Cheching the solubility of molecule in water

Load Data

```
import pandas as pd
df  = pd.read_csv('https://raw.githubusercontent.com/dataprofessor/data/master/delaney_solubility_with_descriptors.csv')
df.head()
```

	MolLogP	MolWt	NumRotatableBonds	AromaticProportion	logS
0	2.5954	167.850	0.0	0.0	-2.18
1	2.3765	133.405	0.0	0.0	-2.00
2	2.5938	167.850	1.0	0.0	-1.74
3	2.0289	133.405	1.0	0.0	-1.48
4	2.9189	187.375	1.0	0.0	-3.04

Data Preparation

Data Separation as X and y

```
y = df["logS"]
y
```

```
0      -2.180
1      -2.000
2      -1.740
3      -1.480
4      -3.040
        ...
1139    1.144
1140   -4.925
1141   -3.893
1142   -3.790
1143   -2.581
Name: logS, Length: 1144, dtype: float64
```

```
X = df.drop(["logS"], axis=1)
X
```

	MolLogP	MolWt	NumRotatableBonds	AromaticProportion
0	2.59540	167.850	0.0	0.000000
1	2.37650	133.405	0.0	0.000000
2	2.59380	167.850	1.0	0.000000
3	2.02890	133.405	1.0	0.000000
4	2.91890	187.375	1.0	0.000000
...	...	...	...	...
1139	1.98820	287.343	8.0	0.000000
1140	3.42130	286.114	2.0	0.333333
1141	3.60960	308.333	4.0	0.695652
1142	2.56214	354.815	3.0	0.521739
1143	2.02164	179.219	1.0	0.461538

1144 rows × 4 columns

Data Spliting

```
import sklearn
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42)
```

```
X_train.shape
```

```
(915, 4)
```

```
X_test.shape
```

```
(229, 4)
```

Model Building

Linear Regression

Training The Model

```
from sklearn.linear_model import LinearRegression
lr = LinearRegression()
```

```
lr.fit(X_train, y_train)
```

```
LinearRegression
LinearRegression()
```

Applying a model to make a prediction

```
y_lr_train_pred = lr.predict(X_train)
y_lr_test_pred = lr.predict(X_test)
```

```
y_lr_train_pred
```

```
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```

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```

```
y_lr_test_pred
```

```
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       -1.91509076, -3.00635454, -3.10567883, -1.48599039])
```

Evaluate Model Performance

```
from sklearn.metrics import mean_squared_error,r2_score
lr_train_mse = mean_squared_error(y_train, y_lr_train_pred)
lr_train_r2 = r2_score(y_train, y_lr_train_pred)

lr_test_mse = mean_squared_error(y_test, y_lr_test_pred)
lr_test_r2 = r2_score(y_test, y_lr_test_pred)



print("LR MSE (Train):",lr_train_mse)
print("LR R2 (Train):",lr_train_r2)
print("LR MSE (Test):",lr_test_mse)
print("LR R2 (Test):",lr_test_r2)
```

```
LR MSE (Train): 1.0139894491573003
LR R2 (Train): 0.7695127746587307
LR MSE (Test): 0.9990844407075306
LR R2 (Test): 0.7705650058569232
```

```
lr_results = pd.DataFrame(['Linear Regression',lr_train_mse,lr_train_r2,lr_test_mse,lr_test_r2]).transpose()
lr_results.columns = ['Model','Training MSE','Training R2','Testing MSE','Testing R2 ']
lr_results
```

	Model	Training MSE	Training R2	Testing MSE	Testing R2
0	Linear Regression	1.013989	0.769513	0.999084	0.770565

Random Forest

```
from sklearn.ensemble import RandomForestRegressor
rf = RandomForestRegressor(max_depth=2,random_state=100)
```

Training The Model

```
rf.fit(X_train, y_train)
```

```
RandomForestRegressor
RandomForestRegressor(max_depth=2, random_state=100)
```

Applying a model to make a prediction

```
y_rf_train_pred = rf.predict(X_train)
y_rf_test_pred = rf.predict(X_test)
```

```
y_rf_train_pred
```

```
array([-4.39406068, -7.01386075, -4.1790564 , -1.17794119, -2.2850991 ,
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```

```
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```

y_rf_test_pred

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```
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            -2.29709247, -2.66365457, -4.37313972, -1.25181203])
```

