a right-skewed distribution (Figure 1). Applying a log-transformation (Figure 2) did not

serve to create a more normal distribution, instead the data is now left-skewed. Therefore, the analysis proceeded with the original data.

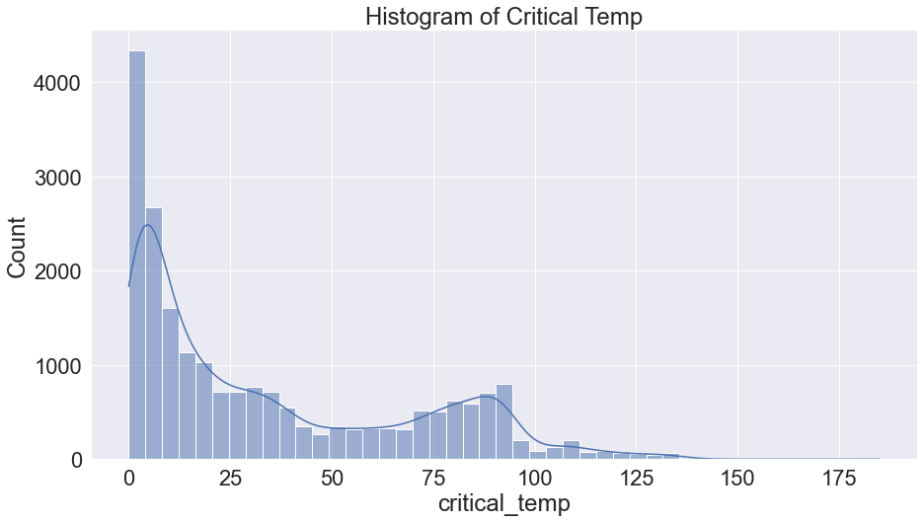


Figure 1: Histogram of Critical Temperature

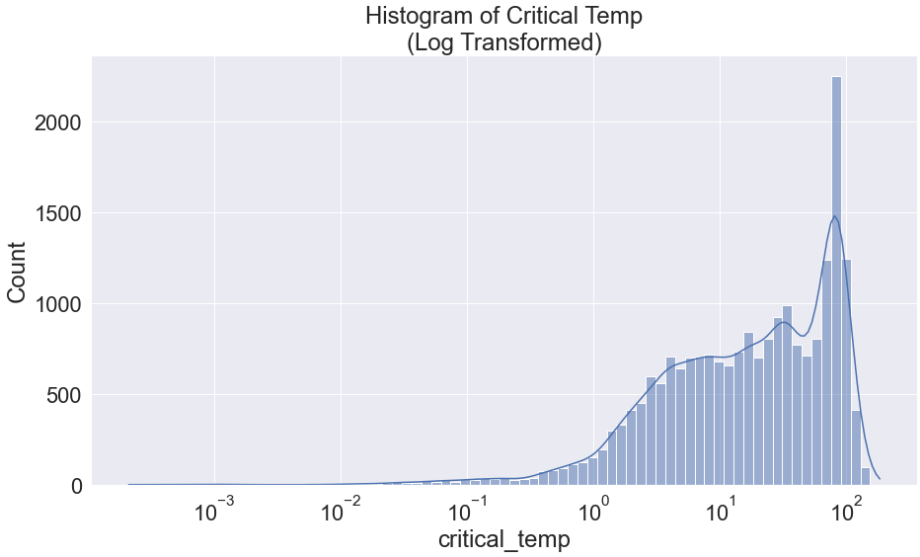


Figure 2: Histogram of Critical Temperature (Log-Transformed)

2.2 Model Preparation & Execution

The response variable, `critical_temp`, was separated from the rest of the data and then both the `X` and `y` data sets were split into test and train data sets using a 75%/25% split. Sklearn's pipeline feature was used to collect the scaler (`RobustScaler`) and model (`Lasso` & `Ridge`) to be used in each model.

A sequence of potential alpha values was defined and then those pieces were wrapped into a `GridSearchCV` process where 10-fold cross validation was performed to determine the most appropriate parameters for the model. After fitting both models, the resulting `neg_mean_absolute_error` and selected alpha value were examined.

Best Score	-12.676
Best Alpha	0.001

Table 1: L1 (LASSO) Model Training Results

Best Score	-12.636
Best Alpha	0.3

Table 2: L2 (Ridge) Model Training Results

3 Results

3.1 Model Results

Once trained, the fitted models were used to make predictions on the testing data that had been held out. For each model, an R^2 value along with the mean absolute error (MAE) were reported for performance comparision.

R^2	0.475
Mean Absolute Error	12.927

Table 3: L1 (LASSO) Model Testing Results

R^2	0.474
Mean Absolute Error	12.912

Table 4: L2 (Ridge) Model Testing Results

Interestingly, both models returned almost identical R^2 and MAE values. It is unclear whether an error was made during the modeling, or if the two models do indeed perform to such a close similarity.

3.2 Coefficient Weights

After completing the linear regression with both L1 (LASSO) and L2 (Ridge) regularlizations, the coefficients were analyzed to determine which coefficients most contributed to each model. The top five for each model are shown below.

Variable	Coefficient
range_ThermalConductivity	30.494
std_ThermalConductivity	29.282
wtd_entropy_Valence	29.185
entropy_fie	27.979
range_fie	25.123

Table 5: L1 (LASSO) Model Top 5 Coefficients

Variable	Coefficient
wtd_gmean_atomic_radius	82.504
wtd_mean_atomic_radius	76.231
wtd_mean_atomic_mass	40.307
wtd_entropy_Valence	36.01
std_ThermalConductivity	33.523

Table 6: L2 (Ridge) Model Top 5 Coefficients

4 Conclusion

In examining the top five coefficients of each model, additional work may have been needed to avoid potential multicollinearity as both models contained high performing coefficients that appear as though they may be correlated. It is also interesting to note that the coefficients of the L1 (LASSO) model have a much narrower distribution; within the L2 (Ridge) model, the top two performing coefficients were significantly separated from the next values.

Appendix

Sources

- Lasso Regression with Python
- How to Use Sklearn Pipelines For Ridiculously Neat Code
- Pre-Process Data with Pipeline to Prevent Data Leakage during Cross-Validation
- sklearn.linear_model.LinearRegression
- How to Develop LASSO Regression Models in Python
- How to create a linear regression model using Scikit-Learn
- Linear Regression in Python

Code

Code begins on the following page.

Case Study 1

Your case study is to build a linear regression model using L1 or L2 regularization (or both) the task to predict the Critical Temperature as closely as possible. In addition, include in your write-up which variable carries the most importance.

