Superconductivity Materials and Critical Temperature

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In [101…
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
import itertools
```

In [102…
```
# Import dataset. Critical temperature unit: K
dataset = pd.read_csv('train.csv')        # Main feature dataset
formula = pd.read_csv('unique_m.csv')     # Formula of materials.
```

In [103…
```
dataset.describe()
```

Out[103]:

	number_of_elements	mean_atomic_mass	wtd_mean_atomic_mass	gmean_atomic_mass	wtd_gmean_atomic_m
count	21263.000000	21263.000000	21263.000000	21263.000000	21263.00
mean	4.115224	87.557631	72.988310	71.290627	58.53
std	1.439295	29.676497	33.490406	31.030272	36.65
min	1.000000	6.941000	6.423452	5.320573	1.96
25%	3.000000	72.458076	52.143839	58.041225	35.24
50%	4.000000	84.922750	60.696571	66.361592	39.91
75%	5.000000	100.404410	86.103540	78.116681	73.11
max	9.000000	208.980400	208.980400	208.980400	208.98

8 rows × 82 columns

In [104…
```
formula.describe()
```

Out[104]:

	H	He	Li	Be	B	C	N	O
count	21263.000000	21263.0	21263.000000	21263.000000	21263.000000	21263.000000	21263.000000	21263.000000
mean	0.017685	0.0	0.012125	0.034638	0.142594	0.384968	0.013284	3.009129
std	0.267220	0.0	0.129552	0.848541	1.044486	4.408032	0.150427	3.811649
min	0.000000	0.0	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
25%	0.000000	0.0	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
50%	0.000000	0.0	0.000000	0.000000	0.000000	0.000000	0.000000	1.000000
75%	0.000000	0.0	0.000000	0.000000	0.000000	0.000000	0.000000	6.800000
max	14.000000	0.0	3.000000	40.000000	105.000000	120.000000	12.800000	66.000000

8 rows × 87 columns

Check if the two datsets have same number of cases.

In [105…
```
dataset.shape[0] == formula.shape[0]
```

Out[105]:
```
True
```

In [106…
```
dataset.columns
```

Out[106]:
```
Index(['number_of_elements', 'mean_atomic_mass', 'wtd_mean_atomic_mass',
       'gmean_atomic_mass', 'wtd_gmean_atomic_mass', 'entropy_atomic_mass',
       'wtd_entropy_atomic_mass', 'range_atomic_mass', 'wtd_range_atomic_mass',
       'std_atomic_mass', 'wtd_std_atomic_mass', 'mean_fie', 'wtd_mean_fie',
       'gmean_fie', 'wtd_gmean_fie', 'entropy_fie', 'wtd_entropy_fie',
       'range_fie', 'wtd_range_fie', 'std_fie', 'wtd_std_fie',
       'mean_atomic_radius', 'wtd_mean_atomic_radius', 'gmean_atomic_radius',
       'wtd_gmean_atomic_radius', 'entropy_atomic_radius',
       'wtd_entropy_atomic_radius', 'range_atomic_radius',
       'wtd_range_atomic_radius', 'std_atomic_radius', 'wtd_std_atomic_radius',
       'mean_Density', 'wtd_mean_Density', 'gmean_Density',
       'wtd_gmean_Density', 'entropy_Density', 'wtd_entropy_Density',
       'range_Density', 'wtd_range_Density', 'std_Density', 'wtd_std_Density',
       'mean_ElectronAffinity', 'wtd_mean_ElectronAffinity',
       'gmean_ElectronAffinity', 'wtd_gmean_ElectronAffinity',
       'entropy_ElectronAffinity', 'wtd_entropy_ElectronAffinity',
       'range_ElectronAffinity', 'wtd_range_ElectronAffinity',
       'std_ElectronAffinity', 'wtd_std_ElectronAffinity', 'mean_FusionHeat',
       'wtd_mean_FusionHeat', 'gmean_FusionHeat', 'wtd_gmean_FusionHeat',
       'entropy_FusionHeat', 'wtd_entropy_FusionHeat', 'range_FusionHeat',
       'wtd_range_FusionHeat', 'std_FusionHeat', 'wtd_std_FusionHeat',
       'mean_ThermalConductivity', 'wtd_mean_ThermalConductivity',
       'gmean_ThermalConductivity', 'wtd_gmean_ThermalConductivity',
       'entropy_ThermalConductivity', 'wtd_entropy_ThermalConductivity',
       'range_ThermalConductivity', 'wtd_range_ThermalConductivity',
       'std_ThermalConductivity', 'wtd_std_ThermalConductivity',
       'mean_Valence', 'wtd_mean_Valence', 'gmean_Valence',
       'wtd_gmean_Valence', 'entropy_Valence', 'wtd_entropy_Valence',
       'range_Valence', 'wtd_range_Valence', 'std_Valence', 'wtd_std_Valence',
       'critical_temp'],
      dtype='object')
```

In [107…
```
dataset.dtypes
```

Out[107]:
```
number_of_elements         int64
mean_atomic_mass         float64
wtd_mean_atomic_mass     float64
gmean_atomic_mass        float64
wtd_gmean_atomic_mass    float64
                          ...
range_Valence              int64
wtd_range_Valence        float64
std_Valence              float64
wtd_std_Valence          float64
critical_temp            float64
Length: 82, dtype: object
```

Save basic info into csv file

In [108…
```
dataset_summary = {
    'Ind': list(range(dataset.shape[1])),
    'Column Name': dataset.columns,
    'Data Type': dataset.dtypes}
d_summary = pd.DataFrame(data = dataset_summary)
d_summary.head()
```

