models

January 21, 2019

0.0.1 Instantiate environment

```
In [50]: from rdkit import Chem
         from rdkit.Chem import Descriptors
         from rdkit.ML.Descriptors import MoleculeDescriptors
         from rdkit.Chem import PandasTools
         import pandas as pd
         from sklearn import preprocessing
         from sklearn.preprocessing import StandardScaler
         from sklearn.feature_selection import VarianceThreshold
         from sklearn.model_selection import train_test_split
         import numpy as np
         import math
```

0.0.2 Read data

```
In [44]: train_df = PandasTools.LoadSDF("data/TR_AOH_516.sdf")
         test_df = PandasTools.LoadSDF("data/TST_AOH_176.sdf")
```

0.0.3 Concatenate data

```
In [45]: AOH = pd.concat([train_df[["Canonical_QSARr", "LogOH"]], test_df[["Canonical_QSARr", "L
```

0.0.4 Calculate features

```
In [47]: nms = [x[0] for x in Descriptors._descList]
         calc = MoleculeDescriptors.MolecularDescriptorCalculator(nms)
         for i in range(len(AOH)):
             descrs = calc.CalcDescriptors(Chem.MolFromSmiles(AOH.iloc[i, 0]))
             for x in range(len(descrs)):
                 AOH.at[i, str(nms[x])] = str(descrs[x])
```

0.0.5 Training & Test Datasets

```
In [51]: X = AOH.drop(columns=["Canonical_QSARr", "LogOH"])
         y = AOH[["LogOH"]]
         X_train, X_test, y_train, y_test = train_test_split(X, y, random_state = 350)
```

```
In [74]: pd.to_numeric(y_train['LogOH']).describe()
```

```
Out[74]: count    519.000000
         mean     -11.433391
         std        1.274721
         min      -16.000000
         25%      -12.000000
         50%      -11.113509
         75%      -10.545918
         max       -9.259637
         Name: LogOH, dtype: float64
```

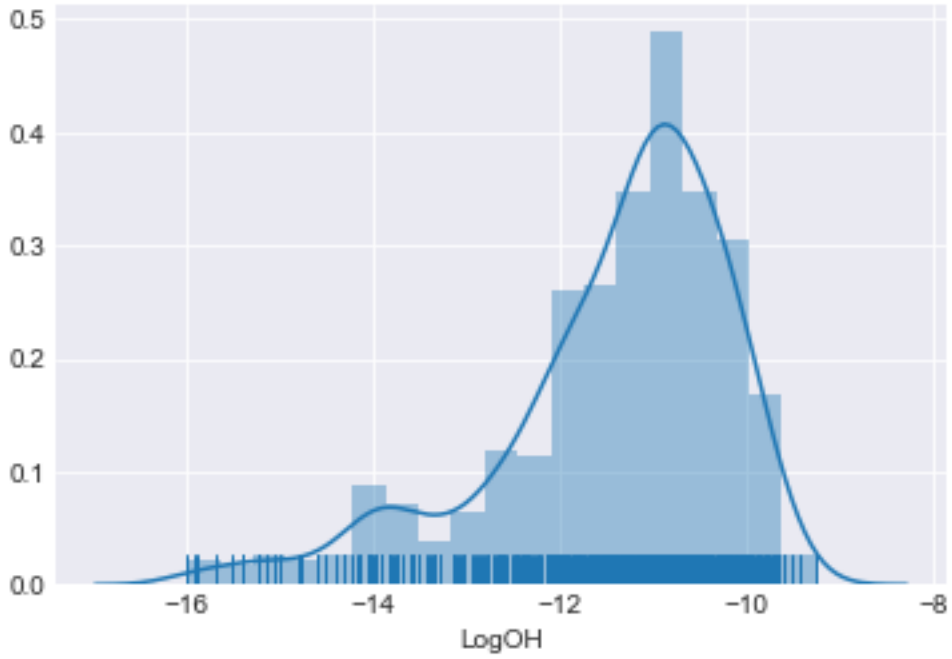
```
In [75]: pd.to_numeric(y_test['LogOH']).describe()
```

```
Out[75]: count    173.000000
         mean     -11.395769
         std        1.329613
         min      -16.221849
         25%      -12.071092
         50%      -11.020907
         75%      -10.424812
         max       -9.537602
         Name: LogOH, dtype: float64
```

```
In [76]: import seaborn as sns
```

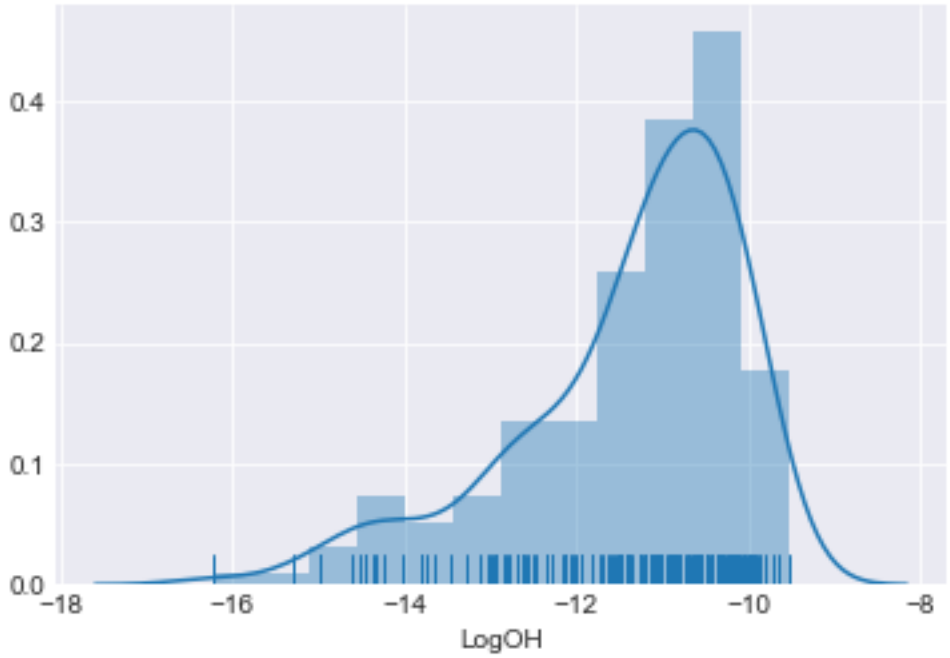
```
In [79]: sns.distplot(pd.to_numeric(y_train['LogOH']), rug = True)
```

```
Out[79]: <matplotlib.axes._subplots.AxesSubplot at 0x1657b1d0>
```

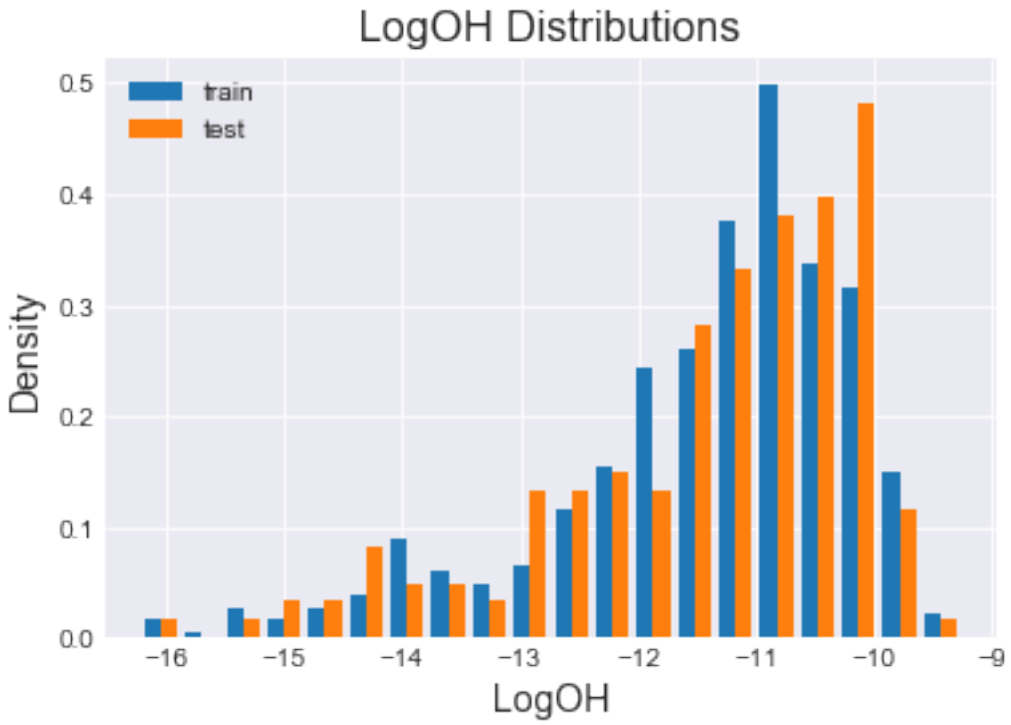


In [80]:
```
sns.distplot(pd.to_numeric(y_test['LogOH']), rug = True)
```

Out[80]:
```
<matplotlib.axes._subplots.AxesSubplot at 0x16d80f98>
```



In [90]:
```
# create dataframe, select columns
df1x = pd.to_numeric(y_train['LogOH'])
df2x = pd.to_numeric(y_test['LogOH'])
#Stack the data
plt.figure()
plt.hist([df1x,df2x], bins = 20, stacked = False, density = True)
plt.title('LogOH Distributions', fontsize = 16)
plt.xlabel('LogOH', fontsize=14)
plt.ylabel('Density', fontsize=14)
plt.legend(['train', 'test'])
plt.show()
```




```
In [92]: type(y['LogOH'])
```

```
Out[92]: pandas.core.series.Series
```