In [ ]:
```
# General libraries
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns

# sklearn libraries
from sklearn.preprocessing import StandardScaler, RobustScaler
from sklearn.linear_model import LinearRegression, Lasso, Ridge
import sklearn.metrics as metrics
from sklearn.model_selection import train_test_split, GridSearchCV
from sklearn.pipeline import make_pipeline
```

In [ ]:
```
# Read in the data
unique = pd.read_csv('unique_m.csv')
train = pd.read_csv('train.csv')

# Drop critical temp since it exists in both data frames
unique = unique.drop(['critical_temp'], axis = 1)

# Merge unique and train
df = pd.concat([train, unique], axis = 1)
```

Examine the Data

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

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 21263 entries, 0 to 21262
Columns: 169 entries, number_of_elements to material
dtypes: float64(156), int64(12), object(1)
memory usage: 27.4+ MB
```

In [ ]:
```
df.head()
```

Out[ ]:

	number_of_elements	mean_atomic_mass	wtd_mean_atomic_mass	gmean_atomic_mass
0	4	88.944468	57.862692	66.361592
1	5	92.729214	58.518416	73.132787
2	4	88.944468	57.885242	66.361592
3	4	88.944468	57.873967	66.361592
4	4	88.944468	57.840143	66.361592

5 rows × 169 columns

In [ ]:
```
df.describe()
```

Out[ ]:

	number_of_elements	mean_atomic_mass	wtd_mean_atomic_mass	gmean_atomic_ma
count	21263.000000	21263.000000	21263.000000	21263.0000
mean	4.115224	87.557631	72.988310	71.2906
std	1.439295	29.676497	33.490406	31.0302
min	1.000000	6.941000	6.423452	5.3205
25%	3.000000	72.458076	52.143839	58.0412
50%	4.000000	84.922750	60.696571	66.3615
75%	5.000000	100.404410	86.103540	78.1166
max	9.000000	208.980400	208.980400	208.9804

8 rows × 168 columns

Material isn't listed in `df.describe()`. How many unique values does it have?

In [ ]:
```
len(df['material'].unique())
```

Out[ ]:
```