```
# d_summary.to_csv('ColumnSummary.csv',index=False)
```

Out[108]:

	Ind	Column Name	Data Type
number_of_elements	0	number_of_elements	int64
mean_atomic_mass	1	mean_atomic_mass	float64
wtd_mean_atomic_mass	2	wtd_mean_atomic_mass	float64
gmean_atomic_mass	3	gmean_atomic_mass	float64
wtd_gmean_atomic_mass	4	wtd_gmean_atomic_mass	float64

EDA

1. Check null values for each column. No null values exist in the given dataset.
2. Check if the target variable ['critical_temp'] has a patterned distribution.
3. Explore the similarity between columns with similiar functions.
4. Check if multi-collinearity exists.

In [109…

```
null_list = {}
for i in dataset.columns:
    null_list[i] = dataset[i].isnull().sum()
    if null_list[i] != 0:
        print(null_list[i])
```

In [110…

```
element = formula.columns
element
```

Out[110]:

```
Index(['H', 'He', 'Li', 'Be', 'B', 'C', 'N', 'O', 'F', 'Ne', 'Na', 'Mg', 'Al',
       'Si', 'P', 'S', 'Cl', 'Ar', 'K', 'Ca', 'Sc', 'Ti', 'V', 'Cr', 'Mn',
       'Fe', 'Co', 'Ni', 'Cu', 'Zn', 'Ga', 'Ge', 'As', 'Se', 'Br', 'Kr', 'Rb',
       'Sr', 'Y', 'Zr', 'Nb', 'Mo', 'Tc', 'Ru', 'Rh', 'Pd', 'Ag', 'Cd', 'In',
       'Sn', 'Sb', 'Te', 'I', 'Xe', 'Cs', 'Ba', 'La', 'Ce', 'Pr', 'Nd', 'Pm',
       'Sm', 'Eu', 'Gd', 'Tb', 'Dy', 'Ho', 'Er', 'Tm', 'Yb', 'Lu', 'Hf', 'Ta',
       'W', 'Re', 'Os', 'Ir', 'Pt', 'Au', 'Hg', 'Tl', 'Pb', 'Bi', 'Po', 'At',
       'Rn', 'critical_temp', 'material'],
      dtype='object')
```

In [111…

```
y = dataset["critical_temp"]
x = dataset.iloc[:,0:dataset.shape[1]-1]
x.shape
```

Out[111]:

```
(21263, 81)
```

Check if key variables are normally distributed.

Following figures shows that the values are not normally distributed, especially for critical temperature. Most of the critical temperature (Y) are low to almost 0K, which is the absolute temperature. As we are looking for the high critical temperature opportunities, we will focus on high critical temperature examples.

In [112…

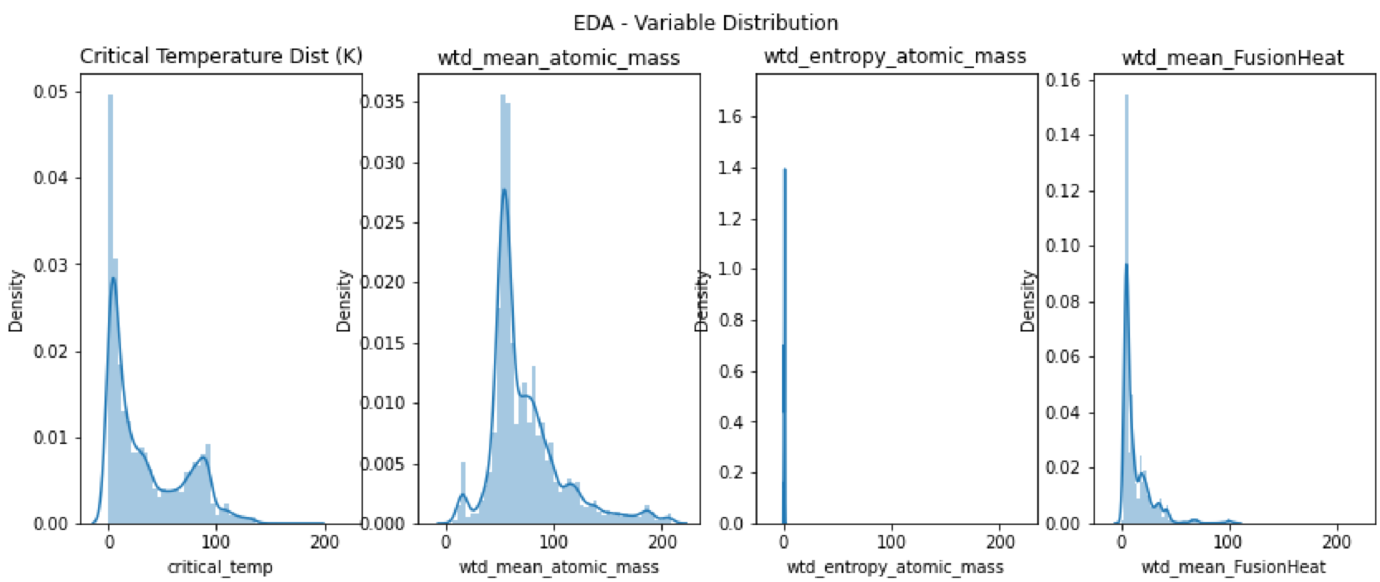
```
fig, axes = plt.subplots(1, 4, sharex=True, figsize=(14,5))
fig.suptitle('EDA - Variable Distribution')

sns.distplot(ax=axes[0],a=y)
axes[0].set_title("Critical Temperature Dist (K)")
sns.distplot(ax=axes[1],a=x['wtd_mean_atomic_mass'])
axes[1].set_title("wtd_mean_atomic_mass")
sns.distplot(ax=axes[2],a=x['wtd_entropy_atomic_mass'])
```

```
axes[2].set_title("wtd_entropy_atomic_mass")
sns.distplot(ax=axes[3],a=x['wtd_mean_FusionHeat'])
axes[3].set_title("wtd_mean_FusionHeat")
```

