Predicting Heat Capacity using ML

In [1]:
```
import os
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from sklearn.model_selection import train_test_split
from sklearn.model_selection import KFold
from collections import OrderedDict
```

In [35]:
```
data = pd.read_csv('downloads/cp_data_cleaned.csv')
```

In [36]:
```
data.head()
```

Out[36]:

	formula	T	Cp
0	B2O3	1400.0	134.306
1	B2O3	1300.0	131.294
2	B2O3	1200.0	128.072
3	B2O3	1100.0	124.516
4	B2O3	1000.0	120.625

In [37]:
```
data.shape
```

Out[37]:
```
(4547, 3)
```

Separate into input and target variables

In [38]:
```
x = data[['formula', 'T']]
y = data['Cp']
```

In [39]:
```
x.shape
```

Out[39]:
```
(4547, 2)
```

In [40]:
```
y.shape
```

Out[40]:
```
(4547,)
```

Separate data into test and train data, make sure that each formula appears ONLY in test, train, or validation

In [41]:
```
uniqueFormula = x['formula'].unique()
numUnique = len(uniqueFormula)
print(numUnique,uniqueFormula)
```

```
244 ['B2O3' 'Be1I2' 'Be1F3Li1' 'Al1Cl4K1' 'Al2Be1O4' 'B2H4O4' 'B2Mg1' 'Be1F2'
 'B1H4Na1' 'Br2Ca1' 'Al1N1' 'Al1Cl6Na3' 'Ba1H2O2' 'Al1Br3' 'Br3Zr1'
 'Br2Ti1' 'B1Ti1' 'Be2O4Si1' 'Br2Pb1' 'Al1' 'Br2Hg2' 'B1H3O3' 'Br3Ti1'
 'C1Cu1N1' 'B1' 'Al1F6Na3' 'Ca1H2O2' 'B2Be3O6' 'Al1Cl4Na1' 'Al1Cl6K3'
 'C0.98Nb1' 'Br2Hg1' 'Al1Cl1O1' 'Cl1H4N1O4' 'Be1F4Li2' 'C1Mg1O3' 'Br1H4N1'
 'Ca1I2' 'Al1F6Li3' 'Br4Mo1' 'Ba1' 'Br4Ti1' 'Ba1Br2' 'Be1O4S1' 'Ba1F2'
 'Ba1I2' 'Cl2Fe1' 'C1K1N1' 'Be1H2O2' 'Cs1' 'Al1H4Li1' 'C1Be2' 'Cr1'
 'Cs2O4S1' 'Cl1Cu1' 'Cu1F2' 'Al2O3' 'B1N1' 'Co1O4S1' 'Cu1O1' 'Br1Na1'
 'Cr2O3' 'Cs1F1' 'Cr2N1' 'Cl1Li1' 'Fe0.877S1' 'Cl1Na1' 'F2Hg1' 'Fe1H2O2'
 'Cs1H1O1' 'Br3Mo1' 'Br2Sr1' 'Cl2Hg2' 'Fe1O1' 'Co1' 'Cl1Cs1' 'Cu1H2O2'
 'Al1Li1O2' 'Co1F2' 'Br2Fe1' 'Fe1I2' 'Ga1' 'Cl1Li1O4' 'Cl2Cu1' 'Fe0.947O1'
 'Be1Cl2' 'Cl1K1' 'F1Na1' 'H3O4P1' 'Fe3O4' 'H1Na1O1' 'Fe2O12S3' 'H1Na1'
 'Cl1Na1O4' 'B1F4K1' 'Cu1O4S1' 'H1Li1' 'F2H1K1' 'B1H4Li1' 'Hg1O1' 'Be3N2'
 'Fe1' 'I2Mo1' 'Cu1F1' 'Cr1N1' 'Fe1H3O3' 'I1Li1' 'Al1I3' 'Fe1S1'
 'Al2Cl9K3' 'I2Pb1' 'I4Zr1' 'Hg1I2' 'H4I1N1' 'Hf1' 'F2Hg2' 'I2Sr1'
 'C1K2O3' 'C1N1Na1' 'H2O4W1' 'Ca1S1' 'K2O4S1' 'I2Mg1' 'Mg1O3Si1' 'Li3N1'
 'I2Zr1' 'H2Mg1' 'I2Ti1' 'H1K1' 'Mg1O4W1' 'I4Ti1' 'H1K1O1' 'I2' 'Mn1'
 'F1K1' 'Li2O3Si1' 'K2O1' 'Mg1O4S1' 'Al1Na1O2' 'Mo1O2.889' 'Mo1O2.750'
 'N0.465V1' 'Mg2O4Ti1' 'K1O2' 'Mo1O3' 'C1Na2O3' 'K2S1' 'Mo1S2' 'Li2O3Ti1'
 'I4Mo1' 'Ba1S1' 'Na2O3Si1' 'I3Mo1' 'Mg1S1' 'Cu2O5S1' 'K2O2' 'Mg1O3Ti1'
 'Na2S2' 'I3Ti1' 'Li2O2' 'I3Zr1' 'Al2Mg1O4' 'N1Ti1' 'N1V1' 'Na1O2' 'Ni1S1'
 'Na2O1' 'I4Si1' 'B1Li1O2' 'O1Ti1' 'H1Li1O1' 'Nb1O1' 'F2Mg1' 'Nb1' 'O3Ti2'
 'Ca1' 'Nb1O2' 'O3Pb1Si1' 'O4Pb3' 'O3W1' 'O7Ti4' 'K1' 'O4V2' 'O2.90W1'
 'Ca1Cl2' 'Pb1' 'Na2O5Si2' 'O5Ti3' 'O5V2' 'Mg3N2' 'Mg2O4Si1' 'Mo1O2.875'
 'Br1K1' 'Br2Mo1' 'Cl1H4N1' 'Cu1' 'F1Li1' 'Fe1S2' 'H2O2Sr1' 'I1K1' 'I1Na1'
 'K2O3Si1' 'Li2O4S1' 'Li2O5Si2' 'Mg1' 'Mg2Si1' 'Mo2S3' 'N1Zr1' 'N2O4'
 'N4Si3' 'N5P3' 'Na2O2' 'Na2S1' 'Nb2O5' 'Ni1' 'Ni1S2' 'Ni3S2' 'Ni3S4'
 'O10P4' 'O1Pb1' 'O1Sr1' 'O1V1' 'O2.72W1' 'O2.96W1' 'O2Pb1' 'O2Si1'
 'O2Ti1' 'O2Zr1' 'O3V2' 'O4Pb2Si1' 'O4S1Zn1' 'O4Si1Zr1' 'P1' 'P4S3'
 'Pb1S1' 'Rb1' 'S1' 'S1Sr1' 'Sr1' 'Ti1' 'V1' 'W1' 'Zn1' 'Zr1']
```