15542
```

Yikes, 15,542 unique strings. I'll drop this column from the data.

In [ ]:
```
df=df.drop(['material'], axis=1)
```

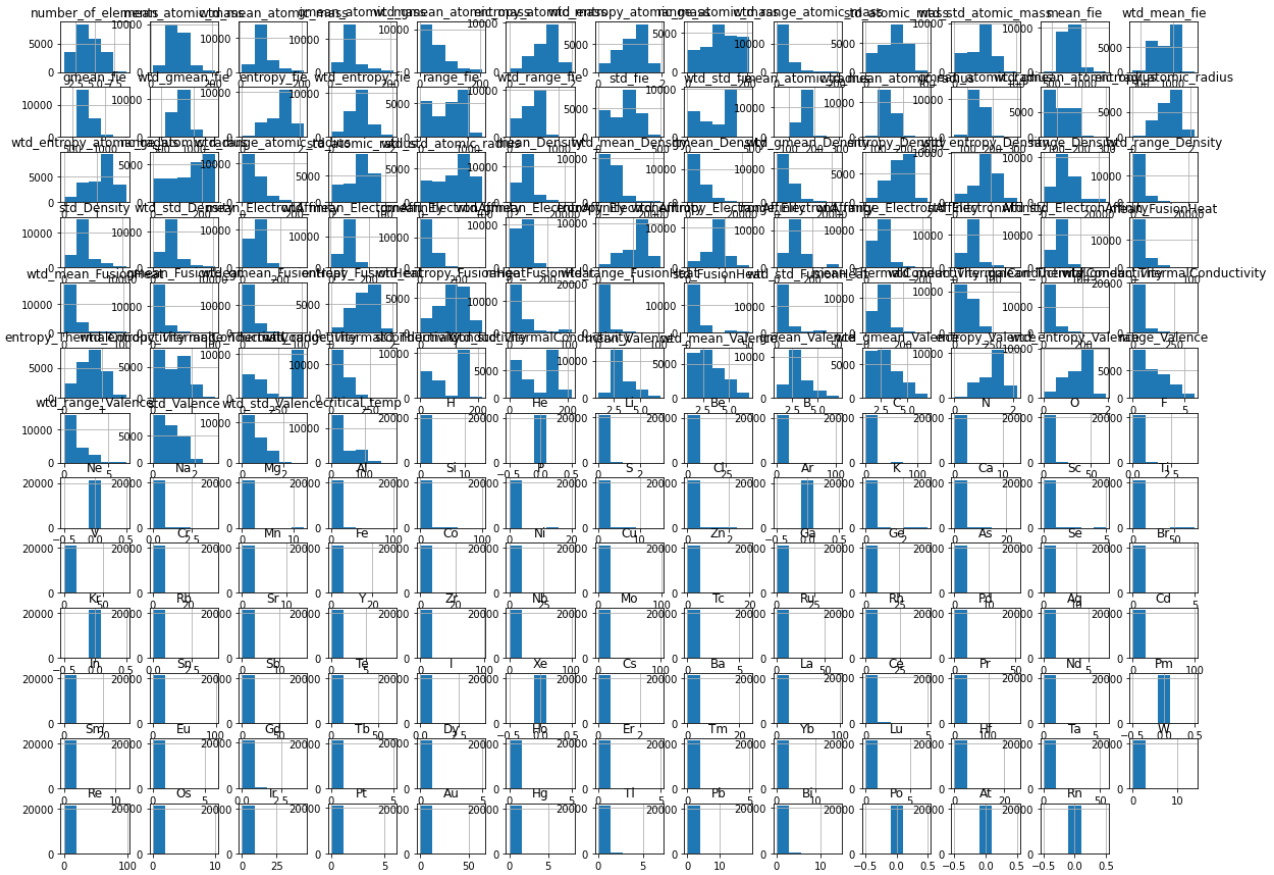
Missing Values

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

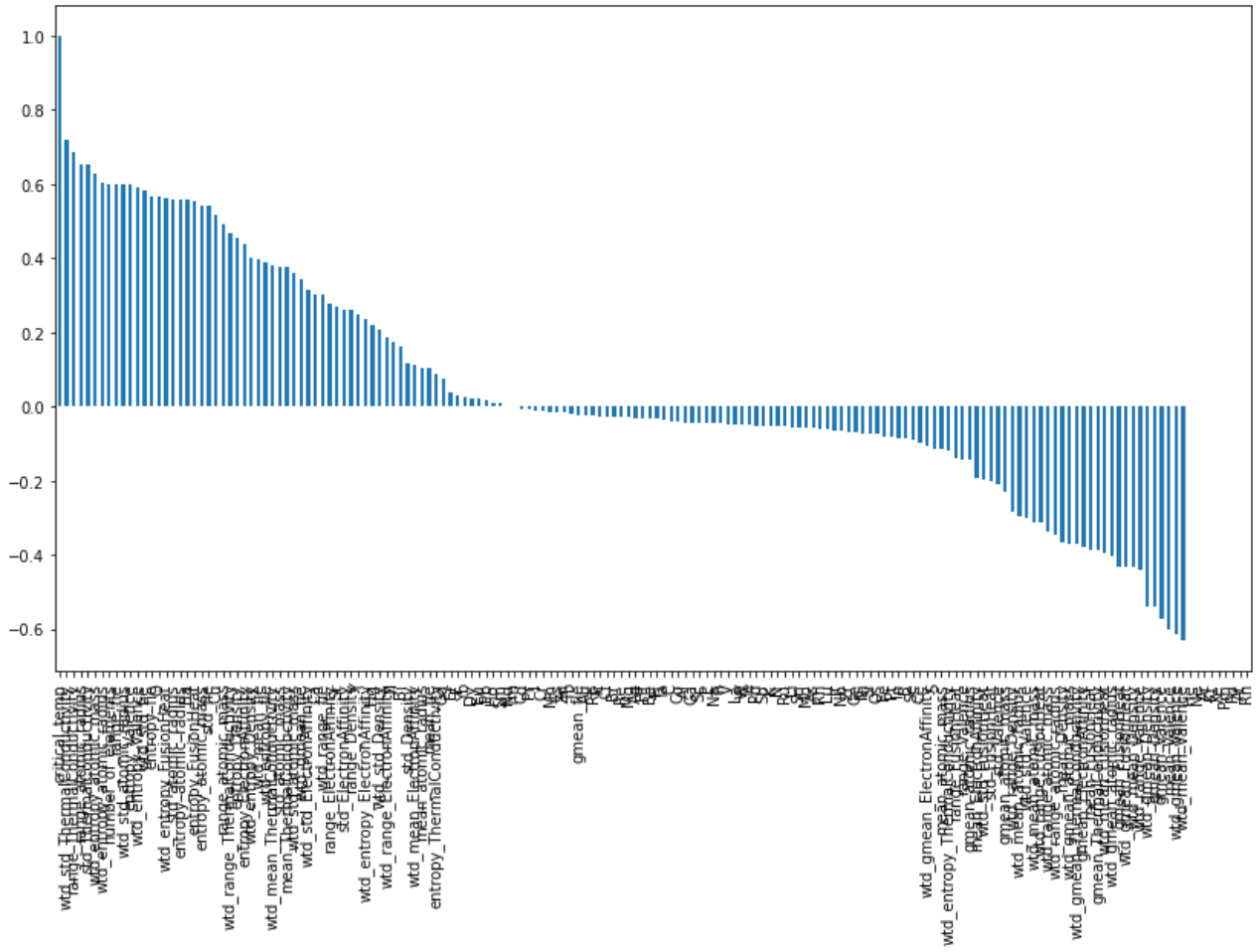
Out[ ]:
```
number_of_elements        0
mean_atomic_mass          0
wtd_mean_atomic_mass      0
gmean_atomic_mass         0
wtd_gmean_atomic_mass     0
                         ..
Pb                        0
Bi                        0
Po                        0
At                        0
Rn                        0
Length: 168, dtype: int64
```

It doesn't appear that there are any missing values in the data.

In [ ]:
```
df.hist(bins=5, figsize=(20,15))
plt.show()
```



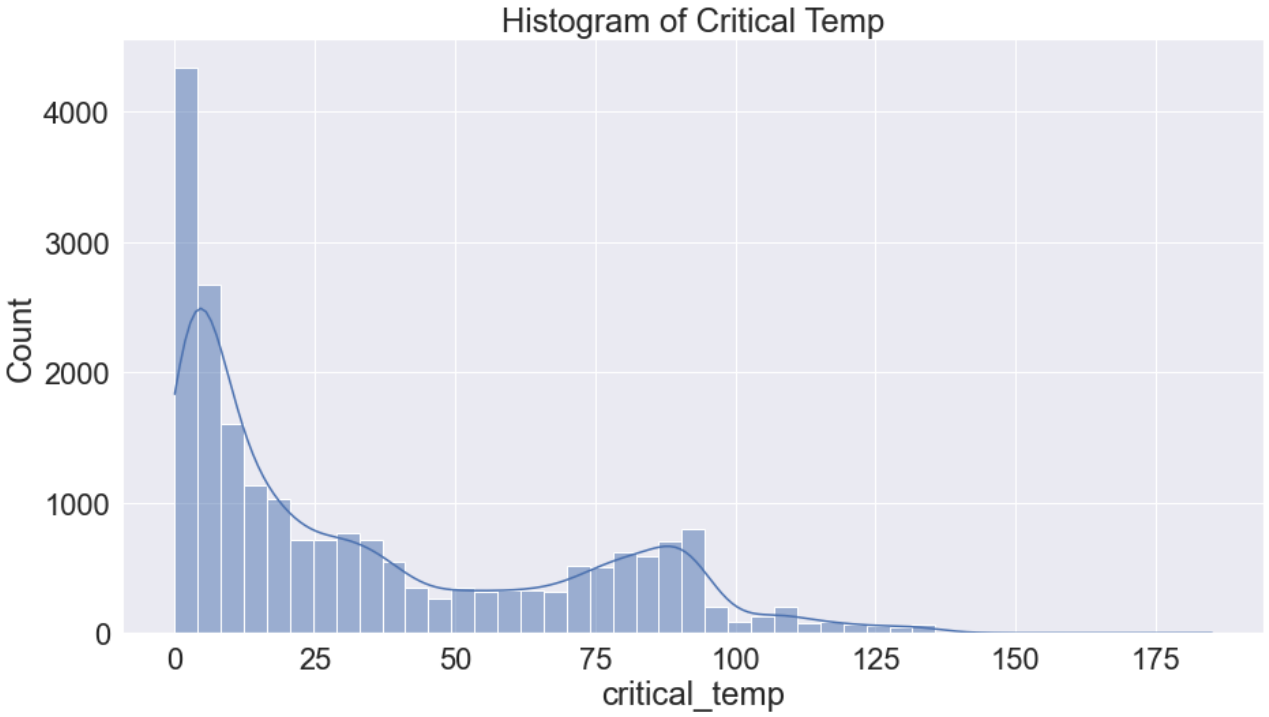
In [ ]:
```
plt.figure(figsize=(14,8))
bars = df.corr()['critical_temp'].sort_values(ascending=False).plot(kind='ba
```



Examine Response Variable

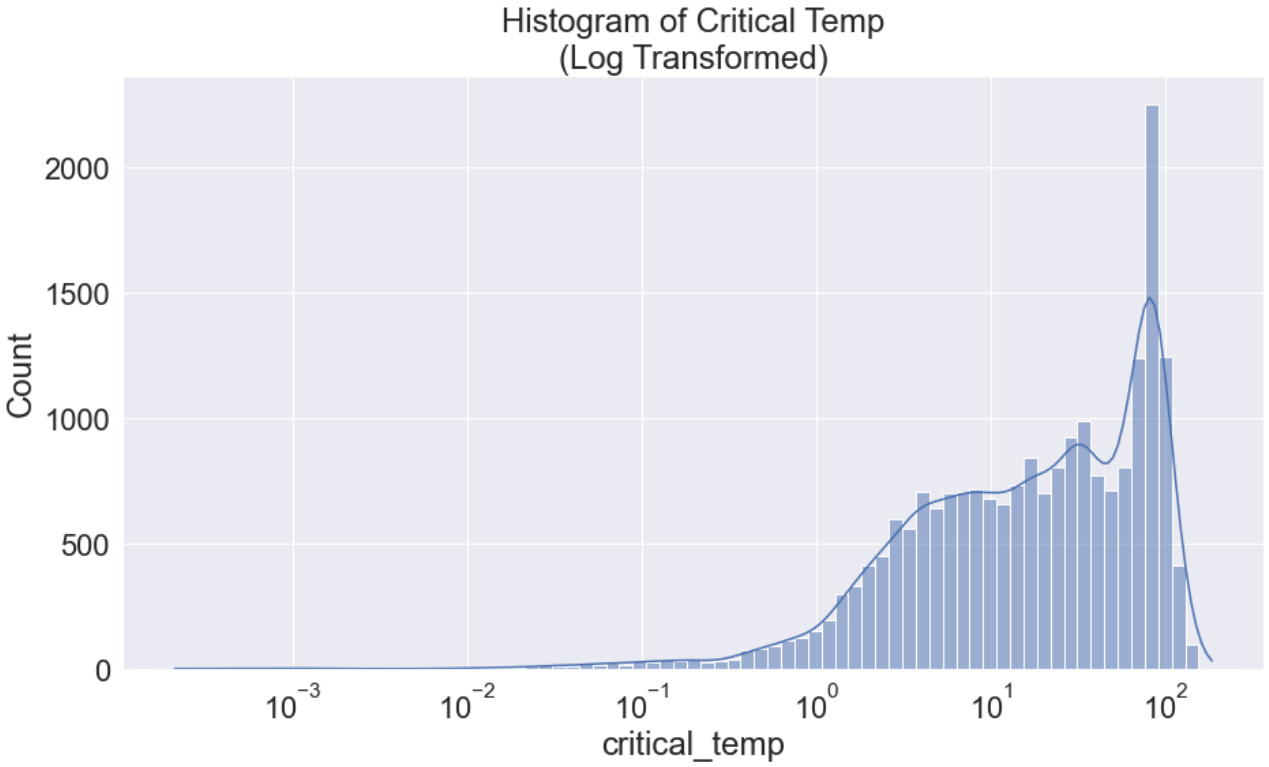
In [ ]:
```
# Examine response variable
sns.set(rc = {'figure.figsize':(15,8)})
sns.set(font_scale = 2)
p=sns.histplot(df['critical_temp'], kde=True)
p.set_title("Histogram of Critical Temp")
```

Out[ ]:
```
Text(0.5, 1.0, 'Histogram of Critical Temp')
```



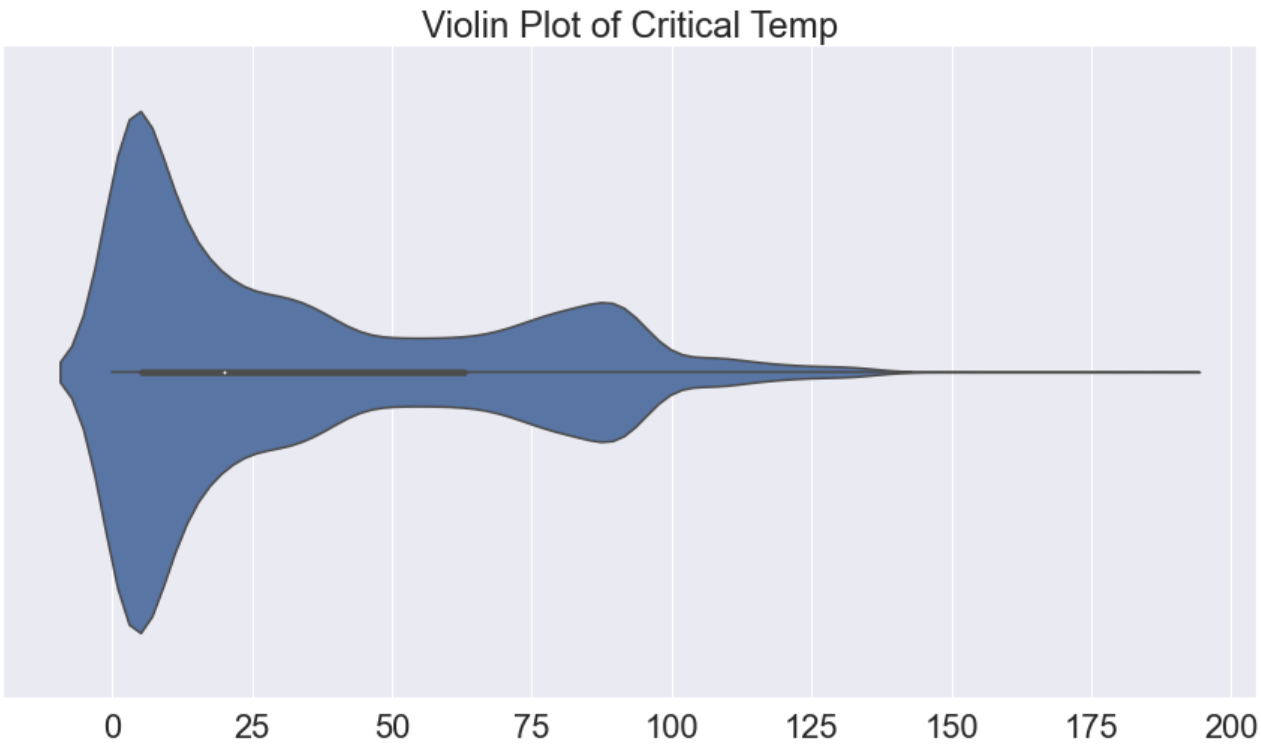
In [ ]:
```
# Does a transformation help?
p=sns.histplot(df['critical_temp'], kde=True, log_scale=True)
p.set_title("Histogram of Critical Temp\n(Log Transformed)")
```

Out[ ]:
```
Text(0.5, 1.0, 'Histogram of Critical Temp\n(Log Transformed)')
```



In [ ]:
```
p=sns.violinplot(x=df['critical_temp'])
p.set_title("Violin Plot of Critical Temp")
p.set(xlabel=None)
```

Out[ ]:
```
[Text(0.5, 0, '')]
```



Model Building

Define & Split the Data

In [ ]:
```
# Define response & feature variables
X = df.drop(labels = ['critical_temp'], axis = 1)
y = df['critical_temp']