```
c:\Users\youyu\AppData\Local\Programs\Python\Python38\lib\site-packages\seaborn\distributions.py:2619: FutureWarning: `distplot` is a deprecated function and will be removed in a future version. Please adapt your code to use either `displot` (a figure-level function with similar flexibility) or `histplot` (an axes-level function for histograms).
  warnings.warn(msg, FutureWarning)
c:\Users\youyu\AppData\Local\Programs\Python\Python38\lib\site-packages\seaborn\distributions.py:2619: FutureWarning: `distplot` is a deprecated function and will be removed in a future version. Please adapt your code to use either `displot` (a figure-level function with similar flexibility) or `histplot` (an axes-level function for histograms).
  warnings.warn(msg, FutureWarning)
c:\Users\youyu\AppData\Local\Programs\Python\Python38\lib\site-packages\seaborn\distributions.py:2619: FutureWarning: `distplot` is a deprecated function and will be removed in a future version. Please adapt your code to use either `displot` (a figure-level function with similar flexibility) or `histplot` (an axes-level function for histograms).
  warnings.warn(msg, FutureWarning)
c:\Users\youyu\AppData\Local\Programs\Python\Python38\lib\site-packages\seaborn\distributions.py:2619: FutureWarning: `distplot` is a deprecated function and will be removed in a future version. Please adapt your code to use either `displot` (a figure-level function with similar flexibility) or `histplot` (an axes-level function for histograms).
  warnings.warn(msg, FutureWarning)
```

Out[112]:

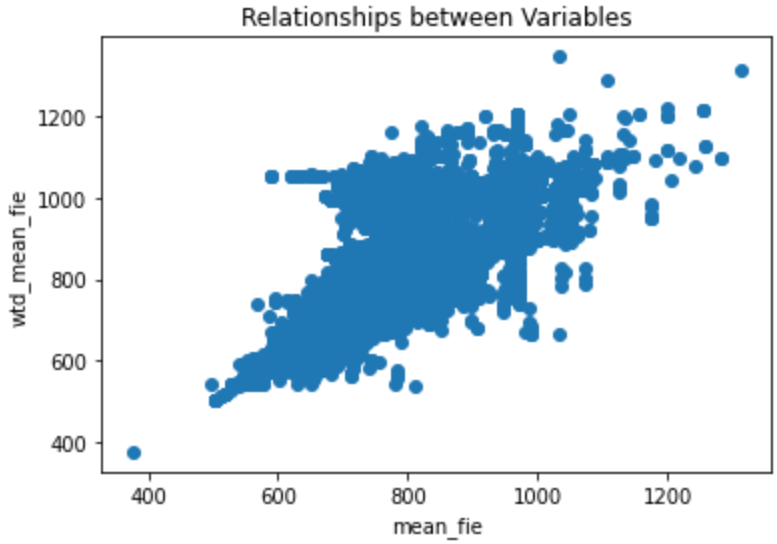
```
Text(0.5, 1.0, 'wtd_mean_FusionHeat')
```



Although the column names looks alike, the values are not 100% linearly related. Following figures indicated the differences between similiar features.

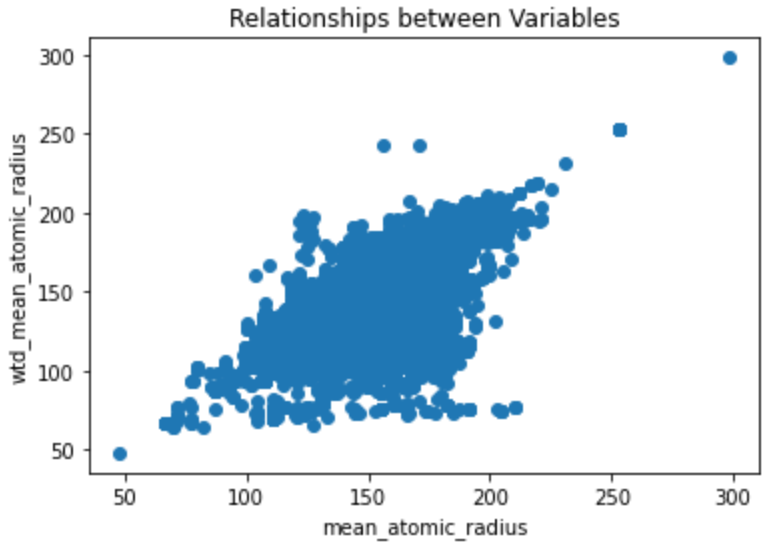
In [113…

```
plt.scatter(x['mean_fie'],x['wtd_mean_fie'])
plt.title('Relationships between Variables')
plt.xlabel('mean_fie')
plt.ylabel('wtd_mean_fie')
plt.show()
```



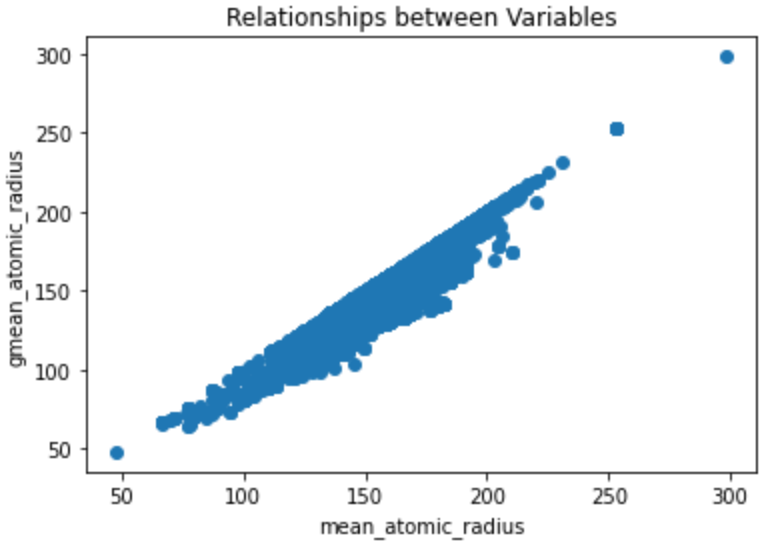
In [114…

```
plt.scatter(x['mean_atomic_radius'],x['wtd_mean_atomic_radius'])
plt.title('Relationships between Variables')
plt.xlabel('mean_atomic_radius')
plt.ylabel('wtd_mean_atomic_radius')
plt.show()
```



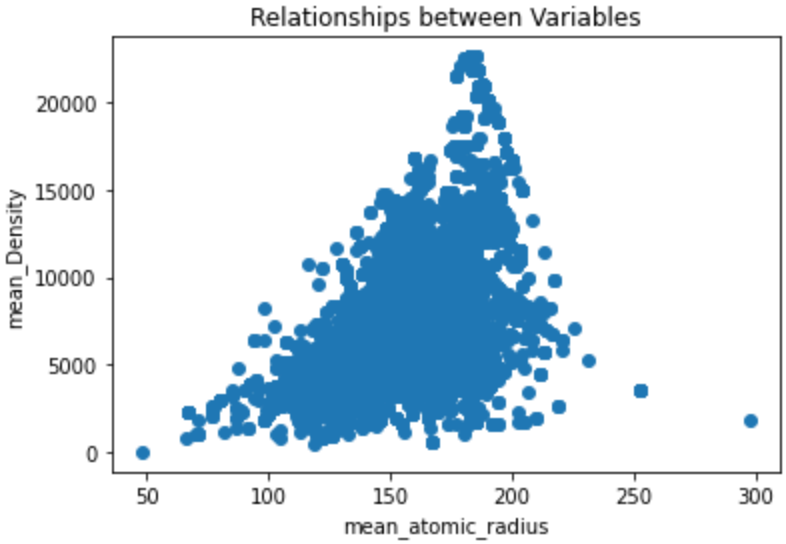
In [115…