In [42]:
```
trainingSet = uniqueFormula.copy()
```

In [43]:
```
#determine ratio of dataset in val, test, and train
val_rat = 0.2
test_rat = 0.1
train_rat = 1 - val_rat - test_rat

#calculate number of formulas in each set
num_val = int(round(val_rat*numUnique))
num_test = int(round(test_rat*numUnique))
num_train = int(round(1 - val_rat - test_rat*numUnique))

#randomly select formulas for val & train data, remove from list
valSet = np.random.choice(trainingSet, size = num_val, replace = False)
trainingSet = [a for a in trainingSet if a not in valSet]

testSet = np.random.choice(trainingSet, size = num_test, replace = False)
trainingSet = [a for a in trainingSet if a not in testSet]
```

In [44]:
```
print('Validation set:', len(valSet))
print('Test set:', len(testSet))
print('Training set:', len(trainingSet))
```

```
Validation set: 49
Test set: 24
Training set: 171
```

Val, test, & train sets have been determined by formula, now dividing dataset

In [45]:
```
df_train = data[data['formula'].isin(trainingSet)]
df_test = data[data['formula'].isin(testSet)]
df_val = data[data['formula'].isin(valSet)]
```

In [46]:
```
df_train.shape
```

Out[46]:
```
(3116, 3)
```

In [47]:
```
df_train.head(10)
```

Out[47]:

	formula	T	Cp
14	Be1I2	1400.0	89.341
15	Be1I2	1300.0	89.115
16	Be1I2	1200.0	88.780
17	Be1I2	1100.0	88.337
18	Be1I2	1000.0	87.789
19	Be1I2	900.0	87.132
20	Be1I2	800.0	86.366
21	Be1I2	753.0	85.944
22	Be1I2	600.0	84.190
23	Be1I2	500.0	81.638

In [48]:
```
df_test.shape
```

Out[48]:
```
(435, 3)
```

In [49]:
```
df_test.head(10)
```

Out[49]:

	formula	T	Cp
145	Al1N1	2900.0	51.845
146	Al1N1	2800.0	51.807
147	Al1N1	2700.0	51.765
148	Al1N1	2600.0	51.718
149	Al1N1	2500.0	51.666
150	Al1N1	2400.0	51.609
151	Al1N1	2300.0	51.543
152	Al1N1	2200.0	51.469
153	Al1N1	2100.0	51.385
154	Al1N1	2000.0	51.290

In [50]:
```
df_val.shape
```
Out[50]:
```
(996, 3)
```

In [51]:
```
df_val.head(10)
```
Out[51]:

	formula	T	Cp
0	B2O3	1400.0	134.306
1	B2O3	1300.0	131.294
2	B2O3	1200.0	128.072
3	B2O3	1100.0	124.516
4	B2O3	1000.0	120.625
5	B2O3	900.0	116.190
6	B2O3	800.0	111.169
7	B2O3	723.0	106.692
8	B2O3	700.0	105.228
9	B2O3	600.0	98.115

CHECK: make sure that there is no intersection between datasets

In [52]:
```
trainCheck = set(df_train['formula'].unique())
testCheck = set(df_test['formula'].unique())
valCheck = set(df_val['formula'].unique())
```

In [53]:
```
check1 = trainCheck.intersection(testCheck)
check2 = trainCheck.intersection(valCheck)
check3 = testCheck.intersection(valCheck)

print('intersections in check 1:', len(check1))
print('intersections in check 2:', len(check2))
print('intersections in check 3:', len(check3))
```
```
intersections in check 1: 0
intersections in check 2: 0
intersections in check 3: 0
```

In [54]:
```
df_train.to_csv('downloads/cp_train.csv')
df_test.to_csv('downloads/cp_test.csv')
df_val.to_csv('downloads/cp_val.csv')
```

Preprocessing

Don't rerun test/train split! Want to make sure the datasets stay the same throughout testing - saved splits to csv for reproducability