# Create a feature list
feature_list = list(X.columns)

# Split the data
X_train, X_test, y_train, y_test =\
    train_test_split(X, y,
    test_size=0.25,
    random_state=1)
```

Instantiate Pipeline

In [ ]:
```
# Source: https://towardsdatascience.com/pre-process-data-with-pipeline-to-p

lasso_pipeline = make_pipeline(RobustScaler(), Lasso(random_state=1))
ridge_pipeline = make_pipeline(RobustScaler(), Ridge(random_state=1))

# Set up alpha search
# https://stackoverflow.com/questions/41899132/invalid-parameter-for-sklearn
alpha_range = [0.0001, 0.001, 0.01, 0.1, 0.3, 0.5, 0.7, 0.9, 1, 3, 5, 7, 9,
lasso_params = [{'lasso__alpha': alpha_range}]
ridge_params = [{'ridge__alpha': alpha_range}]
```

Train Models

LASSO

In [ ]:
```
lasso_train = GridSearchCV(estimator=lasso_pipeline,
                           param_grid=lasso_params,
                           scoring='neg_mean_absolute_error',
                           cv=10,
                           n_jobs=-1)

lasso_train.fit(X_train, y_train)

print("L1 (LASSO) Model")
print("Best Score:", lasso_train.best_score_)
print("Best Alpha:", lasso_train.best_params_)
```