Evaluate Model Performance

```
from sklearn.metrics import mean_squared_error,r2_score
rf_train_mse = mean_squared_error(y_train, y_rf_train_pred)
rf_train_r2 = r2_score(y_train, y_rf_train_pred)

rf_test_mse = mean_squared_error(y_test, y_rf_test_pred)
rf_test_r2 = r2_score(y_test, y_rf_test_pred)


rf_results = pd.DataFrame(['Random Forest',rf_train_mse,rf_train_r2,rf_test_mse,rf_test_r2]).transpose()
rf_results.columns = ['Model','Training MSE','Training R2','Testing MSE','Testing R2 ']
rf_results
```

	Model	Training MSE	Training R2	Testing MSE	Testing R2
0	Random Forest	1.057186	0.759694	1.05209	0.758393

Start coding or generate with AI.

Model Compression

```
df_models = pd.concat([lr_results, rf_results], ignore_index=True , axis = 0)
df_models
```

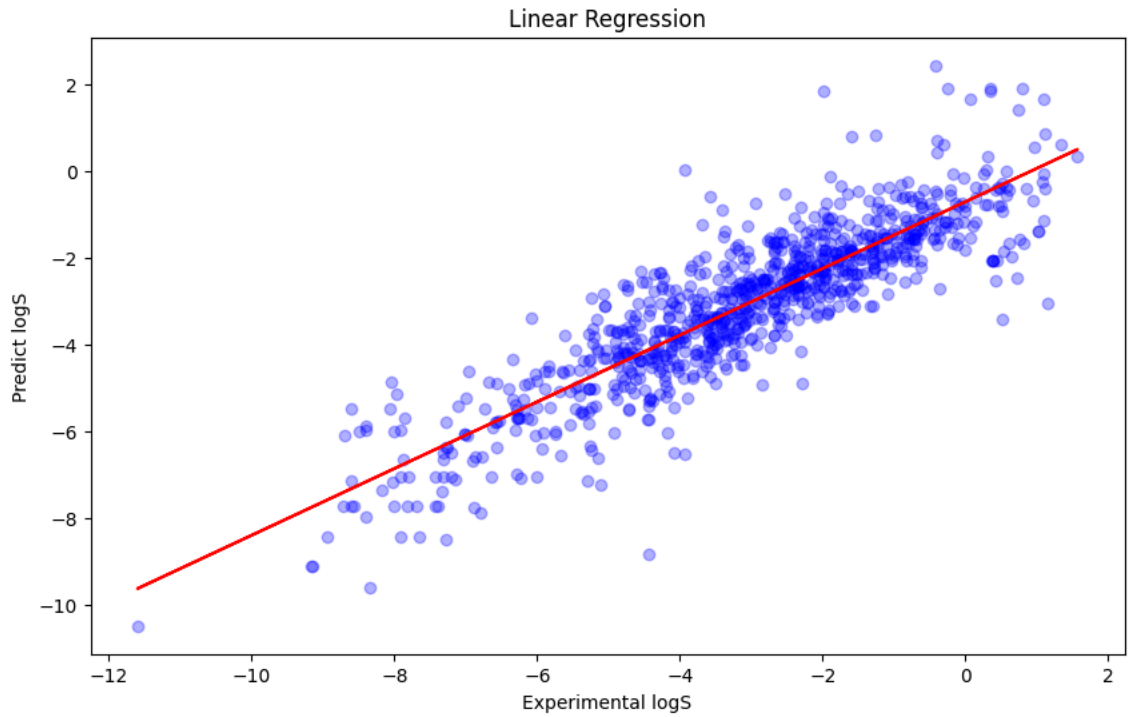
	Model	Training MSE	Training R2	Testing MSE	Testing R2
0	Linear Regression	1.013989	0.769513	0.999084	0.770565
1	Random Forest	1.057186	0.759694	1.05209	0.758393

Data Visualization of prediction Result

```
import matplotlib.pyplot as plt
import numpy as np

plt.figure(figsize=(10, 6))
plt.scatter(y_train, y_lr_train_pred, color='blue', alpha=0.3)
z = np.polyfit(y_train, y_lr_train_pred, 1)
p = np.poly1d(z)
plt.plot(y_train, p(y_train), color='red')
plt.xlabel('Experimental logS')
plt.ylabel('Predict logS')
plt.title('Linear Regression')

plt.show()
```



Start coding or generate with AI.