In [2]:
```
pip install CBFV
```

```
Requirement already satisfied: CBFV in c:\users\alish\anaconda3\lib\site-packages (1.
1.0)
Requirement already satisfied: numpy in c:\users\alish\anaconda3\lib\site-packages (f
rom CBFV) (1.21.5)
Requirement already satisfied: pytest in c:\users\alish\anaconda3\lib\site-packages
(from CBFV) (7.1.1)
Requirement already satisfied: tqdm in c:\users\alish\anaconda3\lib\site-packages (fr
om CBFV) (4.64.0)
Requirement already satisfied: pandas in c:\users\alish\anaconda3\lib\site-packages
(from CBFV) (1.4.2)
Requirement already satisfied: pytz>=2020.1 in c:\users\alish\anaconda3\lib\site-pack
ages (from pandas->CBFV) (2021.3)
Requirement already satisfied: python-dateutil>=2.8.1 in c:\users\alish\anaconda3\lib
\site-packages (from pandas->CBFV) (2.8.2)
Requirement already satisfied: six>=1.5 in c:\users\alish\anaconda3\lib\site-packages
(from python-dateutil>=2.8.1->pandas->CBFV) (1.16.0)
Requirement already satisfied: attrs>=19.2.0 in c:\users\alish\anaconda3\lib\site-pac
kages (from pytest->CBFV) (21.4.0)
Requirement already satisfied: iniconfig in c:\users\alish\anaconda3\lib\site-package
s (from pytest->CBFV) (1.1.1)
Requirement already satisfied: packaging in c:\users\alish\anaconda3\lib\site-package
s (from pytest->CBFV) (21.3)
Requirement already satisfied: pluggy<2.0,>=0.12 in c:\users\alish\anaconda3\lib\site
-packages (from pytest->CBFV) (1.0.0)
Requirement already satisfied: py>=1.8.2 in c:\users\alish\anaconda3\lib\site-package
s (from pytest->CBFV) (1.11.0)
Requirement already satisfied: tomli>=1.0.0 in c:\users\alish\anaconda3\lib\site-pack
ages (from pytest->CBFV) (1.2.2)
Requirement already satisfied: atomicwrites>=1.0 in c:\users\alish\anaconda3\lib\site
-packages (from pytest->CBFV) (1.4.0)
Requirement already satisfied: colorama in c:\users\alish\anaconda3\lib\site-packages
(from pytest->CBFV) (0.4.4)
Requirement already satisfied: pyparsing!=3.0.5,>=2.0.2 in c:\users\alish\anaconda3\l
ib\site-packages (from packaging->pytest->CBFV) (3.0.4)
Note: you may need to restart the kernel to use updated packages.
```

In [2]:
```python
from CBFV.composition import generate_features
```

In [3]:
```python
#save datasplits to csv for reproducability
df_train = pd.read_csv('downloads/cp_train.csv')
df_test = pd.read_csv('downloads/cp_test.csv')
df_val = pd.read_csv('downloads/cp_val.csv')
```

In [4]:
```python
#rename Cp column to target for CBFV
renameDict = {'Cp':'target'}

df_train = df_train.rename(columns=renameDict)
df_test = df_test.rename(columns=renameDict)
df_val = df_val.rename(columns=renameDict)
```

In [5]:
```python
df_train = df_train.drop(columns=['Unnamed: 0'])
df_test = df_test.drop(columns=['Unnamed: 0'])
df_val = df_val.drop(columns=['Unnamed: 0'])
```

In [6]:
```python
X_train_unscaled, y_train, formulae_train, skipped_train = generate_features(df_train,
X_val_unscaled, y_val, formulae_val, skipped_val = generate_features(df_val, elem_prop
X_test_unscaled, y_test, formulae_test, skipped_test = generate_features(df_test, elem
```

```
Processing Input Data: 100%|██████████████████████████████████████████| 31
16/3116 [00:00<00:00, 9983.32it/s]
        Featurizing Compositions...
Assigning Features...: 100%|██████████████████████████████████████████| 31
16/3116 [00:00<00:00, 4011.12it/s]
        Creating Pandas Objects...
Processing Input Data: 100%|███████████████████████████████████████████| 9
96/996 [00:00<00:00, 10416.42it/s]
        Featurizing Compositions...
Assigning Features...: 100%|████████████████████████████████████████████|
996/996 [00:00<00:00, 5103.06it/s]
        Creating Pandas Objects...
Processing Input Data: 100%|████████████████████████████████████████████|
435/435 [00:00<00:00, 8363.88it/s]
        Featurizing Compositions...
Assigning Features...: 100%|████████████████████████████████████████████|
435/435 [00:00<00:00, 3334.84it/s]
        Creating Pandas Objects...
```

In [7]:
```python
X_train_unscaled.head()
```

Out[7]:

	sum_Atomic_Number	sum_Atomic_Weight	sum_Period	sum_group	sum_families	sum_Metal	sum_
0	110.0	262.82112	12.0	36.0	18.0	1.0	
1	110.0	262.82112	12.0	36.0	18.0	1.0	
2	110.0	262.82112	12.0	36.0	18.0	1.0	
3	110.0	262.82112	12.0	36.0	18.0	1.0	
4	110.0	262.82112	12.0	36.0	18.0	1.0	

5 rows × 309 columns

In [8]:
```python
X_train_unscaled.shape
```

Out[8]:
```
(3116, 309)
```

Data scaling/normalization

In [9]:
```python
from sklearn.preprocessing import StandardScaler
from sklearn.preprocessing import normalize
```

In [10]:
```python
scaler = StandardScaler()
```

In [11]:
```python
x_train = scaler.fit_transform(X_train_unscaled)
x_test = scaler.fit_transform(X_test_unscaled)
x_val = scaler.fit_transform(X_val_unscaled)
```

In [12]:
```python
x_train = normalize(x_train)
x_test = normalize(x_test)
x_val = normalize(x_val)
```

Modeling

In [13]:
```
from time import time

from sklearn.dummy import DummyRegressor

from sklearn.linear_model import Ridge

from sklearn.ensemble import AdaBoostRegressor
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.ensemble import ExtraTreesRegressor
from sklearn.ensemble import RandomForestRegressor

from sklearn.neighbors import KNeighborsRegressor

from sklearn.svm import SVR
from sklearn.svm import LinearSVR

from sklearn.metrics import r2_score
from sklearn.metrics import mean_absolute_error
from sklearn.metrics import mean_squared_error
```