```
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 1.956e+06, tolerance: 1.698e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 1.919e+06, tolerance: 1.696e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 1.950e+06, tolerance: 1.690e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 1.964e+06, tolerance: 1.700e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 1.957e+06, tolerance: 1.700e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 1.679e+06, tolerance: 1.698e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
```

```
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 1.650e+06, tolerance: 1.695e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 1.922e+06, tolerance: 1.695e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 1.650e+06, tolerance: 1.696e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 1.952e+06, tolerance: 1.695e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 1.713e+06, tolerance: 1.700e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 1.946e+06, tolerance: 1.687e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 1.663e+06, tolerance: 1.700e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 1.687e+06, tolerance: 1.695e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 1.951e+06, tolerance: 1.698e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 1.936e+06, tolerance: 1.694e+03
```

```
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 2.879e+05, tolerance: 1.698e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 2.984e+05, tolerance: 1.695e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 2.929e+05, tolerance: 1.700e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 3.236e+05, tolerance: 1.695e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 4.497e+05, tolerance: 1.696e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 2.971e+05, tolerance: 1.700e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 3.147e+05, tolerance: 1.690e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 1.700e+06, tolerance: 1.690e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 2.883e+05, tolerance: 1.687e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
```

```
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 2.975e+05, tolerance: 1.698e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 3.667e+05, tolerance: 1.694e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 1.675e+06, tolerance: 1.698e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 1.716e+06, tolerance: 1.694e+03
  model = cd_fast.enet_coordinate_descent(
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 1.686e+06, tolerance: 1.687e+03
  model = cd_fast.enet_coordinate_descent(
L1 (LASSO) Model
Best Score: -12.675935647682858
Best Alpha: {'lasso__alpha': 0.001}
/Library/Frameworks/Python.framework/Versions/3.10/lib/python3.10/site-packa
ges/sklearn/linear_model/_coordinate_descent.py:647: ConvergenceWarning: Obj
ective did not converge. You might want to increase the number of iterations
, check the scale of the features or consider increasing regularisation. Dua
lity gap: 1.869e+06, tolerance: 1.884e+03
  model = cd_fast.enet_coordinate_descent(
```

Ridge

In [ ]:
```
ridge_train = GridSearchCV(estimator=ridge_pipeline,
                           param_grid=ridge_params,
                           scoring='neg_mean_absolute_error',
                           cv=10,
                           n_jobs=-1)

ridge_train.fit(X_train, y_train)

print("L2 (Ridge) Model")
print("Best Score:", ridge_train.best_score_)
print("Best Alpha:", ridge_train.best_params_)
```

```
L2 (Ridge) Model
Best Score: -12.635863718438099
Best Alpha: {'ridge__alpha': 0.3}
```

Test Models

In [ ]:
```
y_lasso_pred = lasso_train.predict(X_test)
y_ridge_pred = ridge_train.predict(X_test)

print("L1 (Lasso) Performance")
print("R2:", metrics.r2_score(y_test, y_lasso_pred))
print("MAE:", metrics.mean_absolute_error(y_test, y_lasso_pred))

print("L2 (Ridge) Performance")
print("R2:", metrics.r2_score(y_test, y_ridge_pred))
print("MAE:", metrics.mean_absolute_error(y_test, y_ridge_pred))
```

```
L1 (Lasso) Performance
R2: 0.4747144301704468
MAE: 12.926775749215134
L2 (Ridge) Performance
R2: 0.4736246385198172
MAE: 12.916091908191113
```

LASSO Coefficients

In [ ]:
```
lasso_train.best_estimator_['lasso'].coef_
```

Out[ ]:
```
array([ 9.57783500e-01,  1.07102790e+01, -2.44358911e+01,  1.04027772e+00,
        8.16278998e+00, -1.53256296e+01,  6.87766444e+00,  1.35714866e+01,
        2.76912117e+00, -7.29225020e+00, -4.71937808e+00, -5.00386011e+00,
        1.11240793e+01,  3.03823513e+00, -1.47706986e-01,  2.79798655e+01,
        1.24165866e+01,  2.51236245e+01,  7.15162495e+00, -2.23953985e+01,
       -9.81364123e-01,  4.40499564e+00,  2.28749791e+01, -1.06063075e+01,
       -1.36852157e+01, -1.87685238e+01,  2.81080137e+00,  1.15680374e+01,
       -2.62937064e+00, -2.14754443e+01,  1.42423094e+01, -8.90430382e+00,
        1.45265338e+01, -2.53589478e+00,  9.48326449e-01, -1.65980781e+00,
       -1.92615392e+00, -2.79048700e+00, -1.49186569e+00,  3.00868899e+00,
       -7.40083286e-01, -2.21373455e+00,  1.65227462e+01,  5.16101130e+00,
       -2.01803338e+01,  2.33521312e+00, -3.17175823e+00, -1.81894675e+01,
       -3.47078488e+00,  2.12717758e+01, -1.05784925e+01,  4.41433965e+00,
       -1.46848711e+01, -7.57258539e-01,  9.28403492e+00, -7.06984796e+00,
        1.08400838e+01, -2.75456654e+00,  4.50022333e+00, -3.74596540e-01,
        1.22957938e+00, -1.06763558e+00,  2.03920295e+01, -3.32826257e+00,
       -1.35831327e+01,  4.36822098e+00,  1.78870150e+00, -3.04940941e+01,
       -1.10573467e+01,  2.92823232e+01,  5.16633945e+00, -3.70894323e+00,
       -2.63565941e+00,  6.33971955e+00,  3.74889889e-01,  9.13386712e+00,
       -2.91985086e+01,  1.22043044e+01, -1.39216655e+00, -3.48766522e+00,
       -1.20790538e+01, -1.59036674e+00,  0.00000000e+00,  2.03980073e+00,
       -2.07088140e-01, -8.96282716e-01, -5.37536627e-02, -8.57234841e-01,
       -2.85888644e+00,  7.85478426e+00,  0.00000000e+00,  4.93087301e+00,
        1.92302465e-01, -1.66773375e-01, -1.63523818e+00, -1.37116598e+00,
       -1.61602981e+00, -6.57462661e+00,  0.00000000e+00,  7.91926303e+00,
        1.52521853e+00,  2.77876592e-01, -6.33380191e-02,  2.70928383e-02,
       -3.40225311e-01, -6.57350325e-01,  1.12988964e+00, -4.90142912e-01,
       -3.90928251e-01, -1.62054044e+00, -6.77624016e-02,  4.15975316e-01,
       -1.03629972e+00, -1.73660252e+00, -9.61018888e-01,  4.49519403e-01,
        0.00000000e+00,  7.99866829e+00,  1.59816293e-01, -2.40118167e-01,
        4.58537181e-03,  8.97130750e-02,  1.12198379e-01,  1.81761821e+00,
        2.69863413e-01, -5.06208729e-02,  4.71838080e-02, -1.07904524e+01,
       -1.30990690e+01,  1.29731285e+00, -4.75534544e-02, -2.09319119e-01,
        6.42825888e-01,  6.97522861e+00,  0.00000000e+00,  5.59681256e+00,
        1.18779051e+01, -3.68035330e-02, -2.36269273e+00, -4.92670364e-02,
       -2.25105371e+00,  0.00000000e+00,  2.99732327e-01, -1.77472869e+00,
       -6.45399400e-01,  1.72880767e+00,  5.38477121e+00,  3.05348872e+00,
        2.29729229e+00,  0.00000000e+00,  2.72754219e+00,  3.89535507e+00,
       -5.56428177e-01, -6.56803226e-02,  2.22277354e-01, -9.26692325e-02,
        1.34390256e+00,  9.35943109e-02,  4.24995960e+00, -5.18340417e-01,
        5.44217393e+00,  5.02505209e+00,  1.82571149e+00,  5.44537540e+00,
        0.00000000e+00,  0.00000000e+00,  0.00000000e+00])
```

In [ ]:
```
lasso_weights = {df.columns[key]:abs(value) for key, value in enumerate(lass
dict(sorted(lasso_weights.items(), key=lambda item: item[1], reverse=True))
```

Out[ ]:
```
{'range_ThermalConductivity': 30.49409411677583,
 'std_ThermalConductivity': 29.282323240875897,
 'wtd_entropy_Valence': 29.198508585454952,
 'entropy_fie': 27.97986546194415,
 'range_fie': 25.123624476195126,
 'wtd_mean_atomic_mass': 24.435891139005925,
 'wtd_mean_atomic_radius': 22.874979120467305,
 'std_fie': 22.39539852273098,
 'std_atomic_radius': 21.475444256410604,
 'std_ElectronAffinity': 21.27177577566263,
 'wtd_mean_ThermalConductivity': 20.392029472833922,
```

```
'wtd_gmean_ElectronAffinity': 20.180333799299305,
'entropy_atomic_radius': 18.76852382229849,
'range_ElectronAffinity': 18.189467525878282,
'wtd_mean_ElectronAffinity': 16.52274622173433,
'entropy_atomic_mass': 15.325629639254325,
'wtd_mean_FusionHeat': 14.6848711033669,
'wtd_mean_Density': 14.52653380481855,
'wtd_std_atomic_radius': 14.242309400501746,
'wtd_gmean_atomic_radius': 13.685215742990312,
'wtd_gmean_ThermalConductivity': 13.583132665970748,
'range_atomic_mass': 13.571486647086104,
'Ag': 13.099068959396925,
'wtd_entropy_fie': 12.416586573489242,
'range_Valence': 12.204304386174638,
'wtd_std_Valence': 12.07905375876434,
'Cs': 11.877905091518043,
'range_atomic_radius': 11.568037372445035,
'wtd_mean_fie': 11.124079338792933,
'wtd_range_ThermalConductivity': 11.057346695129356,
'wtd_entropy_FusionHeat': 10.840083795372646,
'Pd': 10.79045244425821,
'mean_atomic_mass': 10.710278983793811,
'gmean_atomic_radius': 10.606307488553403,
'wtd_std_ElectronAffinity': 10.578492540726353,
'wtd_gmean_FusionHeat': 9.284034916446018,
'entropy_Valence': 9.13386711623424,
'mean_Density': 8.904303815908566,
'wtd_gmean_atomic_mass': 8.162789976403497,
'Kr': 7.998668286799644,
'Ar': 7.919263030464211,
'O': 7.854784255642465,
'std_atomic_mass': 7.292250199264196,
'wtd_range_fie': 7.151624951194831,
'entropy_FusionHeat': 7.069847960411798,
'Te': 6.975228611552435,
'wtd_entropy_atomic_mass': 6.877664441886284,
'S': 6.574626605353182,
'gmean_Valence': 6.339719548522305,
'Xe': 5.596812559503841,
'Pb': 5.445375395590002,
'Au': 5.442173927520701,
'Tb': 5.3847712110203245,
'wtd_std_ThermalConductivity': 5.166339452102838,
'gmean_ElectronAffinity': 5.161011304703671,
'Hg': 5.025052094297533,
'mean_fie': 5.003860109194855,
'Ne': 4.930873010747075,
'wtd_std_atomic_mass': 4.71937808421278,
'wtd_range_FusionHeat': 4.500223329140536,
'mean_FusionHeat': 4.4143396479120405,
'mean_atomic_radius': 4.404995641865948,
'entropy_ThermalConductivity': 4.368220980912161,
'Ir': 4.249959602459216,
'Yb': 3.8953550721372396,
'mean_Valence': 3.7089432296434546,
'std_Valence': 3.4876652164013864,
'wtd_range_ElectronAffinity': 3.4707848762762006,
```

```
'gmean_ThermalConductivity': 3.3282625728437782,
'wtd_entropy_ElectronAffinity': 3.1717582264839423,
'Dy': 3.0534887247597147,
'gmean_fie': 3.038235132476612,
'std_Density': 3.008688992839782,
'N': 2.858886442856935,
'wtd_entropy_atomic_radius': 2.810801374766463,
'range_Density': 2.790487002440247,
'wtd_range_atomic_mass': 2.7691211665542204,
'range_FusionHeat': 2.7545665374504558,
'Tm': 2.7275421938545423,
'wtd_mean_Valence': 2.6356594054954847,
'wtd_range_atomic_radius': 2.6293706373414825,
'gmean_Density': 2.535894783973816,
'La': 2.3626927332742036,
'entropy_ElectronAffinity': 2.335213124448163,
'Ho': 2.2972922880342668,
'Pr': 2.251053708318047,
'mean_ElectronAffinity': 2.2137345508615316,
'He': 2.0398007287297544,
'wtd_entropy_Density': 1.9261539192964232,
'Tl': 1.8257114916233292,
'Mo': 1.8176182121205717,
'wtd_entropy_ThermalConductivity': 1.7887015013073493,
'Sm': 1.774728691803154,
'Ge': 1.7366025169716748,
'Gd': 1.7288076709844695,
'entropy_Density': 1.659807813091683,
'Al': 1.6352381758607275,
'Ni': 1.6205404380715394,
'P': 1.616029813679954,
'critical_temp': 1.5903667437812903,
'K': 1.525218526578877,
'wtd_range_Density': 1.4918656926198284,
'wtd_range_Valence': 1.3921665499578924,
'Si': 1.371165978901978,
'Re': 1.3439025629210517,
'Cd': 1.297312846219618,
'wtd_std_FusionHeat': 1.2295793803452253,
'Mn': 1.1298896361967758,
'mean_ThermalConductivity': 1.0676355781628066,
'gmean_atomic_mass': 1.0402777247214938,
'Ga': 1.0362997224882886,
'wtd_std_fie': 0.9813641226288073,
'As': 0.9610188881101238,
'number_of_elements': 0.9577835001175794,
'wtd_gmean_Density': 0.9483264485778177,
'Be': 0.8962827158736726,
'C': 0.8572348411535096,
'gmean_FusionHeat': 0.7572585387106064,
'wtd_std_Density': 0.7400832860166121,
'Cr': 0.6573503253831036,
'Eu': 0.6453994001876798,
'Sb': 0.6428258884186397,
'Lu': 0.556428177380533,
'Pt': 0.5183404169063515,
'Fe': 0.49014291191209514,
```

```
'Se': 0.4495194031822201,
'Zn': 0.41597531590190345,
'Co': 0.3909282510461157,
'wtd_gmean_Valence': 0.3748898887573451,
'std_FusionHeat': 0.374596539587452,
'V': 0.3402253112823565,
'Pm': 0.29973232715150905,
'Ca': 0.27787659202703113,
'Tc': 0.26986341348455223,
'Sr': 0.2401181674518157,
'Ta': 0.22227735447628277,
'Sn': 0.20931911858524127,
'Li': 0.2070881397680395,
'Na': 0.19230246477019114,
'Mg': 0.16677337486842167,
'Rb': 0.15981629299843023,
'wtd_gmean_fie': 0.14770698615424116,
'Nb': 0.11219837900968294,
'Os': 0.09359431086609563,
'W': 0.09266923248615051,
'Zr': 0.08971307499131446,
'Cu': 0.06776240155316159,
'Hf': 0.06568032258619723,
'Sc': 0.06333801909648593,
'B': 0.05375366268827595,
'Ru': 0.05062087289089685,
'Ce': 0.049267036373158074,
'In': 0.047553454427502306,
'Rh': 0.04718380802698852,
'Ba': 0.03680353296040104,
'Ti': 0.027092838316867224,
'Y': 0.0045853718116380905,
'H': 0.0,
'F': 0.0,
'Cl': 0.0,
'Br': 0.0,
'I': 0.0,
'Nd': 0.0,
'Er': 0.0,
'Bi': 0.0,
'Po': 0.0,
'At': 0.0}
```

Ridge Coefficients

In [ ]:
```
ridge_train.best_estimator_['ridge'].coef_
```

Out[ ]:
```
array([ 1.20324413e+00,  2.20346450e+01, -4.03065560e+01, -6.43441155e+00,
        2.42649729e+01, -1.23044395e+01,  2.44146902e+00,  1.41406662e+01,
        2.82145340e+00, -1.17358604e+01, -2.67478182e-01, -1.52923755e+01,
        4.57257803e+00,  1.36616003e+01,  4.82461363e+00, -2.14090017e+00,
        1.44174043e+01,  2.75633752e+01,  8.35245059e+00, -1.94135515e+01,
       -5.49363845e+00, -7.80156981e+00,  7.62310037e+01,  1.66167608e+00,
       -8.25042373e+01, -1.10509209e+01,  1.20629520e+01,  9.62290305e+00,
       -2.47657895e+00, -1.27932472e+01,  1.66552784e+00, -1.12203557e+01,
        1.69822669e+01,  2.17652782e+00, -2.20888804e+00, -1.53948065e+00,
       -2.18476427e+00, -2.68867123e+00, -1.48661728e+00,  3.40379669e+00,
       -1.15082410e+00, -1.77067822e+00,  1.53468318e+01,  4.85220553e+00,
       -1.90720584e+01,  2.83361737e+00, -3.38763584e+00, -1.78942371e+01,
       -3.27595533e+00,  2.09907883e+01, -1.04204233e+01,  1.12556724e+01,
       -2.32438071e+01, -7.31315106e+00,  1.85161509e+01, -1.04081962e+01,
        1.14808700e+01, -2.03651088e+00,  5.05646180e+00, -3.95770684e+00,
        2.77554515e+00, -1.80387481e+00,  2.05960475e+01, -2.70970471e+00,
       -1.41494817e+01,  5.85949490e+00,  8.48953347e-01, -3.19735952e+01,
       -1.12471641e+01,  3.35231118e+01,  3.06675980e+00,  9.49809581e+00,
       -1.39530319e+01, -4.32589850e+00,  9.30282386e+00,  3.07334771e+01,
       -3.60100904e+01,  1.28969008e+01, -2.14515582e+00, -3.13781443e+00,
       -1.15825733e+01, -5.92094514e-01,  0.00000000e+00,  2.72399882e+00,
       -3.70482965e-01, -1.02466061e+00, -6.55805352e-02, -3.35754197e-01,
       -3.19839342e+00,  9.15132226e+00,  0.00000000e+00,  6.87830668e+00,
        4.44699545e-01, -1.30841389e-01, -1.61286838e+00, -1.54644489e+00,
       -1.70765800e+00, -5.04900290e+00,  0.00000000e+00,  9.49594799e+00,
        1.64150126e+00,  8.47822755e-02, -3.66268712e-02,  3.96890356e-02,
       -3.23138798e-01, -6.04680068e-01,  1.13151166e+00, -4.86576010e-01,
       -4.12884952e-01, -1.56897943e+00, -1.09542386e-01,  3.92842832e-01,
       -1.05760881e+00, -1.73041629e+00, -9.26657745e-01,  1.22348715e+00,
        0.00000000e+00,  9.88329567e+00,  2.99842115e-01, -3.07663866e-01,
        8.76579365e-03,  8.76317644e-02,  1.27955887e-01,  1.99791138e+00,
        3.08501245e-01, -5.66833737e-02,  5.24874917e-02, -1.08189756e+01,
       -1.31058436e+01,  1.15653445e+00, -7.30836442e-02, -1.80117700e-01,
        7.62693657e-01,  7.50936751e+00,  0.00000000e+00,  7.14703854e+00,
        1.16600744e+01, -2.16017250e-02, -2.44367723e+00, -5.23680313e-02,
       -1.98780854e+00,  0.00000000e+00,  3.35297412e-02, -1.92495212e+00,
       -7.09207660e-01,  1.65958931e+00,  5.32793106e+00,  2.86817339e+00,
        2.19810018e+00,  1.80804633e-02,  2.19567468e+00,  3.88613319e+00,
       -5.20957163e-01, -8.61567810e-02,  6.49733832e-01, -9.20539523e-02,
        1.27131574e+00,  1.20267673e-01,  3.97914357e+00, -4.58660680e-01,
        5.78202763e+00,  5.09142213e+00,  1.78190081e+00,  5.49509654e+00,
        0.00000000e+00,  0.00000000e+00,  0.00000000e+00])
```

In [ ]:
```
ridge_weights = {df.columns[key]:abs(value) for key, value in enumerate(ridg
dict(sorted(ridge_weights.items(), key=lambda item: item[1], reverse=True))
```

Out[ ]:
```
{'wtd_gmean_atomic_radius': 82.50423733510665,
 'wtd_mean_atomic_radius': 76.23100370069614,
 'wtd_mean_atomic_mass': 40.30655598944086,
 'wtd_entropy_Valence': 36.010090382187286,
 'std_ThermalConductivity': 33.52311183863332,
 'range_ThermalConductivity': 31.973595153364414,
 'entropy_Valence': 30.733477135522136,
 'range_fie': 27.563375166707345,
 'wtd_gmean_atomic_mass': 24.26497287703653,
 'wtd_mean_FusionHeat': 23.24380714242241,
 'mean_atomic_mass': 22.03464500407608,
```