```
plt.scatter(x['mean_atomic_radius'],x['gmean_atomic_radius'])
plt.title('Relationships between Variables')
plt.xlabel('mean_atomic_radius')
plt.ylabel('gmean_atomic_radius')
plt.show()
```



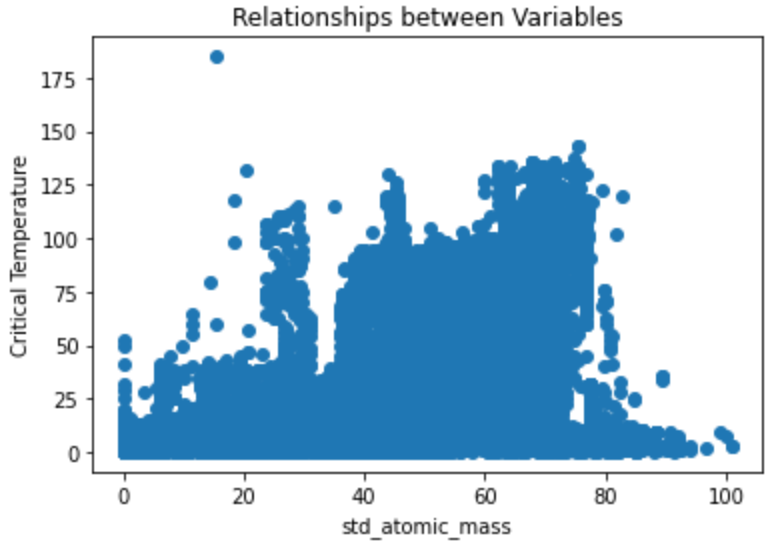
The atomic radius and density relationship is illustrated below. For smaller atoms, the radius and density are positive related. Meanwhile for larger atoms, the radius and density form a negative relationship. And the highest density atoms usually has atomic radius around 180.

In [116…
```
plt.scatter(x['mean_atomic_radius'],x['mean_Density'])
plt.title('Relationships between Variables')
plt.xlabel('mean_atomic_radius')
plt.ylabel('mean_Density')
plt.show()
```

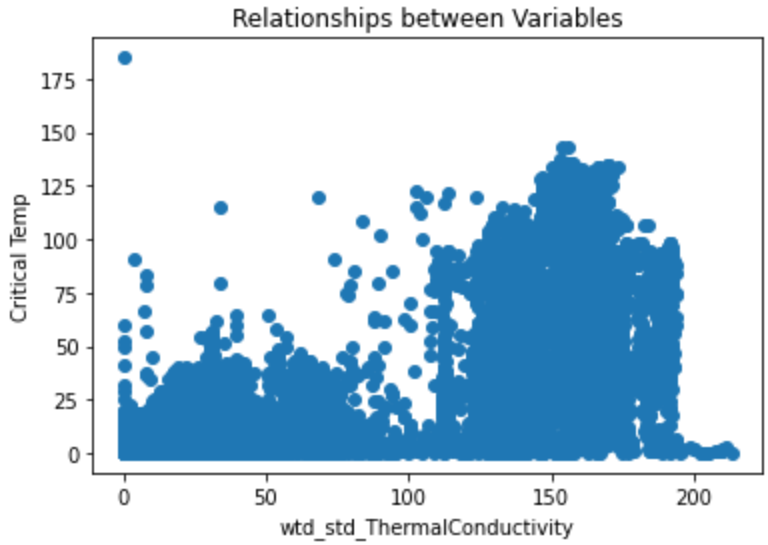


The standard deviation of atomic mass and critical temperature (Y) do not have any obvious relationship.

In [117…
```
plt.scatter(x['std_atomic_mass'],y)
plt.title('Relationships between Variables')
plt.xlabel('std_atomic_mass')
plt.ylabel('Critical Temperature')
plt.show()
```

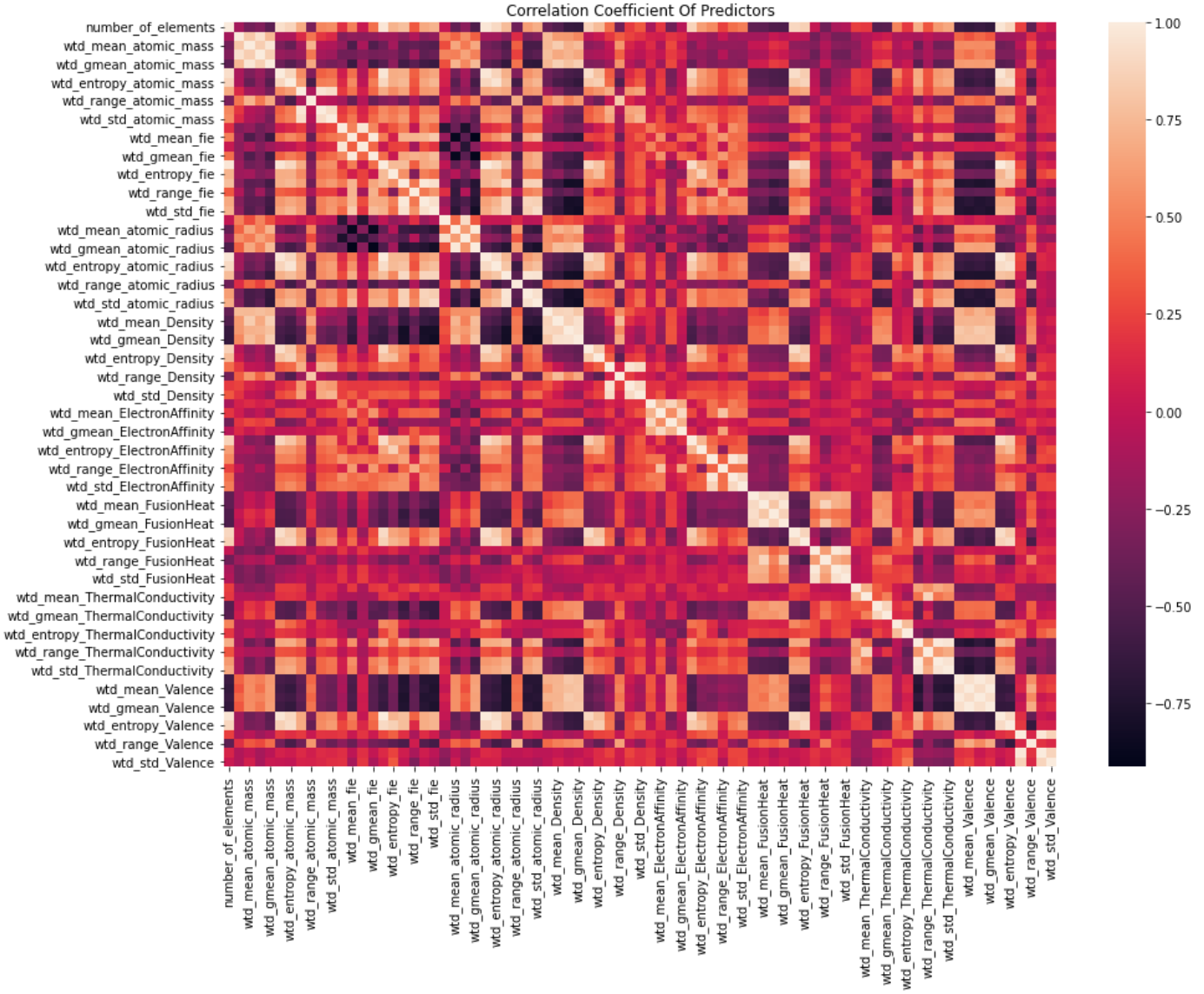


In [118…
```
plt.scatter(x['wtd_std_ThermalConductivity'],y)
plt.title('Relationships between Variables')
plt.xlabel('wtd_std_ThermalConductivity')
plt.ylabel('Critical Temp')
plt.show()
```



The plot above indicated that the critical temperature (Y) is not normally distributed.

In [119…
```
plt.figure(figsize=(15,11))
sns.heatmap(x.corr())
plt.title('Correlation Coefficient Of Predictors')
plt.show()
```



From the plot above we can see that some of the variables are linearly correlated. Those repetitive columns do not need to be removed because they will not affect the modeling part.

In [120…
```
# Feature selection (basic)
from sklearn.feature_selection import SelectFromModel
```

In [121…
```
# Add penalty part for linear regression, ridge and lasso.
# Thos class would be called inside the linear regression.
class Linear:
    def __init__(self, alpha):
        self.a = alpha
    def cost(self,w):
        return 0
    def derivation(self, w):
        return 0

class RidgePenalty:
    """
    This class defines ridge regression penalty, which make it different than lasso.
    """
    def __init__(self, alpha):
        self.a = alpha
    def cost(self, w):
        return self.a*np.sum(np.square(w))
    def derivation(self, w):
        return 2*self.a*w
```

```python
class LassoPenalty:
    """
    This class defines lasso regression penalty.
    """
    def __init__(self, alpha):
        self.a = alpha
    def cost(self,w):
        return self.a*np.sum(np.abs(w))
    def derivation(self, w):
        return self.a*np.sign(w)
```

In [122…

```python
class LinearRegression():
    """
    Suggestion: scaling x before train.
    This class is used for multivariate linear regression.
    """
    def __init__(self,x:pd.DataFrame,y:pd.Series,
                 lr:float,epo:int, alpha:float =0,
                 regulation=Linear):
        self.x = x
        self.y = y
        self.w = np.zeros(x.shape[1])
        self.b = 0
        self.lr = lr
        self.epo = epo
        self.alpha = alpha
        self.regularization = regulation

    def loss_function(self):
        loss = 0
        n = len(self.y)
        for i in range(n):
            loss += (self.y[i]-(np.dot(self.w,self.x.iloc[i])+self.b))**2
        return loss/2/float(n)

    def gradient_descend(self):
        z = self.x.dot(self.w) + self.b
        loss = z - self.y

        weight_gradient = self.x.T.dot(loss) / len(self.y)
        bias_gradient = np.sum(loss) / len(self.y)
        # Ridge or lasso will add this part
        # reg = self.regularization(alpha=self.alpha)
        # weight_gradient = self.x.T.dot(loss) / len(self.y)+reg.derivation(self.w)

        self.w = np.array(self.w - self.lr*weight_gradient)
        self.b = self.b - self.lr*bias_gradient
        return self.w, self.b

    def train(self):
        """
        w: input slope trial starting point
        b: input intersect trial starting point
        learning rate: suggested from 0.001 to 0.05
        epochs: suggested larger than 100
        """
        cost_list = [0] * self.epo
        for epoch in range(self.epo):
            self.w, self.b = self.gradient_descend()
            cost = self.loss_function(self.x, self.y, self.w, self.b)
            cost_list[epoch] = cost
            if (epoch%(self.epo/5)==0):
                print("Cost at epoch",epoch,"is:",cost)
        print(f"w = {self.w}, b = {self.b}")
```

```
        return self.w, self.b, cost_list

    def predict(self):
        return np.dot(self.x,self.w) + self.b
```

In [123…
```
# p =LinearRegression(x,y,lr=0.01,epo=3)
# y_pred_test = p.predict(x_test, w, b)
# cost_test = (y_test-y_pred_test)**2
# prediction = pd.DataFrame({"Y": y_test, "Y_predict": y_pred_test,"cost":cost_test})
```

In [124…
```
# rmse1 = np.sqrt(sum(cost_test)/len(cost_test))
# r2_1 = 1-sum(cost_test)/sum((y_test-sum(y_test)/len(y_test))**2)
# rmse_r2_summary = pd.DataFrame({'Method':['1','2'],
#                                 'RMSE':[rmse1,rmse2],
#                                 'R2 score':[r2_1,r2_2]})
# rmse_r2_summary
```

Find Subset And Feature Selection

In [125…
```
q1 = LinearRegression()

def processSubset(x,y,feature_set,learningrate,epochs):
    # Select features
    x = x[list(feature_set)]
    w, b, cost_list= q1.train(x, y, np.zeros(x.shape[1]), 0, learningrate=learningrate,e
    # regr = model.train()
    predict = q1.predict(x=x, w=w, b=b)
    rss = ((predict-y)**2).sum()
    return {"w":w,"b":b, "RSS":rss}

def getBest(k,x,y,epo):
    results = []
    combo_list = []
    for combo in itertools.combinations(x.columns, k):
        results.append(processSubset(x=x,y=y,feature_set=combo,learningrate=0.01,epochs=
        combo_list.append(combo)
    # Wrap everything up in a nice dataframe
    models = pd.DataFrame(results)
    models['Combo'] = combo_list
    # Choose the model with the highest RSS
    best_model = models.loc[models['RSS'].argmin()]
    #print("Processed", models.shape[0], "models on", k)
    # Return the best model, along with some other useful information about the model
    return best_model
```

```
---------------------------------------------------------------------------
TypeError                                 Traceback (most recent call last)
~\AppData\Local\Temp/ipykernel_28816/382791111.py in <module>
----> 1 q1 = LinearRegression()
      2
      3 def processSubset(x,y,feature_set,learningrate,epochs):
      4     # Select features
      5     x = x[list(feature_set)]

TypeError: __init__() missing 4 required positional arguments: 'x', 'y', 'lr', and 'epo'
```

In [ ]:
```
# models_best = pd.DataFrame(columns=["w", "b","RSS","Combo"])
# for i in range(1,7):
#     models_best.loc[i] = getBest(i,x,y,epo=250)
```

In [ ]:
```
def forward(x,y,predictors, lr, epo):
    # Pull out predictors we still need to process
    remaining_predictors = [p for p in x.columns if p not in predictors]
```

```
    results = []
    combo_list = []

    for p in remaining_predictors:
        results.append(processSubset(x,y,predictors+[p], learningrate=lr, epochs=epo))
        combo_list.append(predictors+[p])

    # # Wrap everything up in a nice dataframe
    models = pd.DataFrame(results)
    models['Predictors'] = combo_list

    # # Choose the model with the highest RSS
    best_model = models.loc[models['RSS'].argmin()]

    # Return the best model, along with some other useful information about the model
    return best_model

def backward(x,y,predictors,lr,epo):
    results = []
    combo_list = []

    for combo in itertools.combinations(predictors, len(predictors)-1):
        results.append(processSubset(x,y,combo,learningrate=lr, epochs=epo))
        combo_list.append(combo)

    # Wrap everything up in a nice dataframe
    models = pd.DataFrame(results)
    models['Predictors'] = combo_list
    # Choose the model with the highest RSS
    best_model = models.loc[models['RSS'].argmin()]

    # Return the best model, along with some other useful information about the model
    return best_model
```

In [ ]:

```
# models_fwd = pd.DataFrame(columns=["w", "b","RSS","Predictors"])
# predictors = []

# for i in range(1,len(features_order)):
#     predictors = features_order[0:i]
#     models_fwd.loc[i] = forward(x,y,predictors,lr=0.01,epo=250)

# models_fwd

# models_bwd = pd.DataFrame(columns=["w", "b","RSS","Predictors"], index = range(1,len(x
# features_order = ['SqFt','Bathrooms','Neighborhood','Brick','Bedrooms','Offers']

# while(len(features_order) > 0):
#     models_bwd.loc[len(features_order)] = backward(x,y,features_order,lr=0.01,epo=250)
#     features_order.pop()

# models_bwd
```