In [23]:
```
#helper functions
def instantiate_model(model_name):
    model = model_name()
    return model

def fit_model(model, X_train, y_train):
    ti = time()
    model = instantiate_model(model)
    model.fit(X_train, y_train)
    fit_time = time() - ti
    return model, fit_time

def evaluate_model(model, X, y_act):
    y_pred = model.predict(X)
    r2 = r2_score(y_act, y_pred)
    mae = mean_absolute_error(y_act, y_pred)
    rmse_val = mean_squared_error(y_act, y_pred, squared=False)
    return r2, mae, rmse_val

def fit_evaluate_model(model, model_name, X_train, y_train, X_val, y_act_val):
    model, fit_time = fit_model(model, X_train, y_train)
    r2_train, mae_train, rmse_train = evaluate_model(model, X_train, y_train)
    r2_val, mae_val, rmse_val = evaluate_model(model, X_val, y_act_val)
    result_dict = {
        'model_name': model_name,
        'model_name_pretty': type(model).__name__,
        'model_params': model.get_params(),
        'fit_time': fit_time,
        'r2_train': r2_train,
        'mae_train': mae_train,
        'rmse_train': rmse_train,
        'r2_val': r2_val,
        'mae_val': mae_val,
        'rmse_val': rmse_val}
    return model, result_dict
```

```
def append_result_df(df, result_dict):
    df_result_appended = df.append(result_dict, ignore_index=True)
    return df_result_appended

def append_model_dict(dic, model_name, model):
    dic[model_name] = model
    return dic
```

In [34]:

```
#empty DF to store model results
df_classics = pd.DataFrame(columns=['model_name',
                                    'model_name_pretty',
                                    'model_params',
                                    'fitTime',
                                    'r2_train',
                                    'mae_train',
                                    'rsme_train',
                                    'r2_val',
                                    'mae_val','rsme_val'])
df_classics
```

Out[34]:

model_name	model_name_pretty	model_params	fitTime	r2_train	mae_train	rsme_train	r2_val	m

In [35]:

```
#dictionary of model names used
classic_model_names = OrderedDict({
    'dum': DummyRegressor,
    'rr': Ridge,
    'abr':AdaBoostRegressor,
    'gbr':GradientBoostingRegressor,
    'rfr':RandomForestRegressor,
    'etr':ExtraTreesRegressor,
    'svr':SVR,
    'lsvr':LinearSVR,
    'knn':KNeighborsRegressor
})
```

In [36]:

```
classic_models = OrderedDict()
t=time()
```

In [37]:

```
for model_name, model in classic_model_names.items():
    print(f'Now fitting and evaluating model {model_name}: {model.__name__}')
    model, result_dict = fit_evaluate_model(model, model_name, x_train, y_train, x_val
    df_classics = append_result_df(df_classics, result_dict)
    classic_models = append_model_dict(classic_models, model_name, model)

dt = time() - t
print(f'Finished fitting {len(classic_models)} models, total time: {dt:0.2f} s')
```

```
Now fitting and evaluating model dum: DummyRegressor
Now fitting and evaluating model rr: Ridge
Now fitting and evaluating model abr: AdaBoostRegressor
```

```
C:\Users\alish\AppData\Local\Temp\ipykernel_44280\2708434257.py:38: FutureWarning: Th
e frame.append method is deprecated and will be removed from pandas in a future versi
on. Use pandas.concat instead.
  df_result_appended = df.append(result_dict, ignore_index=True)
C:\Users\alish\AppData\Local\Temp\ipykernel_44280\2708434257.py:38: FutureWarning: Th
e frame.append method is deprecated and will be removed from pandas in a future versi
on. Use pandas.concat instead.
  df_result_appended = df.append(result_dict, ignore_index=True)
C:\Users\alish\AppData\Local\Temp\ipykernel_44280\2708434257.py:38: FutureWarning: Th
e frame.append method is deprecated and will be removed from pandas in a future versi
on. Use pandas.concat instead.
  df_result_appended = df.append(result_dict, ignore_index=True)
Now fitting and evaluating model gbr: GradientBoostingRegressor
C:\Users\alish\AppData\Local\Temp\ipykernel_44280\2708434257.py:38: FutureWarning: Th
e frame.append method is deprecated and will be removed from pandas in a future versi
on. Use pandas.concat instead.
  df_result_appended = df.append(result_dict, ignore_index=True)
Now fitting and evaluating model rfr: RandomForestRegressor
C:\Users\alish\AppData\Local\Temp\ipykernel_44280\2708434257.py:38: FutureWarning: Th
e frame.append method is deprecated and will be removed from pandas in a future versi
on. Use pandas.concat instead.
  df_result_appended = df.append(result_dict, ignore_index=True)
Now fitting and evaluating model etr: ExtraTreesRegressor
C:\Users\alish\AppData\Local\Temp\ipykernel_44280\2708434257.py:38: FutureWarning: Th
e frame.append method is deprecated and will be removed from pandas in a future versi
on. Use pandas.concat instead.
  df_result_appended = df.append(result_dict, ignore_index=True)
Now fitting and evaluating model svr: SVR
C:\Users\alish\AppData\Local\Temp\ipykernel_44280\2708434257.py:38: FutureWarning: Th
e frame.append method is deprecated and will be removed from pandas in a future versi
on. Use pandas.concat instead.
  df_result_appended = df.append(result_dict, ignore_index=True)
C:\Users\alish\AppData\Local\Temp\ipykernel_44280\2708434257.py:38: FutureWarning: Th
e frame.append method is deprecated and will be removed from pandas in a future versi
on. Use pandas.concat instead.
  df_result_appended = df.append(result_dict, ignore_index=True)
Now fitting and evaluating model lsvr: LinearSVR
Now fitting and evaluating model knn: KNeighborsRegressor
Finished fitting 9 models, total time: 103.45 s
C:\Users\alish\AppData\Local\Temp\ipykernel_44280\2708434257.py:38: FutureWarning: Th
e frame.append method is deprecated and will be removed from pandas in a future versi
on. Use pandas.concat instead.
  df_result_appended = df.append(result_dict, ignore_index=True)
```

In [38]:
```
df_classics = df_classics.sort_values('r2_val', ignore_index=True)
df_classics
```