```
'std_ElectronAffinity': 20.9907882840034,
'wtd_mean_ThermalConductivity': 20.596047543511407,
'std_fie': 19.413551483808554,
'wtd_gmean_ElectronAffinity': 19.07205841254293,
'wtd_gmean_FusionHeat': 18.516150931227177,
'range_ElectronAffinity': 17.894237113706332,
'wtd_mean_Density': 16.982266859423316,
'wtd_mean_ElectronAffinity': 15.346831797066539,
'mean_fie': 15.292375456462747,
'wtd_entropy_fie': 14.417404282907794,
'wtd_gmean_ThermalConductivity': 14.149481717128543,
'range_atomic_mass': 14.140666241169422,
'wtd_mean_Valence': 13.953031890072314,
'gmean_fie': 13.661600275605622,
'Ag': 13.105843630481445,
'range_Valence': 12.896900802682287,
'std_atomic_radius': 12.793247170520273,
'entropy_atomic_mass': 12.304439463852427,
'wtd_entropy_atomic_radius': 12.062951965890003,
'std_atomic_mass': 11.735860413275395,
'Cs': 11.6600744382917,
'wtd_std_Valence': 11.582573279653054,
'wtd_entropy_FusionHeat': 11.480869992011158,
'mean_FusionHeat': 11.255672400613115,
'wtd_range_ThermalConductivity': 11.247164099420255,
'mean_Density': 11.22035571751498,
'entropy_atomic_radius': 11.050920938098947,
'Pd': 10.818975577499792,
'wtd_std_ElectronAffinity': 10.420423262643894,
'entropy_FusionHeat': 10.408196159105955,
'Kr': 9.883295671758162,
'range_atomic_radius': 9.622903050655621,
'mean_Valence': 9.498095813038935,
'Ar': 9.495947985901113,
'wtd_gmean_Valence': 9.30282385733451,
'O': 9.151322262798242,
'wtd_range_fie': 8.352450586707699,
'mean_atomic_radius': 7.801569810205453,
'Te': 7.509367514891667,
'gmean_FusionHeat': 7.313151063543804,
'Xe': 7.147038543619432,
'Ne': 6.878306683019584,
'gmean_atomic_mass': 6.434411547223428,
'entropy_ThermalConductivity': 5.859494902934971,
'Au': 5.7820276277569915,
'Pb': 5.495096544551145,
'wtd_std_fie': 5.493638453572816,
'Tb': 5.3279310575015355,
'Hg': 5.091422127436061,
'wtd_range_FusionHeat': 5.056461796068855,
'S': 5.0490029024770955,
'gmean_ElectronAffinity': 4.852205532799202,
'wtd_gmean_fie': 4.824613626594694,
'wtd_mean_fie': 4.572578033628301,
'gmean_Valence': 4.325898500560551,
'Ir': 3.9791435693446893,
'std_FusionHeat': 3.957706838806994,
```

```
'Yb': 3.886133185279942,
'std_Density': 3.403796691747466,
'wtd_entropy_ElectronAffinity': 3.3876358417785863,
'wtd_range_ElectronAffinity': 3.2759553278455487,
'N': 3.1983934169938997,
'std_Valence': 3.137814432358151,
'wtd_std_ThermalConductivity': 3.066759795578775,
'Dy': 2.8681733896871577,
'entropy_ElectronAffinity': 2.83361737034622,
'wtd_range_atomic_mass': 2.8214534021231765,
'wtd_std_FusionHeat': 2.775545145152581,
'He': 2.7239988209679544,
'gmean_ThermalConductivity': 2.7097047060217156,
'range_Density': 2.688671229516349,
'wtd_range_atomic_radius': 2.476578947198765,
'La': 2.44367722887337,
'wtd_entropy_atomic_mass': 2.441469015768297,
'wtd_gmean_Density': 2.2088880386686385,
'Ho': 2.198100184514838,
'Tm': 2.1956746756273757,
'wtd_entropy_Density': 2.18476426849969,
'gmean_Density': 2.176527815541163,
'wtd_range_Valence': 2.1451558154296495,
'entropy_fie': 2.1409001732245008,
'range_FusionHeat': 2.0365108825989995,
'Mo': 1.9979113762295582,
'Pr': 1.9878085390622042,
'Sm': 1.9249521213067178,
'mean_ThermalConductivity': 1.8038748071839,
'Tl': 1.7819008083846928,
'mean_ElectronAffinity': 1.770678224956746,
'Ge': 1.7304162929630587,
'P': 1.7076580005004118,
'wtd_std_atomic_radius': 1.665527837265629,
'gmean_atomic_radius': 1.661676080697901,
'Gd': 1.6595893067067595,
'K': 1.641501256750352,
'Al': 1.6128683757915894,
'Ni': 1.5689794280307592,
'Si': 1.5464448895433245,
'entropy_Density': 1.5394806548454576,
'wtd_range_Density': 1.4866172764681747,
'Re': 1.2713157378617894,
'Se': 1.2234871458145533,
'number_of_elements': 1.2032441290584106,
'Cd': 1.1565344516443263,
'wtd_std_Density': 1.1508241026344765,
'Mn': 1.131511662090882,
'Ga': 1.0576088138978954,
'Be': 1.0246606126999513,
'As': 0.9266577450597306,
'wtd_entropy_ThermalConductivity': 0.8489533472971035,
'Sb': 0.7626936574273563,
'Eu': 0.7092076601274739,
'Ta': 0.6497338324638403,
'Cr': 0.6046800680790798,
'critical_temp': 0.5920945136520607,
```

'Lu': 0.5209571626836677,
'Fe': 0.4865760097630898,
'Pt': 0.4586606798933014,
'Na': 0.4446995452341047,
'Co': 0.41288495225960375,
'Zn': 0.39284283160655326,
'Li': 0.37048296493134236,
'C': 0.33575419739723905,
'V': 0.3231387979596321,
'Tc': 0.3085012451591725,
'Sr': 0.3076638659470038,
'Rb': 0.29984211474783373,
'wtd_std_atomic_mass': 0.26747818172496235,
'Sn': 0.18011769958809024,
'Mg': 0.1308413892168927,
'Nb': 0.1279558868584092,
'Os': 0.12026767318856164,
'Cu': 0.10954238558510367,
'W': 0.09205395231182723,
'Zr': 0.08763176437368028,
'Hf': 0.08615678102718098,
'Ca': 0.08478227548101774,
'In': 0.07308364419531818,
'B': 0.06558053522385868,
'Ru': 0.056683373705555276,
'Rh': 0.05248749168577969,
'Ce': 0.05236803128972188,
'Ti': 0.039689035605733836,
'Sc': 0.03662687117883952,
'Pm': 0.033529741194744334,
'Ba': 0.02160172499564086,
'Er': 0.018080463299312347,
'Y': 0.00876579364589835,
'H': 0.0,
'F': 0.0,
'Cl': 0.0,
'Br': 0.0,
'I': 0.0,
'Nd': 0.0,
'Bi': 0.0,
'Po': 0.0,
'At': 0.0}