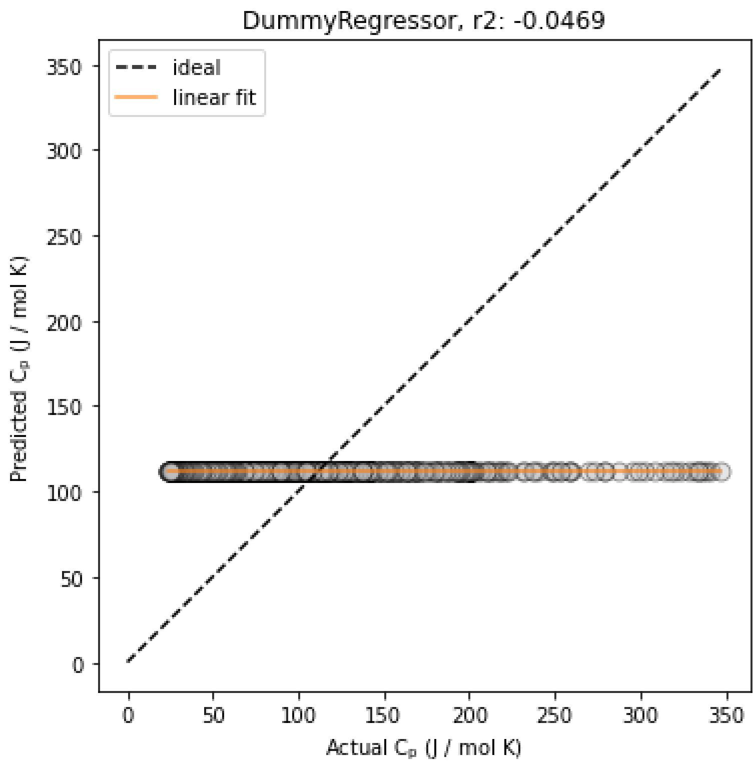
Out[38]:

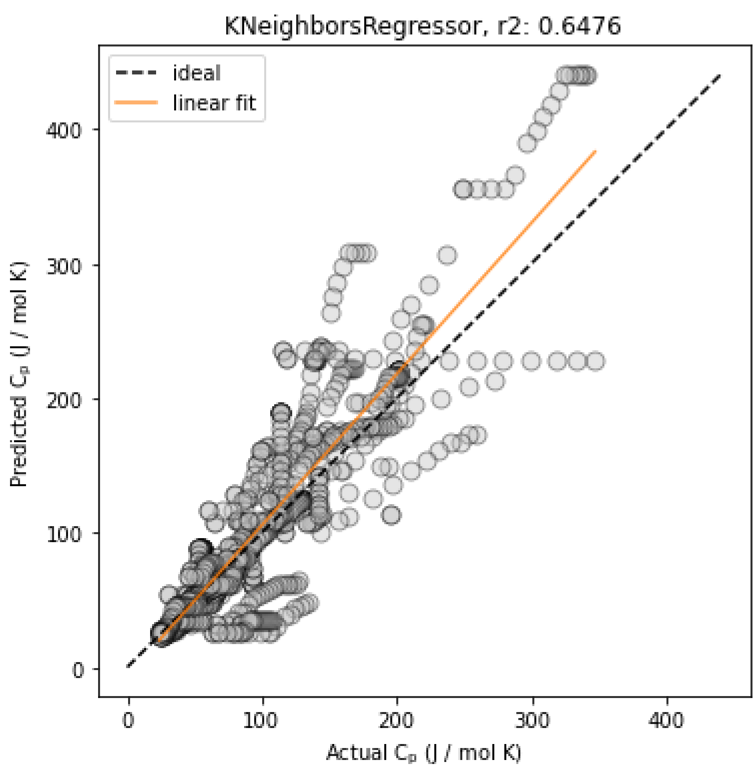
	model_name	model_name_pretty	model_params	fitTime	r2_train	mae_train	rsme_train
0	dum	DummyRegressor	{'constant': None, 'quantile': None, 'strategy...	NaN	0.0	52.532407	NaN
1	knn	KNeighborsRegressor	{'algorithm': 'auto', 'leaf_size': 30, 'metric...	NaN	0.993752	2.221375	NaN
2	abr	AdaBoostRegressor	{'base_estimator': None, 'learning_rate': 1.0,...	NaN	0.912564	17.309772	NaN
3	svr	SVR	{'C': 1.0, 'cache_size': 200, 'coef0': 0.0, 'd...	NaN	0.740108	18.74941	NaN
4	rr	Ridge	{'alpha': 1.0, 'copy_X': True, 'fit_intercept'...	NaN	0.90125	14.225094	NaN
5	lsvr	LinearSVR	{'C': 1.0, 'dual': True, 'epsilon': 0.0, 'fit_...	NaN	0.758191	18.048634	NaN
6	rfr	RandomForestRegressor	{'bootstrap': True, 'ccp_alpha': 0.0, 'criteri...	NaN	0.999056	0.998996	NaN
7	etr	ExtraTreesRegressor	{'bootstrap': False, 'ccp_alpha': 0.0, 'criter...	NaN	0.999765	0.099014	NaN
8	gbr	GradientBoostingRegressor	{'alpha': 0.9, 'ccp_alpha': 0.0, 'criterion': ...	NaN	0.984781	6.284942	NaN

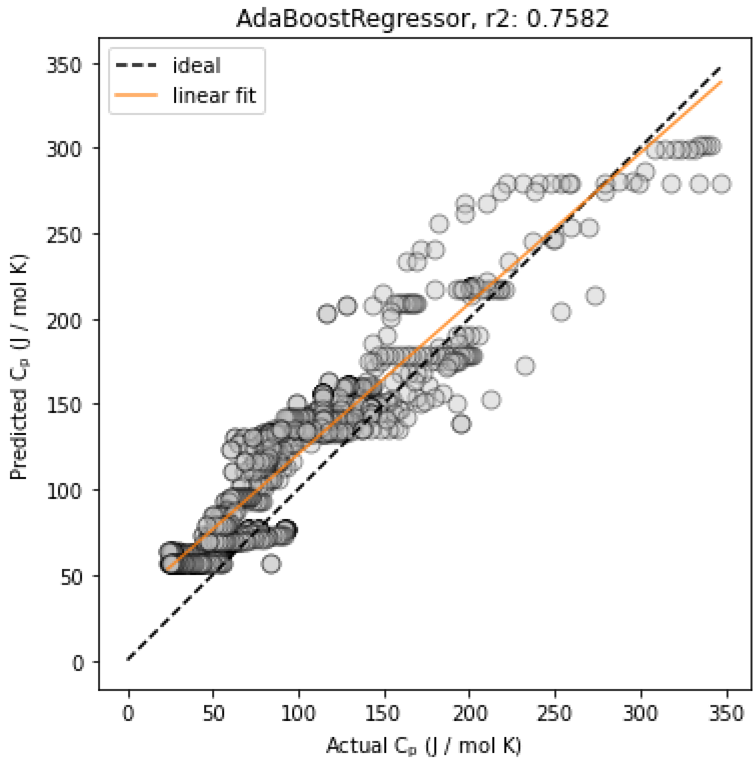
In [39]:

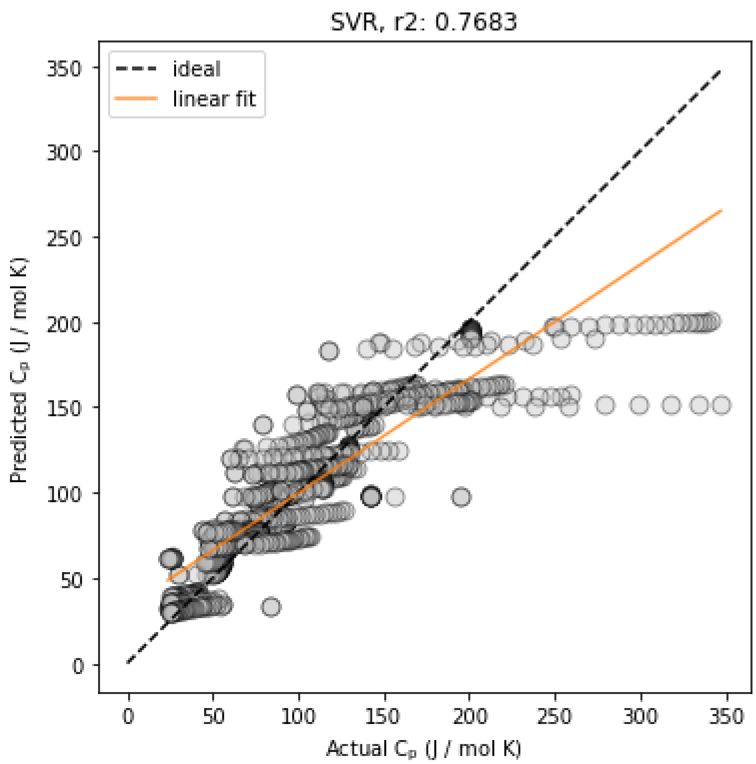
```
def plot_pred_act(act, pred, model, reg_line=True, label=''):
    xy_max = np.max([np.max(act), np.max(pred)])

    plot = plt.figure(figsize=(6,6))
    plt.plot(act, pred, 'o', ms=9, mec='k', mfc='silver', alpha=0.4)
    plt.plot([0, xy_max], [0, xy_max], 'k--', label='ideal')
    if reg_line:
        polyfit = np.polyfit(act, pred, deg=1)
        reg_ys = np.poly1d(polyfit)(np.unique(act))
        plt.plot(np.unique(act), reg_ys, alpha=0.8, label='linear fit')
    plt.axis('scaled')
    plt.xlabel(f'Actual {label}')
    plt.ylabel(f'Predicted {label}')
    plt.title(f'{type(model).__name__}, r2: {r2_score(act, pred):0.4f}')
    plt.legend(loc='upper left')

    return plot
```

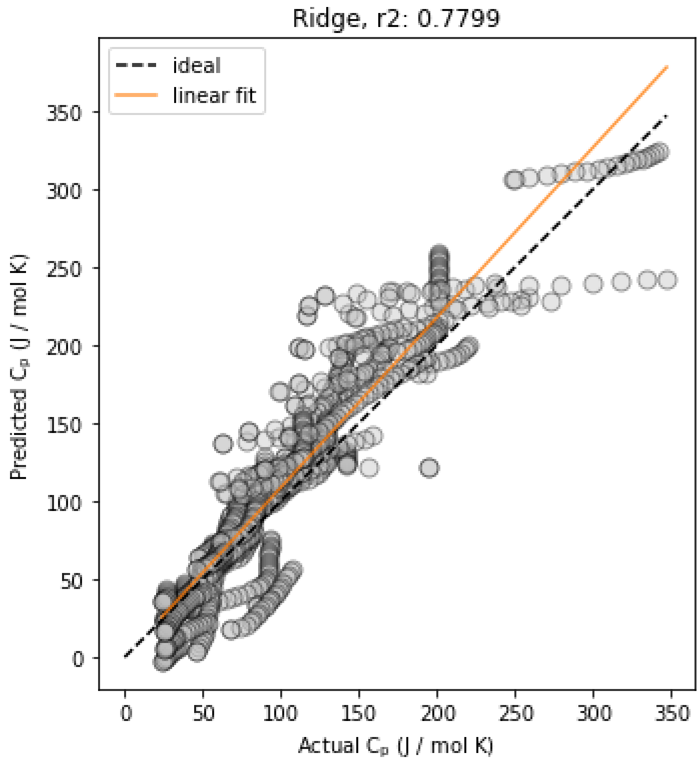
In [40]:
```
for row in range(df_classics.shape[0]):
    model_name = df_classics.iloc[row]['model_name']

    model = classic_models[model_name]
    y_act_val = y_val
    y_pred_val = model.predict(x_val)

    plot = plot_pred_act(y_act_val, y_pred_val, model, reg_line=True, label='$\mathrm{
```

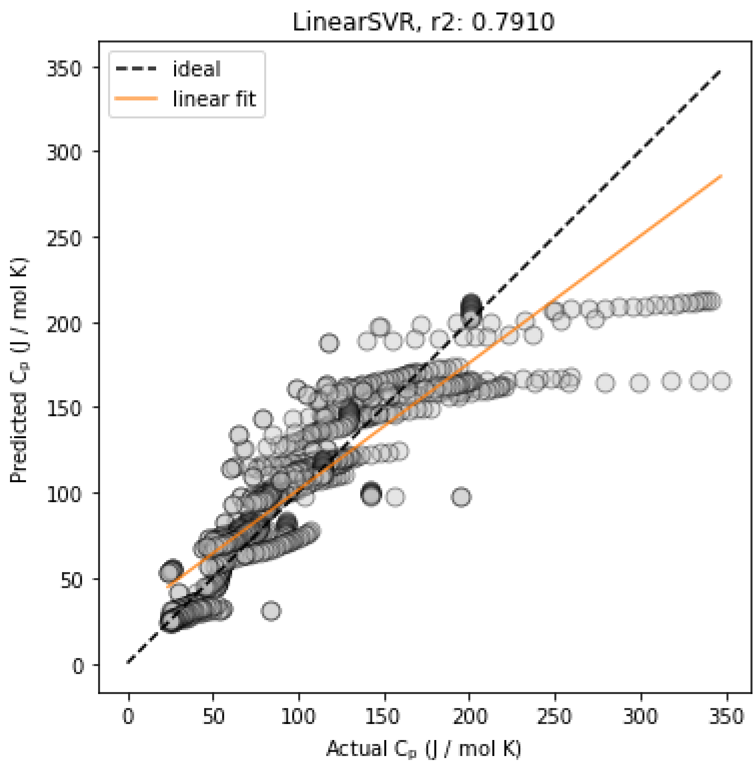


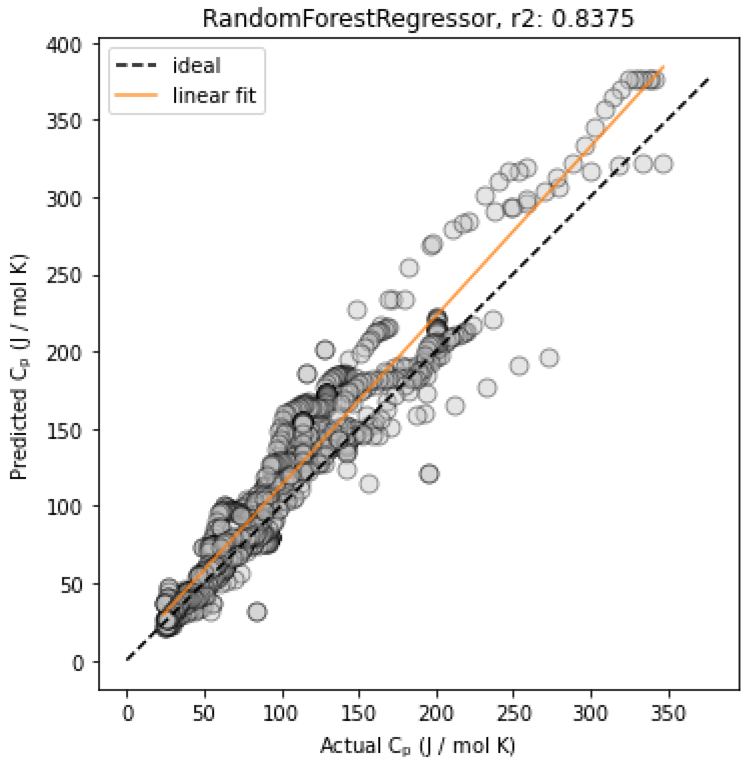


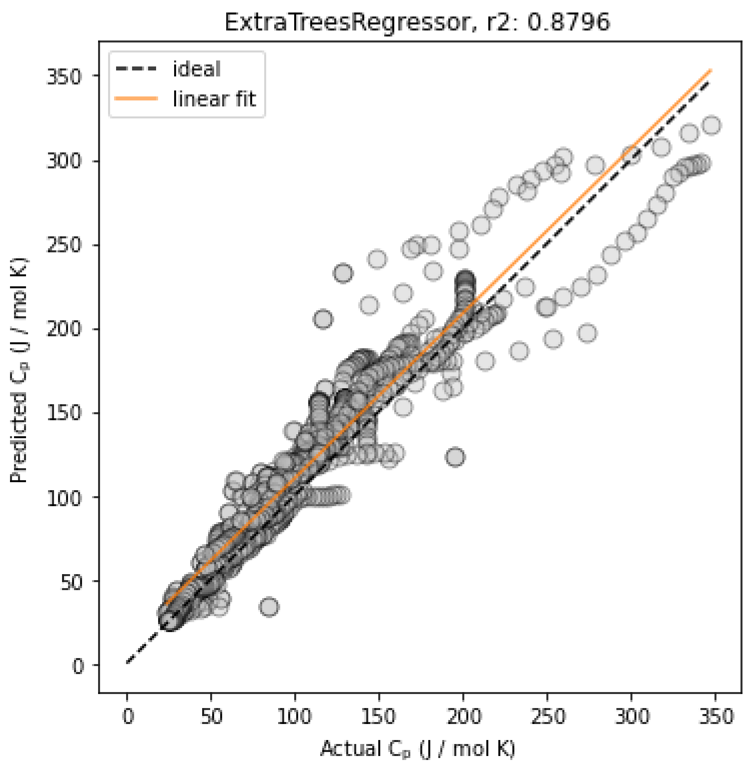

AdaBoostRegressor, r2: 0.7582
ideal
linear fit
Predicted C_p (J / mol K)
Actual C_p (J / mol K)
0
50
100
150
200
250
300
350

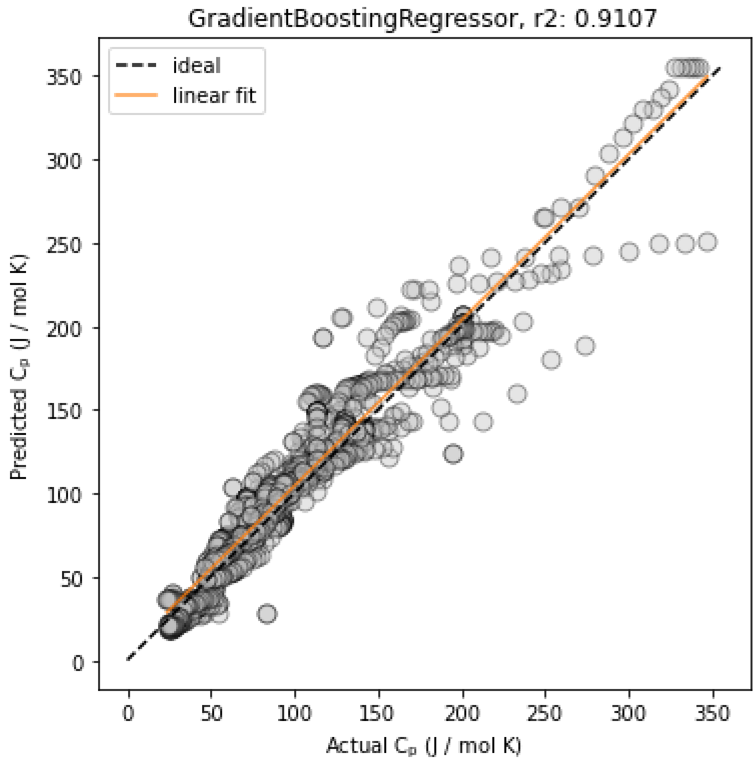

SVR, r2: 0.7683
ideal
linear fit
Predicted C_p (J / mol K)
Actual C_p (J / mol K)
0
50
100
150
200
250
300
350


Ridge, r2: 0.7799
ideal
linear fit
Predicted C_p (J / mol K)
Actual C_p (J / mol K)
0
50
100
150
200
250
300
350


LinearSVR, r2: 0.7910
ideal
linear fit
Predicted C_p (J / mol K)
Actual C_p (J / mol K)
0
50
100
150
200
250
300
350


RandomForestRegressor, r2: 0.8375
ideal
linear fit
Predicted C_p (J / mol K)
Actual C_p (J / mol K)


ExtraTreesRegressor, r2: 0.8796
ideal
linear fit
Predicted C_p (J / mol K)
Actual C_p (J / mol K)



Determining the best model

In [51]:
```
best_model = df_classics.iloc[-1].copy()
best_name = best_model['model_name']
best_params = best_model['model_params']

model = classic_model_names[best_name](**best_params)
print(model)
```

```
GradientBoostingRegressor()
```

Add validation dataset to the training set to retrain before final test

In [52]:
```
x_train_new = np.concatenate((x_train, x_val), axis=0)
y_train_new = np.concatenate((y_train, y_val), axis=0)

print(x_train_new.shape)
```

```
(4112, 309)
```

In [54]:
```
t = time()
model.fit(x_train_new, y_train_new)

dt = time()-t

print('Fit best trained model in:', dt)
```

```
Fit best trained model in: 38.279815435409546
```

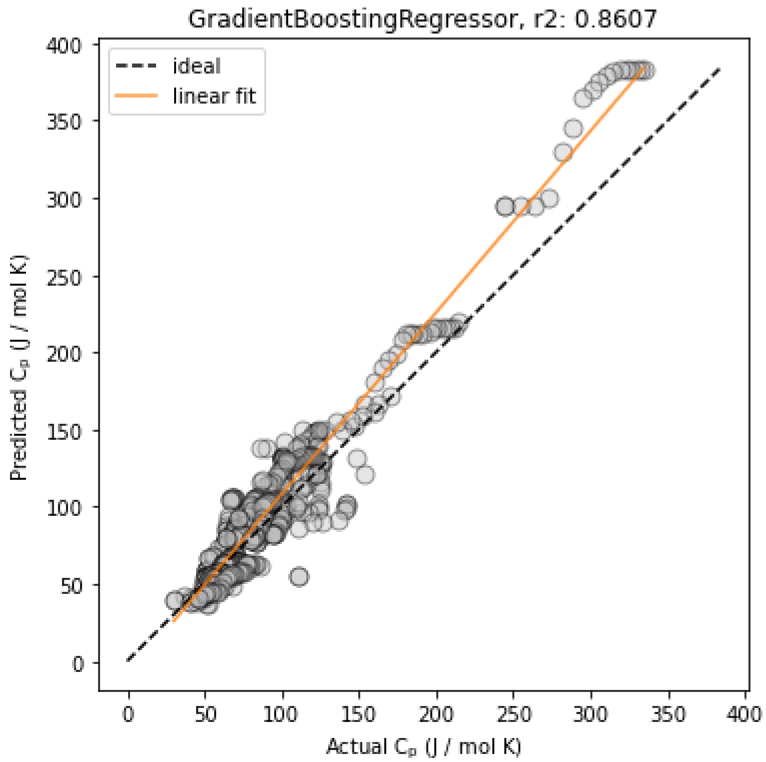
Running retrained model with test data

only run this once - otherwise the model will train with the test set

In [55]:
```
y_actual_test = y_test
y_pred_test = model.predict(x_test)

r2, mae, rsme = evaluate_model(model, x_test, y_test)
```

In [57]:
```
print('r2:', r2)
print('mae:', mae)
print('rsme:', rsme)

plot = plot_pred_act(y_actual_test, y_pred_test, model, reg_line=True, label='$\mathrm
```

```
r2: 0.8607119437701974
mae: 14.715074700761356
rsme: 20.124807045616695
```



Citations

Wang, Anthony Yu-Tung; Murdock, Ryan J.; Kauwe, Steven K.; Oliynyk, Anton O.; Gurlo, Aleksander; Brgoch, Jakoah; Persson, Kristin A.; Sparks, Taylor D., Machine Learning for Materials Scientists: An Introductory Guide toward Best Practices, Chemistry of Materials 2020, 32 (12): 4954–4965. DOI: 10.1021/acs.chemmater.0c01907.

In [ ]: