

Problem statement

To develop a machine learning model capable of predicting the groundwater potential of aquifers, quantified on a scale of 0 to 1, indicating the yield of an aquifer.

Background and Rationale

- Transmissivity: Defined as the measure of the ease of groundwater flow through an aquifer, calculated by multiplying the hydraulic conductivity by the thickness of the aquifer. This metric serves as a comprehensive indicator of water flow ease, rendering hydraulic conductivity as a feature is redundant when transmissivity is available.
- The following features are what are considered in predicting aquifer storage in this project.
 - Aquifer thickness
 - Transimisivity
 - hydraulic conductivty
 - Fracture contrast
 - Transverse resistance
 - longitudinal conductance
 - Overburden thickness
 - aquifer resistivity
 - Reflection co-efficient

```
In [ ]: import pandas as pd
import matplotlib.pyplot as plt
import numpy as np
from sklearn.preprocessing import RobustScaler
import seaborn as sns
import matplotlib.pyplot as plt
from scipy.stats import pearsonr, spearmanr, kendalltau
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import train_test_split, cross_val_score
from sklearn.metrics import mean_squared_error
from sklearn.linear_model import LinearRegression
from sklearn.tree import DecisionTreeRegressor
from sklearn.ensemble import RandomForestRegressor
from sklearn.svm import LinearSVR

np.random.seed(42) # Ensure reproducibility for scipy.stats operations i
```

Section 1: Load up and describe data

```
In [ ]: # Settings
pd.set_option('display.max_columns', None)
```

```
In [ ]: # load up the datasets
df_1 = pd.read_excel("data/dataset_2.xlsx")
df_1.head()
```

Out[]:

	VES S/N	Easting (Min)	Northing (Min)	Elev(m)	No. of Layer	Curve Types	Thickness Topsoil h1(m)	Thickness Laterite h2(m)	Thickness weathered h3 (m)
0	1	36.94	28.00	343.0	4	KH	1.1	4.9	23
1	2	36.73	28.80	359.0	4	KH	0.8	1.6	22
2	3	36.60	28.75	397.0	3	A	0.8	0.0	9
3	4	36.84	29.58	342.0	3	H	0.9	0.0	6
4	5	36.60	29.54	348.0	3	H	2.5	0.0	62

```
In [ ]: df_1.columns
```

```
Out[ ]: Index(['VES S/N', 'Easting (Min)', 'Northing (Min)', 'Elev(m)', 'No. of Layer',
       'Curve Types', 'Thickness Topsoil h1(m)', 'Thickness Laterite h2 (m)',
       'Thickness weathered h3 (m)', 'Corrected Thick. weathered (m) H 3',
       'Thickness Fractured h4 (m)', 'Corrected Thick. Fractured (m) H 4',
       'Thick. Overb.\nB1=h1+h2', 'Total Aquifer Thick. B2=h3+h4',
       'Corrected Total Aquifer Thick', 'p1', 'p2', 'p3', 'p4', 'p5',
       'Res. Of Topsoil', 'Res. Of Laterite', 'Long. Cond. (mhos) Topsoi l',
       'Long. Cond. (mhos) Laterite', 'Long. Cond. (mhos) OVERBURRDEN',
       'Logarithm of Topsoil', 'RESISTIVITY OF FRESH BASEMENT',
       'Logarithm Fresh Basement', 'AQUIFER RES of Weathered. \n(Ohm-M)',
       'Logarithm Weathered', 'Hydraulic Conductivity (K)',
       'Transmissivity (T)', 'Wrong', 'Aquifer storage '],
      dtype='object')
```

```
In [ ]: df_1.describe()
```

Out[]:

	VES S/N	Easting (Min)	Northing (Min)	Elev(m)	No. of Layer	Thickness Topsoil h1(m)
count	253.000000	253.000000	253.000000	253.000000	253.000000	253.000000
mean	127.000000	33.721700	30.040079	329.477075	3.379447	2.248221
std	73.179004	2.190428	1.293328	56.739089	0.510109	2.456100
min	1.000000	29.340000	27.600000	143.000000	3.000000	0.300000
25%	64.000000	32.060000	29.050000	305.000000	3.000000	1.000000
50%	127.000000	33.780000	29.950000	323.000000	3.000000	1.500000
75%	190.000000	35.520000	30.820000	343.000000	4.000000	2.200000
max	253.000000	37.080000	33.540000	930.000000	5.000000	12.700000

In []: df_1.info()

```

<class 'pandas.core.frame.DataFrame'>
RangeIndex: 253 entries, 0 to 252
Data columns (total 34 columns):
 #   Column           Non-Null Count Dtype  
 --- 
 0   VES S/N          253 non-null   int64  
 1   Easting (Min)    253 non-null   float64 
 2   Northing (Min)   253 non-null   float64 
 3   Elev(m)          253 non-null   float64 
 4   No. of Layer     253 non-null   int64  
 5   Curve Types      252 non-null   object  
 6   Thickness Topsoil h1(m) 253 non-null   float64 
 7   Thickness Laterite h2(m) 253 non-null   float64 
 8   Thickness weathered h3 (m) 253 non-null   float64 
 9   Corrected Thick. weathered (m) H3 253 non-null   float64 
 10  Thickness Fractured h4 (m) 253 non-null   float64 
 11  Corrected Thick. Fractured (m) H4 253 non-null   float64 
 12  Thick. Overb.    253 non-null   float64 
B1=h1+h2          253 non-null   float64 
 13 Total Aquifer Thick. B2=h3+h4 253 non-null   float64 
 14 Corrected Total Aquifer Thick 253 non-null   float64 
 15 p1               253 non-null   float64 
 16 p2               253 non-null   float64 
 17 p3               253 non-null   float64 
 18 p4               90 non-null   float64 
 19 p5               4 non-null   float64 
 20 Res. Of Topsoil  253 non-null   float64 
 21 Res. Of Laterite 253 non-null   float64 
 22 Long. Cond. (mhos) Topsoil 253 non-null   float64 
 23 Long. Cond. (mhos) Laterite 253 non-null   float64 
 24 Long. Cond. (mhos) OVERBURRDEN 253 non-null   float64 
 25 Logarithm of Topsoil   253 non-null   float64 
 26 RESISTIVITY OF FRESH BASEMENT 253 non-null   float64 
 27 Logarithm Fresh Basement 253 non-null   float64 
 28 AQUIFER RES of Weathered. (Ohm-M) 253 non-null   float64 
 29 Logarithm Weathered   253 non-null   float64 
 30 Hydraulic Conductivity (K) 253 non-null   float64 
 31 Transmissivity (T)      253 non-null   float64 
 32 Wrong              253 non-null   float64 
 33 Aquifer storage      253 non-null   float64 
dtypes: float64(31), int64(2), object(1)
memory usage: 67.3+ KB

```

Insights from description and info

- The average value for aquifer storage is found to be 22.4. According to the literature, it is recommended that an aquifer storage exceeding 60 percent is indicative of a good water-bearing capacity. This recommendation is from W.O. Raji and K.A. Abdulkadir in their 2020 study.
- Most of the values we want to use for the study are not null

Section 2: Feature Selection

In order to select the features that would be used in this project, plotting to visualize the data is essential. This will help visualize similarities between the features if any

Assumptions:

1. Easting: Represents longitude values. (X axis)
2. Northing: Represents latitude values. (Y axis)

```
In [ ]: cols_to_plot = [
    'Thickness Topsoil h1(m)', 'Thickness Laterite h2(m)',
    'Thickness weathered h3 (m)',
    'Thickness Fractured h4 (m)',
    'Thick. Overb.\nB1=h1+h2', 'Total Aquifer Thick. B2=h3+h4',
    'Corrected Total Aquifer Thick',
    'Res. Of Topsoil', 'Res. Of Laterite', 'Long. Cond. (mhos) Topsoil',
    'Long. Cond. (mhos) Laterite', 'Long. Cond. (mhos) OVERBURDEN',
    'Logarithm of Topsoil', 'RESISTIVITY OF FRESH BASEMENT',
    'Logarithm Fresh Basement', 'AQUIFER RES of Weathered. \n(Ohm-M)',
    'Logarithm Weathered', 'Hydraulic Conductivity (K)',
    'Transmissivity (T)', 'Aquifer storage '
]
```

```
In [ ]: # Create a function for making plots
def plot_features(df, cols_to_plot, scale_data=False, title="", add_scatt
.....
    Plot data for specified columns. Optionally scale the data before plot

Parameters:
- df: DataFrame containing the data
- cols_to_plot: list of columns to plot
- scale_data: boolean, if True, scale the data in cols_to_plot before
.....
# Copy the DataFrame to avoid modifying the original
df_to_plot = df.copy()

if scale_data:
    # Initialize StandardScaler
    scaler = RobustScaler()
    # Apply StandardScaler only to the specified columns
    df_to_plot[cols_to_plot] = scaler.fit_transform(df[cols_to_plot])

n_plots = len(cols_to_plot)
max_plots_per_row = 3

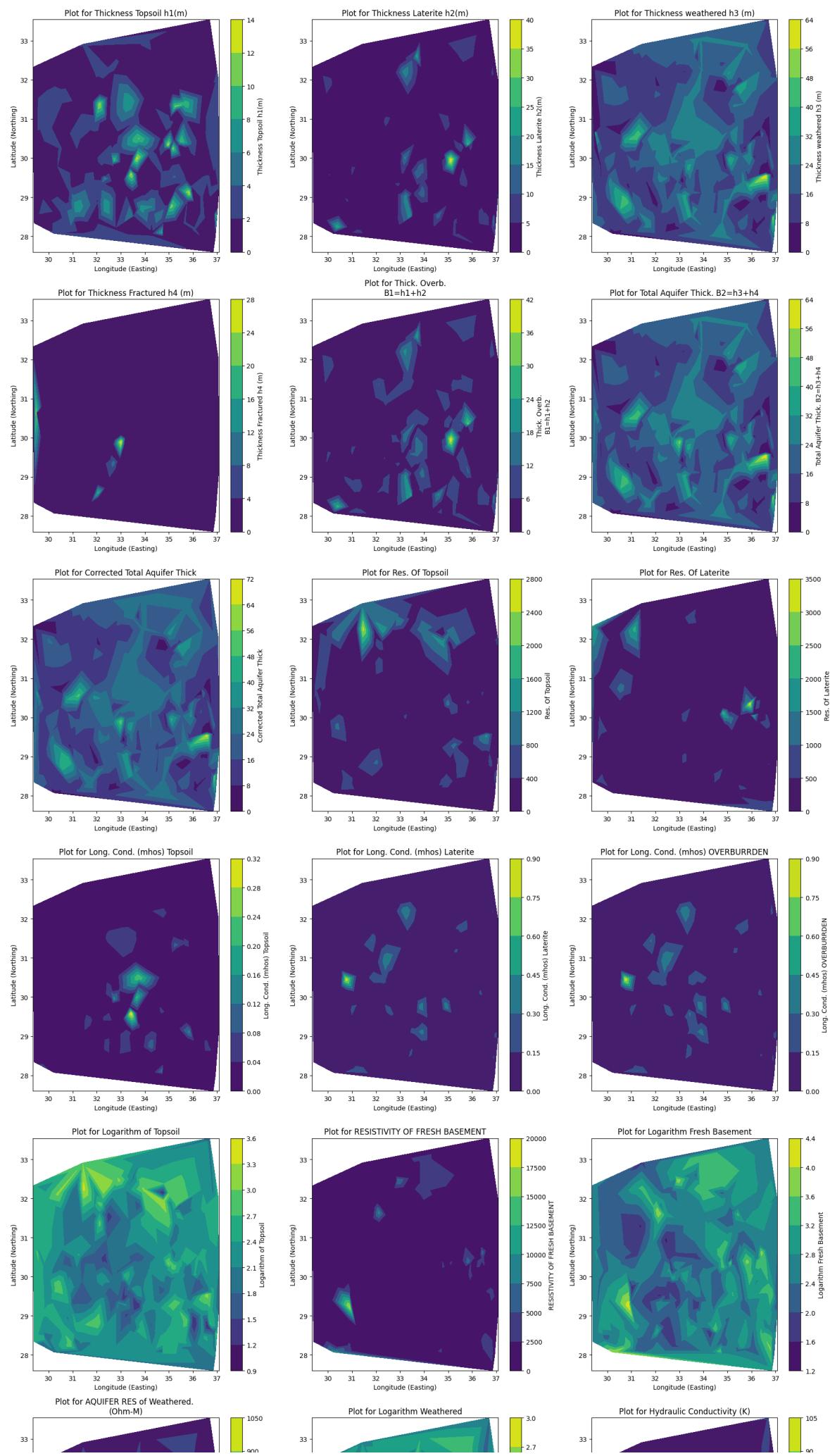
# Calculate nrows and ncols for subplots
ncols = min(n_plots, max_plots_per_row)
nrows = (n_plots + max_plots_per_row - 1) // max_plots_per_row

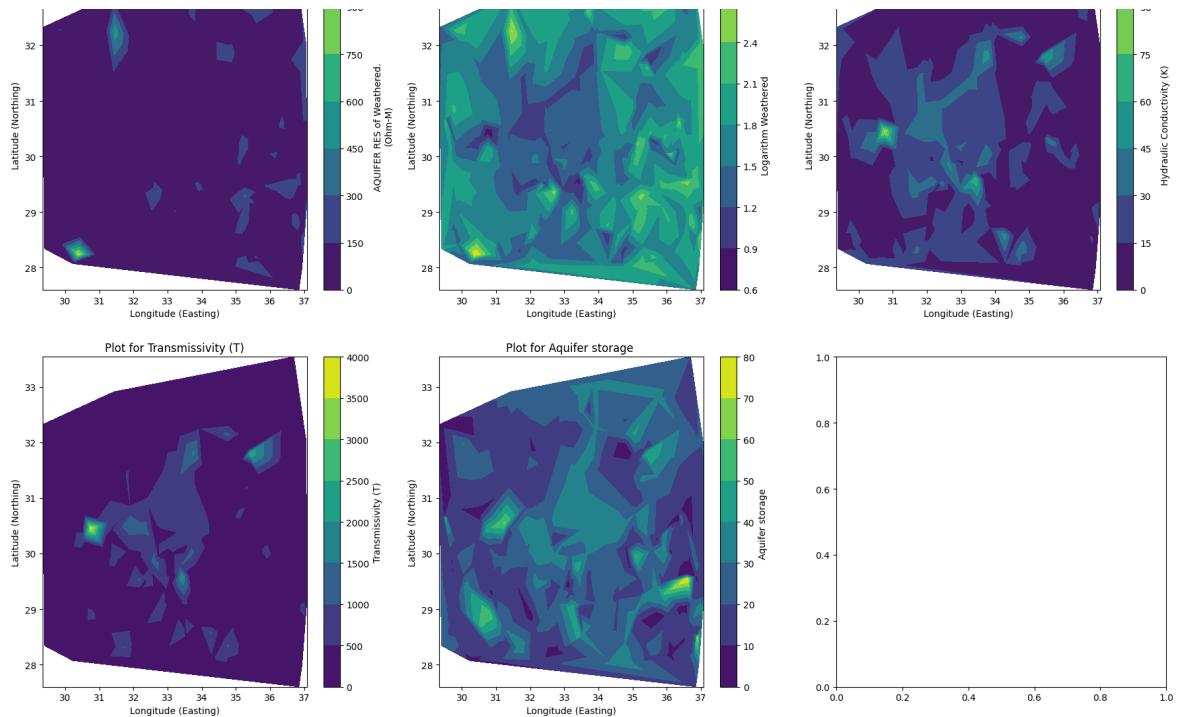
# Plotting the data on the same image
fig, axs = plt.subplots(nrows=nrows, ncols=ncols, figsize=(ncols*6, n
.....
# Add a general title for the entire plot
if title:
    fig.suptitle(title, fontsize=16)

for i, col in enumerate(cols_to_plot):
    # Calculate row and column index for subplot
    row = i // ncols
    col_idx = i % ncols
```

```
ax = axs[row, col_idx]
# Plot using original or scaled data as per the scale_data flag
contour = ax.tricontourf(df['Easting (Min)'], df['Northing (Min)'])
fig.colorbar(contour, ax=ax, label=col)
ax.set_title(f'Plot for {col}' + (' (Scaled)' if scale_data else ''))
ax.set_xlabel('Longitude (Easting)')
ax.set_ylabel('Latitude (Northing)')
# If add_scatter is True, superimpose a scatter plot
# If add_text_markers is True, use text to represent the scatter
if add_scatter:
    # Loop through data points to annotate with text
    for _, row_data in df.iterrows():
        ax.annotate(
            row_data['VES S/N'], # Text to represent the data point
            (row_data['Easting (Min)'], row_data['Northing (Min)']),
            color='black', # Color of the text
            fontsize=9, # Font size
            ha='center', # Horizontal alignment
            va='center', # Vertical alignment
        )
plt.tight_layout()
plt.show()
```

```
In [ ]: # Plot the raw features
plot_features(df_1, cols_to_plot, False)
```





Plot db on the map to visualize VES points

```
In [ ]: def plot_locations(df):
    # Create a scatter plot
    fig, ax = plt.subplots(figsize=(6,7))

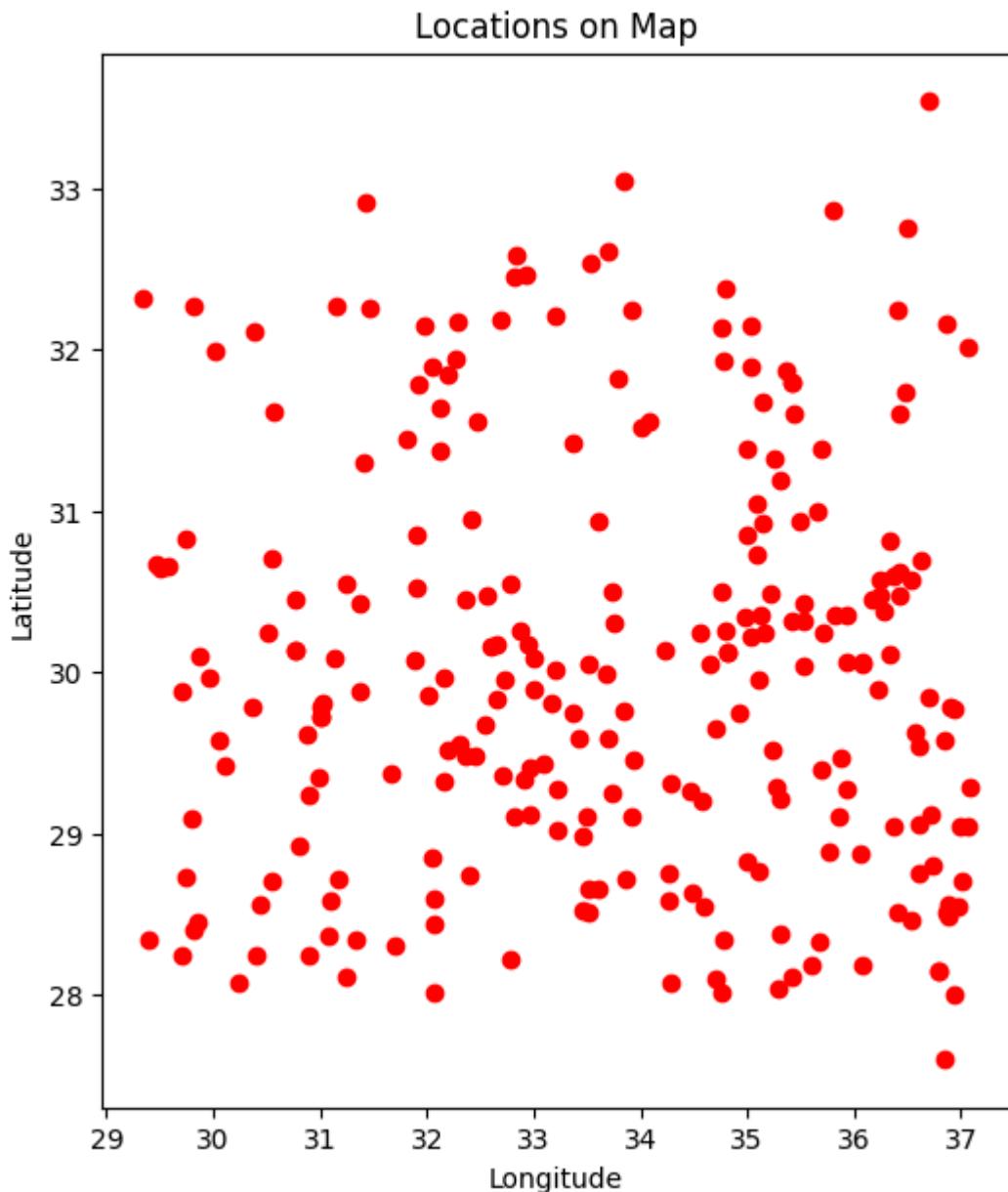
    ax.scatter(df['Easting (Min)'], df['Northing (Min)'], marker='o', color='red')

    # Set labels and title
    ax.set_xlabel('Longitude')
    ax.set_ylabel('Latitude')
    ax.set_title('Locations on Map')

    # Show plot
    plt.show()
```



```
In [ ]: plot_locations(df_1)
```



Plot Insights

- The plot for the thickness of the weathered layer is very similar to the plot for the aquifer storage. The goal of the final model is to predict the aquifer storage. This is insightful because this project can investigate how the final model would be improved or impaired by that feature.
- This same distinction can be seen when comparing the total aquifer thickness with the aquifer storage (this is logical as the larger the aquifer, the larger the expected yield of the aquifer.)
- From the plots some features could be removed, as they seem to be duplicates from a prediction point of view. e.g, corrected thicknesses, fracture thickness

Rank Features

Rank the features with different methods, in order to decide which features would be the most important for the study. Three correlation methods are considered for this;

- Pearson
- Spearman
- Kendall

```
In [ ]: # Create a function to plot correlation analysis
def plot_correlation_analysis(df, columns_to_check, column_to_correlate_aga
...
    Perform and plot correlation analysis between specified columns and a

Parameters:
- df (pandas.DataFrame): The DataFrame containing the data.
- columns_to_check (list of str): A list of column names to calculate
- column_to_correlate_against (str): The name of the column to correl
...
# Initialize a DataFrame to store the correlation results
correlation_results = []

# Loop through each column to calculate correlation coefficients
for column in columns_to_check:
    pearson_corr, _ = pearsonr(df[column], df[column_to_correlate_ag
    spearman_corr, _ = spearmanr(df[column], df[column_to_correlate_a
    kendall_corr, _ = kendalltau(df[column], df[column_to_correlate_a

    # Append the results to the list as a dictionary
    correlation_results.append({
        'Variable': column,
        'Pearson': pearson_corr,
        'Spearman': spearman_corr,
        'Kendall': kendall_corr
    })

# Convert the list to a DataFrame
correlation_results_df = pd.DataFrame(correlation_results)
correlation_results_df = correlation_results_df.melt(id_vars=['Variab
print(correlation_results_df)

# Plotting
sns.catplot(x='Coefficient', y='Variable', hue='Correlation Type', da
plt.title(f'Correlation Analysis with {column_to_correlate_against}')
plt.xlabel('Correlation Coefficient')
plt.ylabel('Variables')
plt.tight_layout()
plt.show()
```

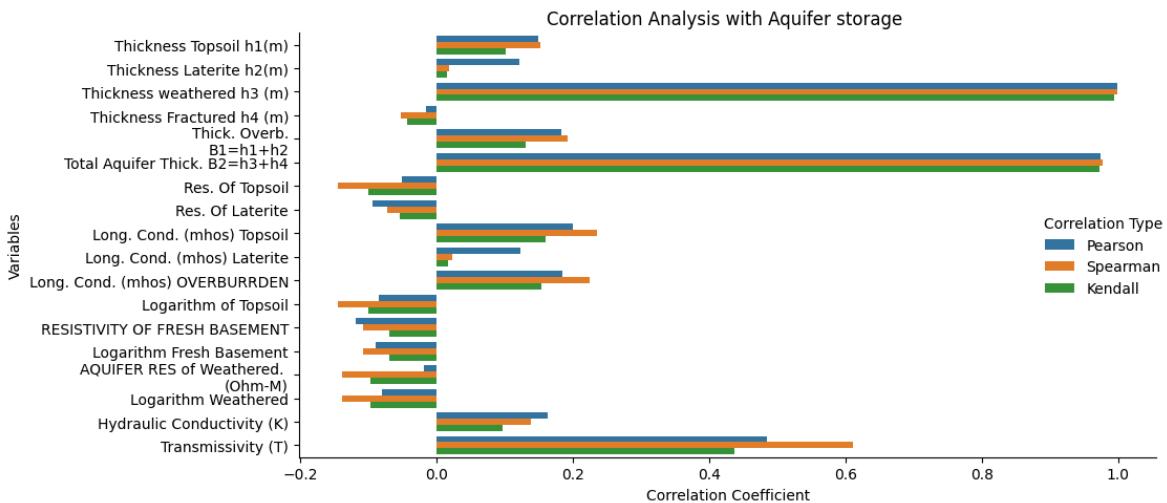
```
In [ ]: features_to_corr = [
    'Thickness Topsoil h1(m)', 'Thickness Laterite h2(m)',
    'Thickness weathered h3 (m)',
    'Thickness Fractured h4 (m)',
    'Thick. Overb.\nB1=h1+h2', 'Total Aquifer Thick. B2=h3+h4',
    'Res. Of Topsoil', 'Res. Of Laterite', 'Long. Cond. (mhos) Topsoil',
    'Long. Cond. (mhos) Laterite', 'Long. Cond. (mhos) OVERBURRDEN',
    'Logarithm of Topsoil', 'RESISTIVITY OF FRESH BASEMENT',
    'Logarithm Fresh Basement', 'AQUIFER RES of Weathered. \n(Ohm-M)',
    'Logarithm Weathered', 'Hydraulic Conductivity (K)',
```

'Transmissivity (T)',

]

In []: plot_correlation_analysis(df_1, features_to_corr, 'Aquifer storage')

	Variable	Correlation	Type	Coefficient
0	Thickness Topsoil h1(m)	Pearson	0.149565	
1	Thickness Laterite h2(m)	Pearson	0.121427	
2	Thickness weathered h3 (m)	Pearson	0.999225	
3	Thickness Fractured h4 (m)	Pearson	-0.016601	
4	Thick. Overb.\nB1=h1+h2	Pearson	0.182830	
5	Total Aquifer Thick. B2=h3+h4	Pearson	0.974173	
6	Res. Of Topsoil	Pearson	-0.051762	
7	Res. Of Laterite	Pearson	-0.093737	
8	Long. Cond. (mhos) Topsoil	Pearson	0.199653	
9	Long. Cond. (mhos) Laterite	Pearson	0.121976	
10	Long. Cond. (mhos) OVERBURRDEN	Pearson	0.184247	
11	Logarithm of Topsoil	Pearson	-0.084771	
12	RESISTIVITY OF FRESH BASEMENT	Pearson	-0.119565	
13	Logarithm Fresh Basement	Pearson	-0.089655	
14	AQUIFER RES of Weathered. \n(Ohm-M)	Pearson	-0.019119	
15	Logarithm Weathered	Pearson	-0.080903	
16	Hydraulic Conductivity (K)	Pearson	0.162177	
17	Transmissivity (T)	Pearson	0.484136	
18	Thickness Topsoil h1(m)	Spearman	0.152381	
19	Thickness Laterite h2(m)	Spearman	0.017991	
20	Thickness weathered h3 (m)	Spearman	0.999122	
21	Thickness Fractured h4 (m)	Spearman	-0.052515	
22	Thick. Overb.\nB1=h1+h2	Spearman	0.192251	
23	Total Aquifer Thick. B2=h3+h4	Spearman	0.977808	
24	Res. Of Topsoil	Spearman	-0.145283	
25	Res. Of Laterite	Spearman	-0.072456	
26	Long. Cond. (mhos) Topsoil	Spearman	0.234784	
27	Long. Cond. (mhos) Laterite	Spearman	0.022671	
28	Long. Cond. (mhos) OVERBURRDEN	Spearman	0.224567	
29	Logarithm of Topsoil	Spearman	-0.145283	
30	RESISTIVITY OF FRESH BASEMENT	Spearman	-0.108986	
31	Logarithm Fresh Basement	Spearman	-0.108986	
32	AQUIFER RES of Weathered. \n(Ohm-M)	Spearman	-0.138672	
33	Logarithm Weathered	Spearman	-0.138672	
34	Hydraulic Conductivity (K)	Spearman	0.138672	
35	Transmissivity (T)	Spearman	0.610228	
36	Thickness Topsoil h1(m)	Kendall	0.101673	
37	Thickness Laterite h2(m)	Kendall	0.015624	
38	Thickness weathered h3 (m)	Kendall	0.994315	
39	Thickness Fractured h4 (m)	Kendall	-0.043257	
40	Thick. Overb.\nB1=h1+h2	Kendall	0.129861	
41	Total Aquifer Thick. B2=h3+h4	Kendall	0.972838	
42	Res. Of Topsoil	Kendall	-0.100154	
43	Res. Of Laterite	Kendall	-0.054790	
44	Long. Cond. (mhos) Topsoil	Kendall	0.159451	
45	Long. Cond. (mhos) Laterite	Kendall	0.017110	
46	Long. Cond. (mhos) OVERBURRDEN	Kendall	0.153257	
47	Logarithm of Topsoil	Kendall	-0.100154	
48	RESISTIVITY OF FRESH BASEMENT	Kendall	-0.069306	
49	Logarithm Fresh Basement	Kendall	-0.069306	
50	AQUIFER RES of Weathered. \n(Ohm-M)	Kendall	-0.097077	
51	Logarithm Weathered	Kendall	-0.097077	
52	Hydraulic Conductivity (K)	Kendall	0.097077	
53	Transmissivity (T)	Kendall	0.436888	



Insights from the plot

Two features, weathered thickness and aquifer thickness seem to be very highly correlated with aquifer storage. The following features will be selected for training from the plots; the features selected generally have correlation greater than or equal to 0.2

1. Thickness Topsoil h1(m)
2. Thickness weathered h3 (m) (high correlation)
3. Thick. Overb.\nB1=h1+h2
4. Total Aquifer Thick. B2=h3+h4 (high correlation)
5. Long. Cond. (mhos) OVERBURRDEN
6. Long. Cond. (mhos) Topsoil
7. Transmissivity (T)

```
In [ ]: # The following features will be used for the rest of the analysis.
all_selected_features = [
    'Thickness Topsoil h1(m)',
    'Thickness weathered h3 (m)',
    'Thick. Overb.\nB1=h1+h2',
    'Total Aquifer Thick. B2=h3+h4',
    'Long. Cond. (mhos) OVERBURRDEN',
    'Long. Cond. (mhos) Topsoil',
    'Transmissivity (T)',
]

features_without_high_corr = [
    'Thickness Topsoil h1(m)',
    'Thick. Overb.\nB1=h1+h2',
    'Long. Cond. (mhos) Topsoil',
    'Long. Cond. (mhos) OVERBURRDEN',
    'Transmissivity (T)',
]

features_without_weathered_thick = [
    'Thickness Topsoil h1(m)',
    'Thick. Overb.\nB1=h1+h2',
    'Total Aquifer Thick. B2=h3+h4',
    'Long. Cond. (mhos) OVERBURRDEN',
]
```

```

'Long. Cond. (mhos) Topsoil',
'Transmissivity (T)',

]

features_without_aquifer_thick = [
    'Thickness Topsoil h1(m)',
    'Thickness weathered h3 (m)',
    'Thick. Overb.\nB1=h1+h2',
    'Long. Cond. (mhos) OVERBURDEN',
    'Long. Cond. (mhos) Topsoil',
    'Transmissivity (T)',
]

```

Section 3: Preprocessing data

The selected features have been broken down into categories. In order to preprocess the data, two major step taken is to transform the features.

Transform features

It is important to do some level of feature transformation in any machine learning project. The idea is to modify the features in the dataset to improve the performance and accuracy of the machine learning models.

```
In [ ]: # function to scale features as needed
def scale_features(df, feature_columns, label):
    """
    Scales the specified features in the DataFrame using StandardScaler.

    Parameters:
    - df: pandas DataFrame containing the data.
    - feature_columns: List of column names to be scaled.
    - label: String name of the label column

    """
    scaler = StandardScaler()

    # Copy the original DataFrame to avoid modifying it directly
    df_scaled = df.copy()

    df_scaled[feature_columns] = scaler.fit_transform(df_scaled[feature_c

    df_scaled['Aquifer Storage'] = df[label]
    df_scaled["VES S/N"] = df["VES S/N"]
    df_scaled[["Easting (Min)", "Northing (Min)"]] = df[["Easting (Min)"]
    return df_scaled

In [ ]: # feature scaling for all feature groups
# creating scaled version of all feature groups
```

```
df_all_predicted = scale_features(df_1, all_selected_features, 'Aquifer s
df_without_high_corr = scale_features(df_1, features_without_high_corr,
df_without_weathered_thick = scale_features(df_1, features_without_weath
df_without_aquifer_thick = scale_features(df_1, features_without_aquifer_
```

In []: df_all_predicted.head()

	Thickness Topsoil h1(m)	Thickness weathered h3 (m)	Thick. Overb.\nB1=h1+h2	Total Aquifer Thick. B2=h3+h4	Long. Cond. (mhos) OVERBURRDEN	Long Cond (mhos Topsoi
0	-0.468424	0.641042	0.273002	0.596086	-0.234145	-0.309435
1	-0.590811	0.565512	-0.407114	0.522118	-0.505891	-0.519935
2	-0.590811	-0.858771	-0.709387	-0.872713	0.098037	1.365838
3	-0.550016	-1.160891	-0.690495	-1.168587	-0.523319	-0.479188
4	0.102715	4.827571	-0.388222	4.696045	-0.533278	-0.508759

In []: df_without_high_corr.head()

	Thickness Topsoil h1(m)	Thick. Overb.\nB1=h1+h2	Long. Cond. (mhos) Topsoil	Long. Cond. (mhos) OVERBURRDEN	Transmissivity (T)	Aqui Stora
0	-0.468424	0.273002	-0.309435	-0.234145	-0.179934	30.017
1	-0.590811	-0.407114	-0.519935	-0.505891	-0.657226	29.119
2	-0.590811	-0.709387	1.365838	0.098037	-0.598868	12.186
3	-0.550016	-0.690495	-0.479188	-0.523319	-0.738212	8.594
4	0.102715	-0.388222	-0.508759	-0.533278	-0.465206	79.790

Key insights

- Features are now scaled as seen in the printed out values of the data
- Aquifer storage has been renamed to label just for clarity and to make it easy to work with

Split data and train ML model

The scaled data will be split at a ratio of 70:30.

- 70% of the data will be used for training the model
- 30% of the data will be used for testing the data

Multiple ML models will be tested to evaluate which works best. This is a regression problem so the major regression models will be evaluated on effectiveness;

1. Linear Regression

2. Decision Tree Regression
3. Random Forest Regressor
4. Linear SVR

```
In [ ]: def evaluate_models(df, features, target, models=None, title=""):  
    # Split the data into features (X) and target (y)  
    features_with_sn = features + ["VES S/N"]  
    X = df[features_with_sn]  
    y = df[target]  
  
    default_models = [  
        ('Linear Regression', LinearRegression()),  
        ('Decision Tree Regressor', DecisionTreeRegressor()),  
        ('Random Forest Regressor', RandomForestRegressor()),  
        ("Linear SVR", LinearSVR())  
    ]  
  
    # If no models are provided, use the default models  
    if models is None:  
        models = default_models  
  
    # Split data into training and testing sets  
    X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0  
X_train_with_sn = X_train.copy()  
X_test_with_sn = X_test.copy()  
X_train = X_train.drop("VES S/N", axis=1)  
X_test = X_test.drop("VES S/N", axis=1)  
results = []  
best_score = float('-inf')  
best_model = None  
  
for name, model in models:  
    # Perform cross-validation  
    cv_scores = cross_val_score(model, X_train, y_train, cv=5)  
    cv_mean = np.mean(cv_scores)  
  
    # Fit the model on the full training data and evaluate on the test data  
    model.fit(X_train, y_train)  
    y_pred = model.predict(X_test)  
  
    test_df = df.loc[X_test.index].copy()  
    predicted_col_name = f'Predicted {target}'  
    test_df[predicted_col_name] = y_pred  
    test_df["VES S/N"] = X_test_with_sn["VES S/N"]  
    plot_features(test_df, [target, predicted_col_name], title=f'{name} Model')  
  
    test_score = mean_squared_error(y_test, y_pred, squared=False) #  
  
    results.append({  
        'Model': name,  
        'Average Accuracy (CV Mean Score)': cv_mean,  
        'Test Score': test_score  
    })  
  
    # Update the best model if this model has a better score  
    if cv_mean > best_score:  
        best_score = cv_mean  
        best_model = model
```

```

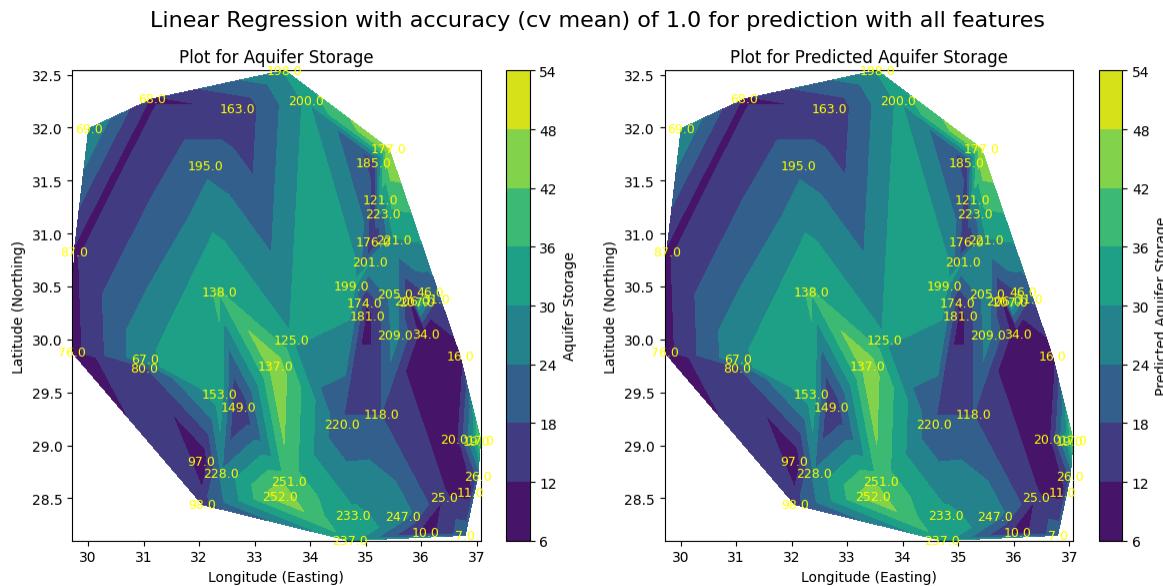
results_df = pd.DataFrame(results)

# Print the best model
print(f'{best_model} is the best model with a CV mean score / accuracy of {cv_mean:.4f} %')
# Predict with the best model for the test dataset
predicted_col_name = f'Predicted {target}'
test_predictions = best_model.predict(X_test)
test_df = df.loc[X_test.index].copy()
test_df[predicted_col_name] = test_predictions
test_df["VES S/N"] = X_test_with_sn["VES S/N"]

# Return the evaluation results and the DataFrame with predictions on
return results_df, test_df

```

In []: results, df_pred = evaluate_models(df_all_predicted, all_selected_feature)

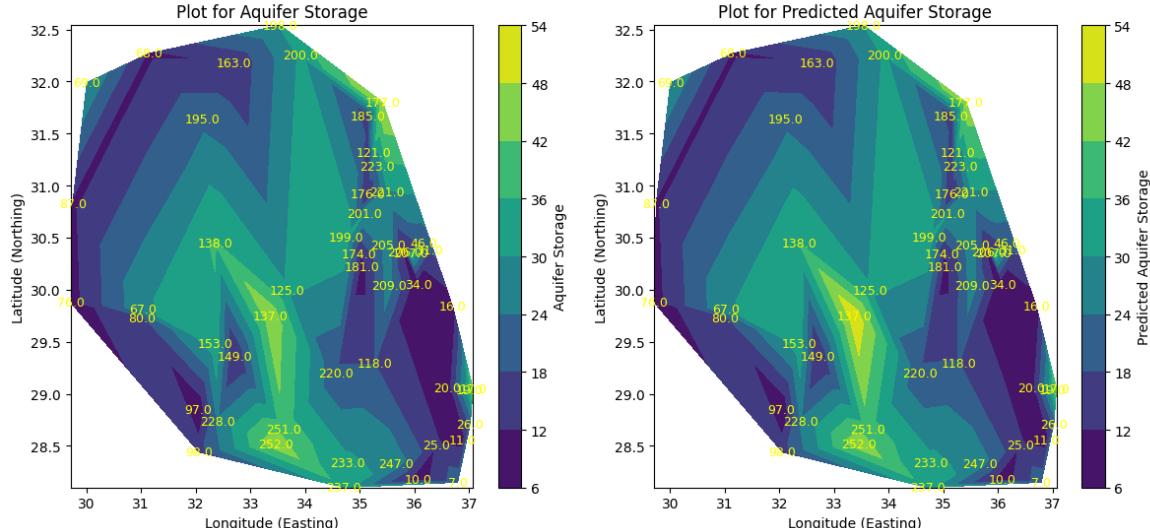


```

/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/metrics/_regression.py:483: FutureWarning: 'squared' is deprecated in version 1.4 and will be removed in 1.6. To calculate the root mean squared error, use the function 'root_mean_squared_error'.
warnings.warn(

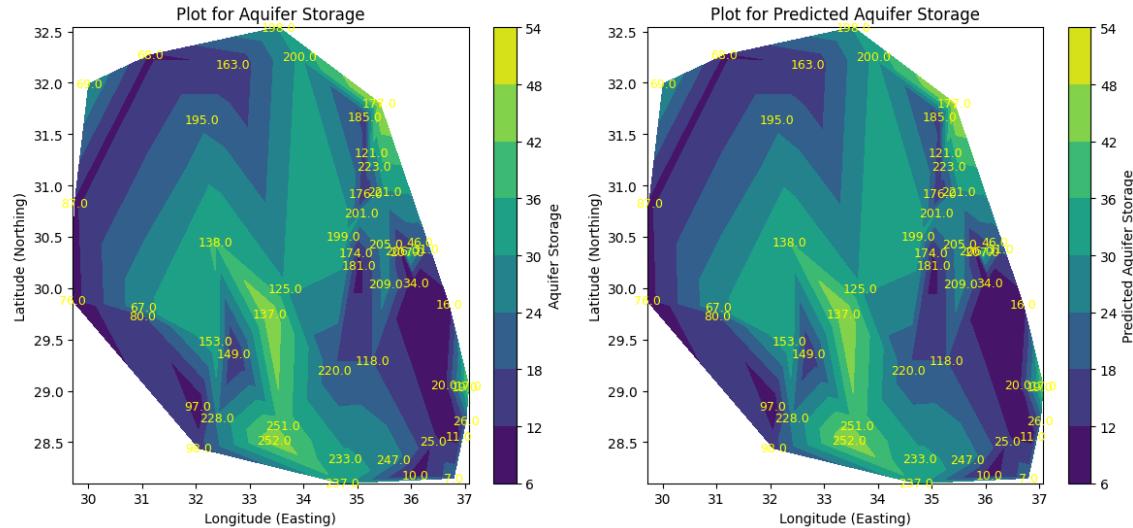
```

Decision Tree Regressor with accuracy (cv mean) of 0.9801431828371798 for prediction with all features



```
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/metrics/_regression.py:483: FutureWarning: 'squared' is deprecated in version 1.4 and will be removed in 1.6. To calculate the root mean squared error, use the function 'root_mean_squared_error'.
  warnings.warn(
```

Random Forest Regressor with accuracy (cv mean) of 0.9639842744264708 for prediction with all features



```
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/metrics/_regression.py:483: FutureWarning: 'squared' is deprecated in version 1.4 and will be removed in 1.6. To calculate the root mean squared error, use the function 'root_mean_squared_error'.
  warnings.warn(
```

```
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `auto` in 1.5. Set the value of `dual` explicitly to suppress the warning.
  warnings.warn(
```

```
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `auto` in 1.5. Set the value of `dual` explicitly to suppress the warning.
  warnings.warn(
```

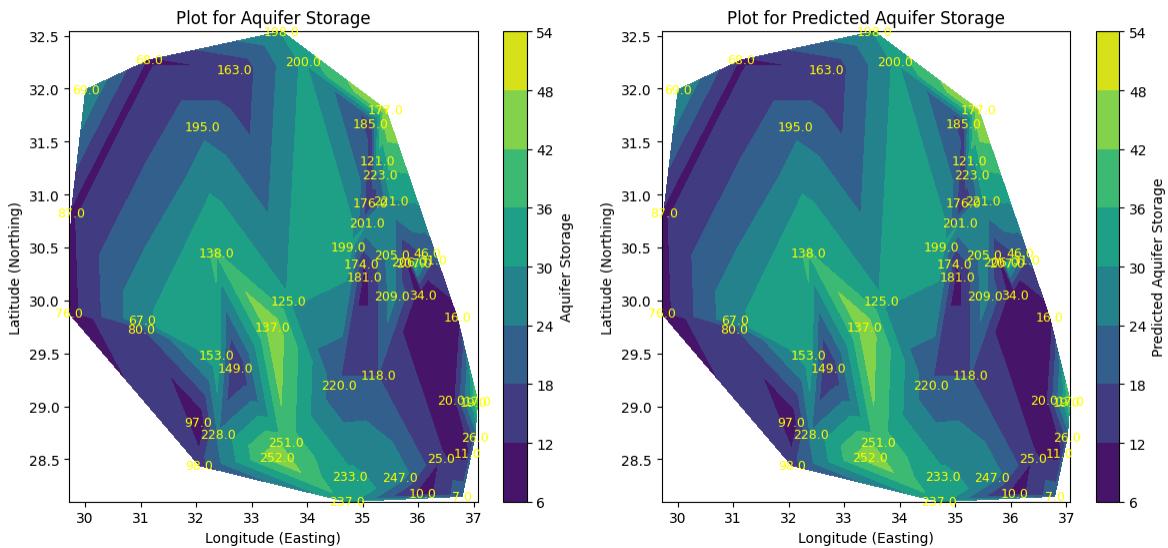
```
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `auto` in 1.5. Set the value of `dual` explicitly to suppress the warning.
  warnings.warn(
```

```
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `auto` in 1.5. Set the value of `dual` explicitly to suppress the warning.
  warnings.warn(
```

```
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `auto` in 1.5. Set the value of `dual` explicitly to suppress the warning.
  warnings.warn(
```

```
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `auto` in 1.5. Set the value of `dual` explicitly to suppress the warning.
  warnings.warn(
```

Linear SVR with accuracy (cv mean) of 0.9962738714621449 for prediction with all features



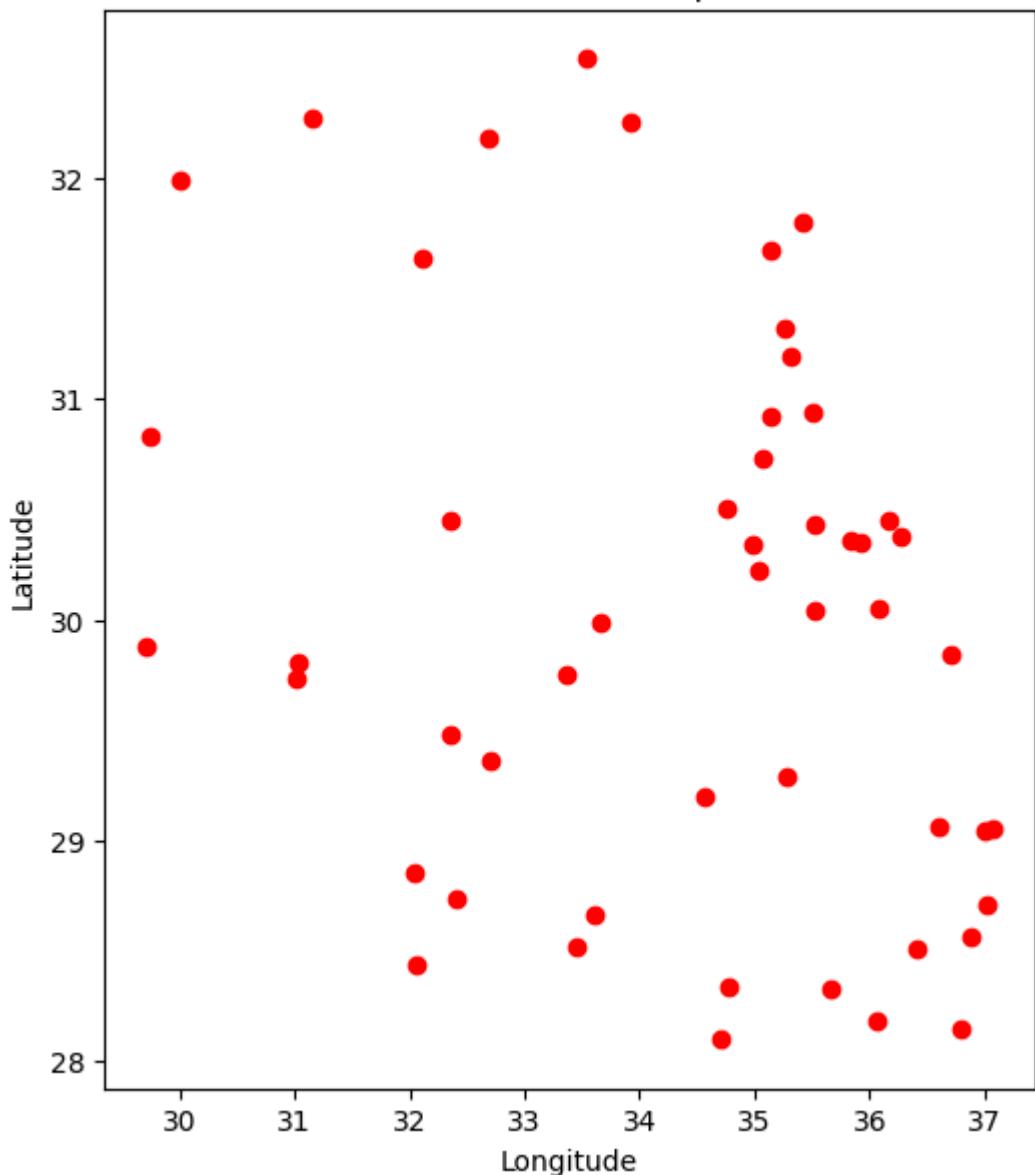
LinearRegression() is the best model with a CV mean score / accuracy score of 1.0.

```
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/metrics/_regression.py:483: FutureWarning: 'squared' is deprecated in version 1.4 and will be removed in 1.6. To calculate the root mean squared error, use the function 'root_mean_squared_error'.
    warnings.warn(
```

Plot data points of predicted values

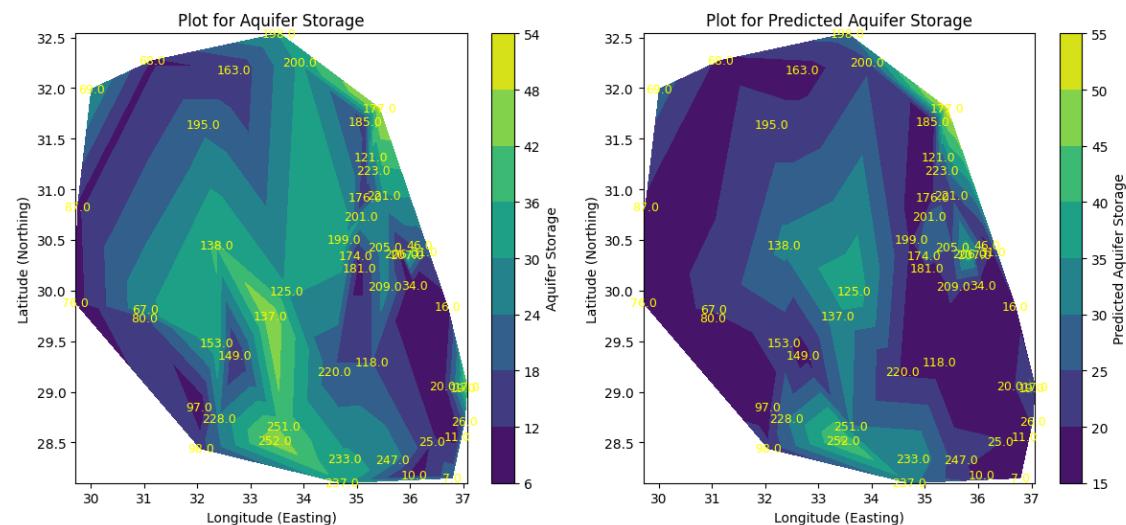
```
In [ ]: plot_locations(df_pred)
```

Locations on Map



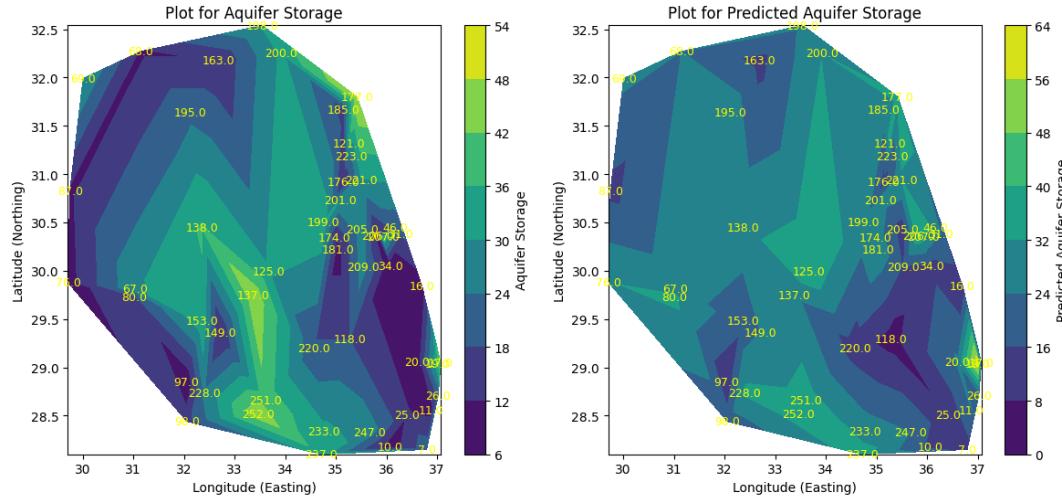
```
In [ ]: results_whc, df_pred_whc = evaluate_models(df_without_high_corr, feature
```

Linear Regression with accuracy (cv mean) of 0.18017291862228846 for prediction without high correlators



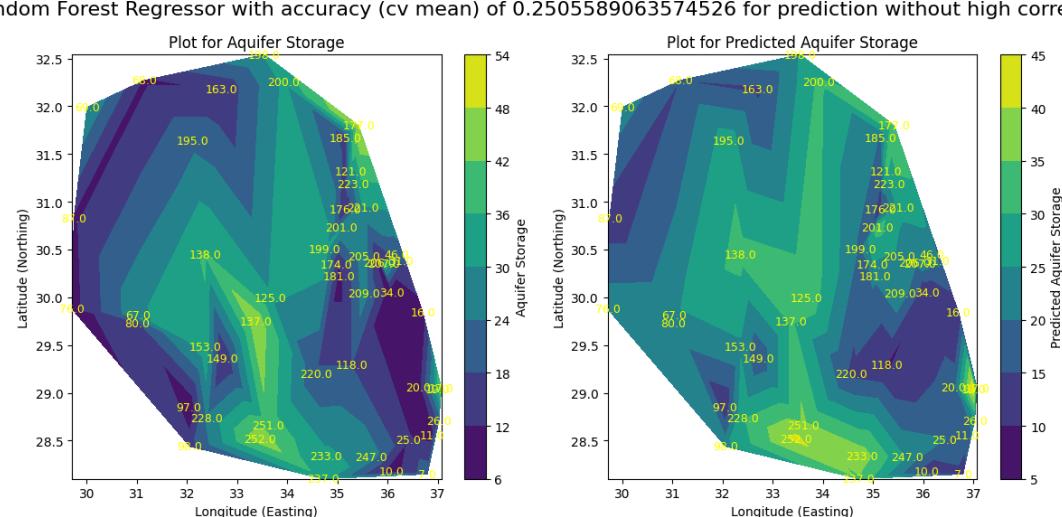
```
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/metrics/_regression.py:483: FutureWarning: 'squared' is deprecated in version 1.4 and will be removed in 1.6. To calculate the root mean squared error, use the function 'root_mean_squared_error'.
warnings.warn(
```

Decision Tree Regressor with accuracy (cv mean) of -0.2513922181530209 for prediction without high correlators



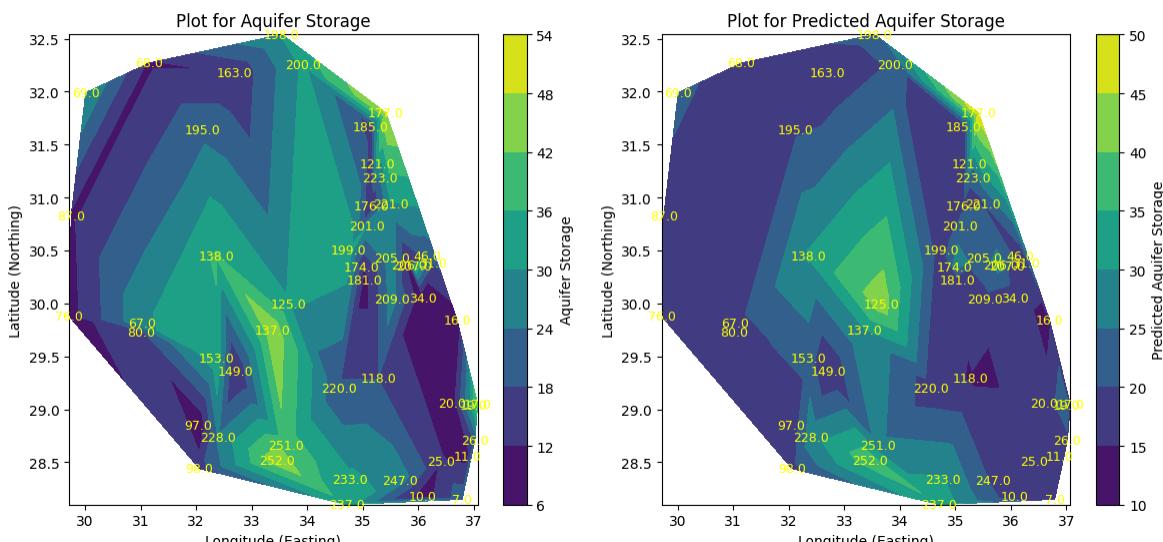
```
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/metrics/_regression.py:483: FutureWarning: 'squared' is deprecated in version 1.4 and will be removed in 1.6. To calculate the root mean squared error, use the function 'root_mean_squared_error'.
warnings.warn(
```

Random Forest Regressor with accuracy (cv mean) of 0.2505589063574526 for prediction without high correlators



```
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/metrics/_regression.py:483: FutureWarning: 'squared' is deprecated in version 1.4 and will be removed in 1.6. To calculate the root mean squared error, use the function 'root_mean_squared_error'.
    warnings.warn(
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `auto` in 1.5. Set the value of `dual` explicitly to suppress the warning.
    warnings.warn(
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `auto` in 1.5. Set the value of `dual` explicitly to suppress the warning.
    warnings.warn(
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `auto` in 1.5. Set the value of `dual` explicitly to suppress the warning.
    warnings.warn(
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `auto` in 1.5. Set the value of `dual` explicitly to suppress the warning.
    warnings.warn(
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `auto` in 1.5. Set the value of `dual` explicitly to suppress the warning.
    warnings.warn(
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `auto` in 1.5. Set the value of `dual` explicitly to suppress the warning.
    warnings.warn(
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `auto` in 1.5. Set the value of `dual` explicitly to suppress the warning.
    warnings.warn(
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `auto` in 1.5. Set the value of `dual` explicitly to suppress the warning.
```

Linear SVR with accuracy (cv mean) of 0.12221561022021629 for prediction without high correlators

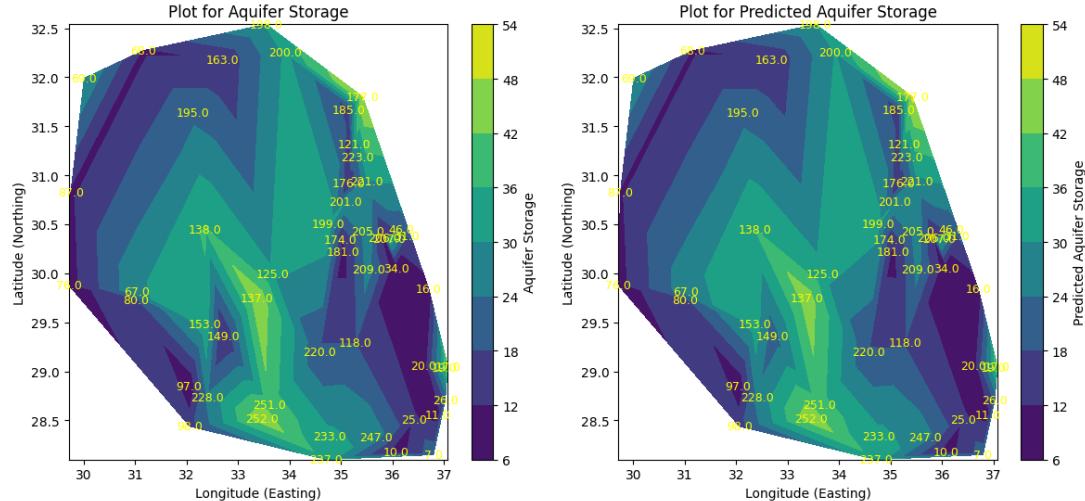


RandomForestRegressor() is the best model with a CV mean score / accuracy score of 0.2505589063574526.

```
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/metrics/_regression.py:483: FutureWarning: 'squared' is deprecated in version 1.4 and will be removed in 1.6. To calculate the root mean squared error, use the function 'root_mean_squared_error'.
    warnings.warn(
```

```
In [ ]: results_wwt, df_pred_wwt = evaluate_models(df_without_weathered_thick, f
```

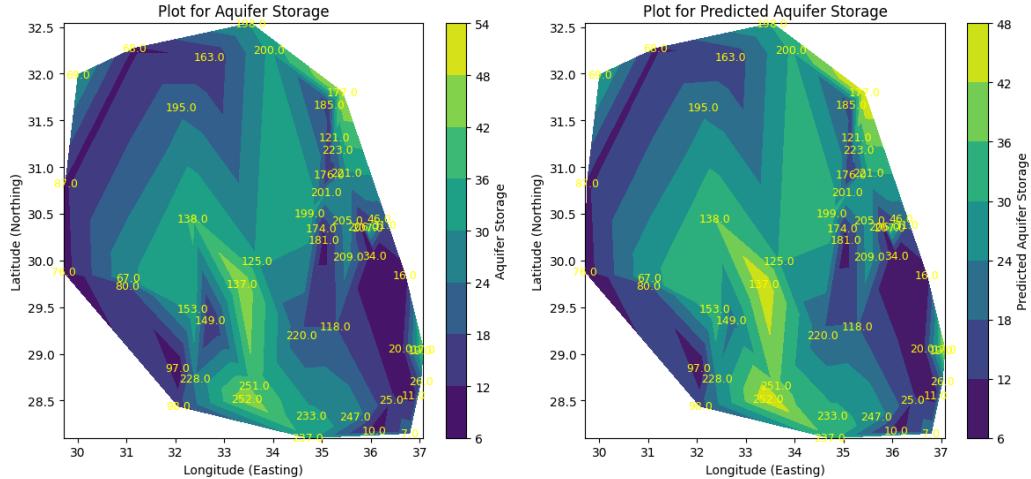
Linear Regression with accuracy (cv mean) of 0.9109362093015712 for prediction without weathered thickness



/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/metrics/_regression.py:483: FutureWarning: 'squared' is deprecated in version 1.4 and will be removed in 1.6. To calculate the root mean squared error, use the function 'root_mean_squared_error'.

```
warnings.warn(
```

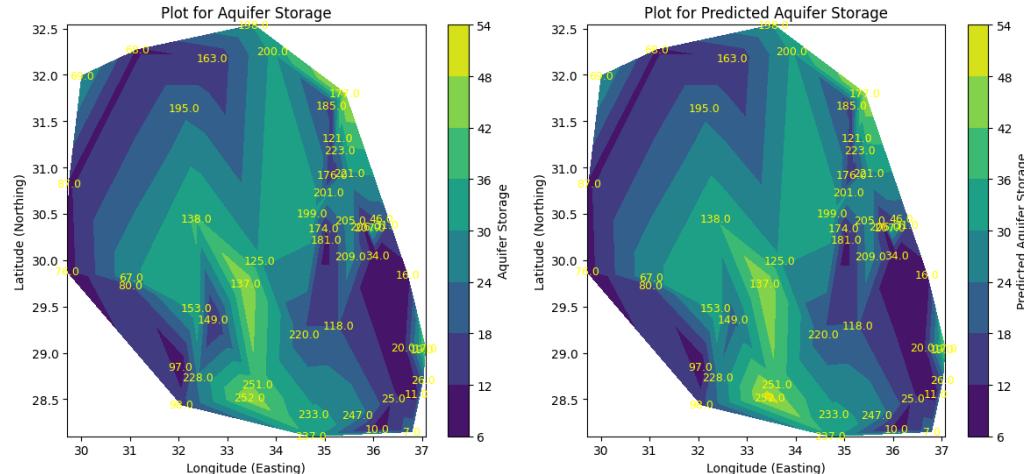
Decision Tree Regressor with accuracy (cv mean) of 0.8473775945645793 for prediction without weathered thickness



/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/metrics/_regression.py:483: FutureWarning: 'squared' is deprecated in version 1.4 and will be removed in 1.6. To calculate the root mean squared error, use the function 'root_mean_squared_error'.

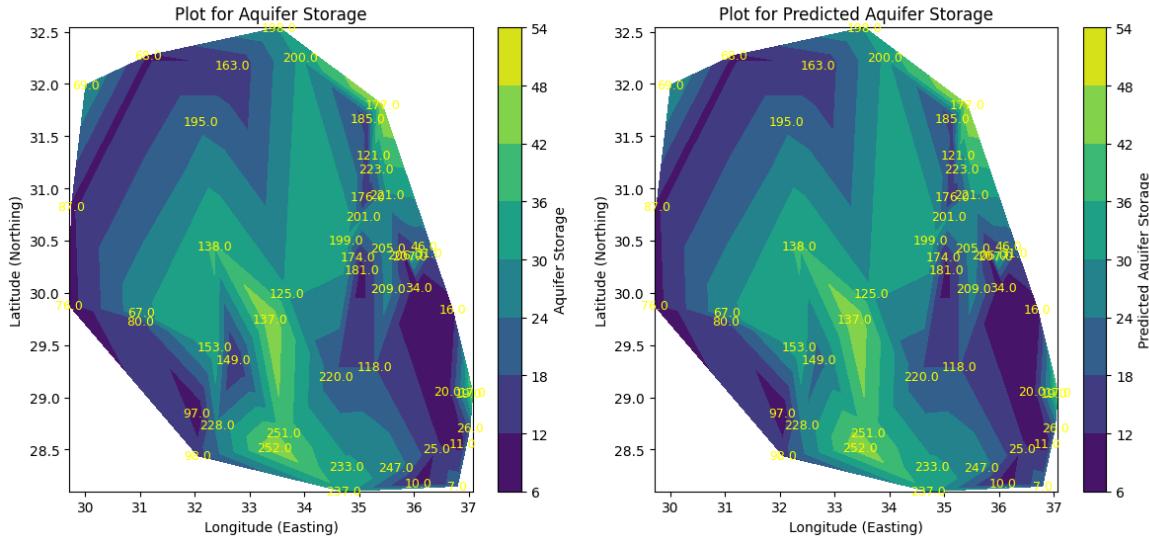
```
warnings.warn(
```

Random Forest Regressor with accuracy (cv mean) of 0.869792986195699 for prediction without weathered thickness



```
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/metrics/_regression.py:483: FutureWarning: 'squared' is deprecated in version 1.4 and will be removed in 1.6. To calculate the root mean squared error, use the function 'root_mean_squared_error'.
    warnings.warn(
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `'auto'` in 1.5. Set the value of `dual` explicitly to suppress the warning.
    warnings.warn(
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `'auto'` in 1.5. Set the value of `dual` explicitly to suppress the warning.
    warnings.warn(
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `'auto'` in 1.5. Set the value of `dual` explicitly to suppress the warning.
    warnings.warn(
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `'auto'` in 1.5. Set the value of `dual` explicitly to suppress the warning.
    warnings.warn(
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `'auto'` in 1.5. Set the value of `dual` explicitly to suppress the warning.
    warnings.warn(
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `'auto'` in 1.5. Set the value of `dual` explicitly to suppress the warning.
```

Linear SVR with accuracy (cv mean) of 0.9094173670295447 for prediction without weathered thickness

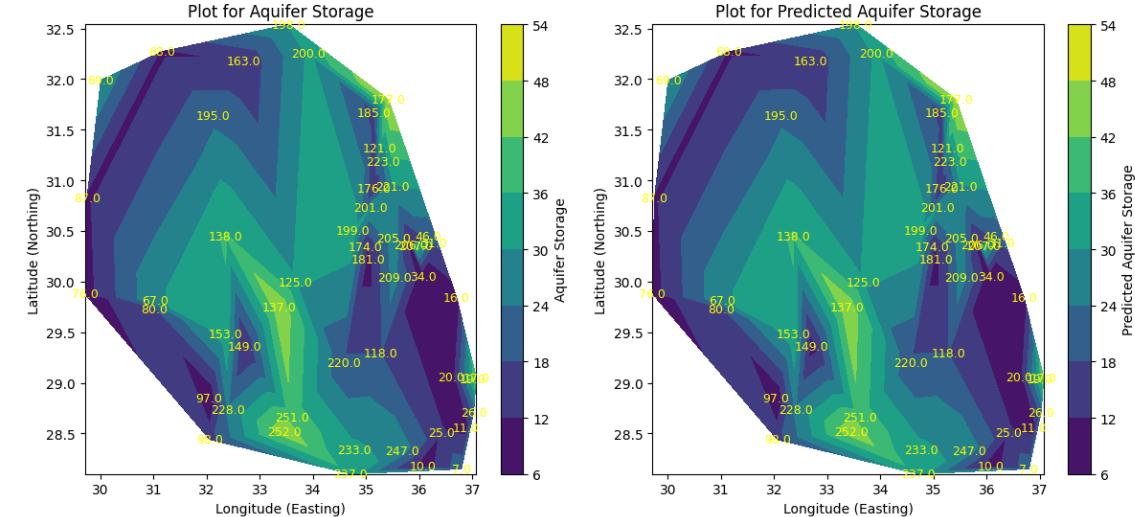


LinearRegression() is the best model with a CV mean score / accuracy score of 0.9109362093015712.

```
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/metrics/_regression.py:483: FutureWarning: 'squared' is deprecated in version 1.4 and will be removed in 1.6. To calculate the root mean squared error, use the function 'root_mean_squared_error'.
warnings.warn(
```

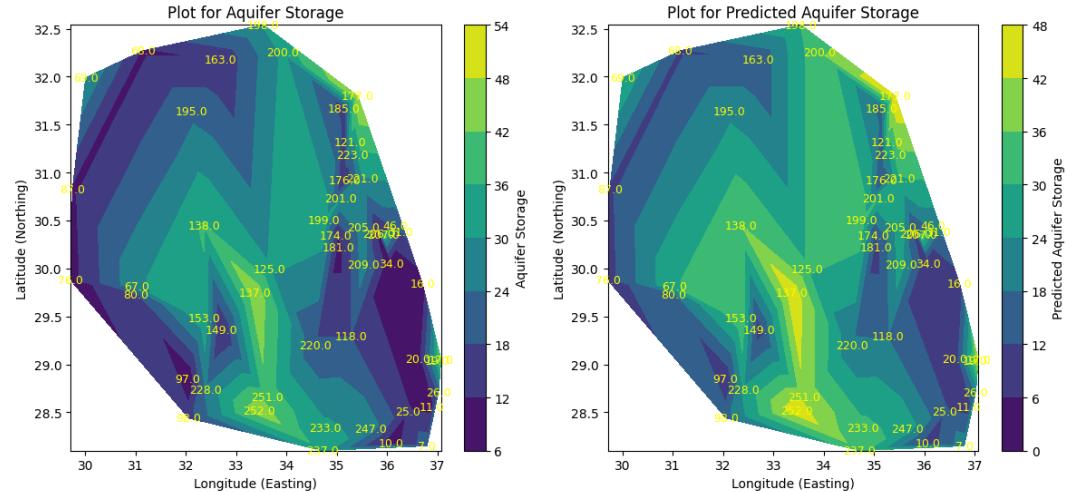
In []: results_wat, df_pred_wat = evaluate_models(df_without_aquifer_thick, fea

Linear Regression with accuracy (cv mean) of 0.9973361885316774 for prediction without aquifer thickness



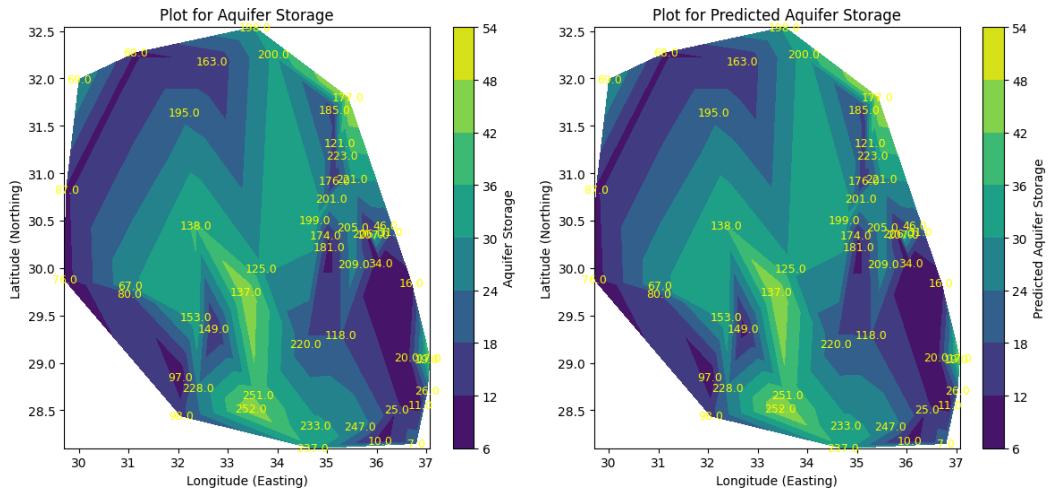
```
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/metrics/_regression.py:483: FutureWarning: 'squared' is deprecated in version 1.4 and will be removed in 1.6. To calculate the root mean squared error, use the function 'root_mean_squared_error'.
warnings.warn(
```

Decision Tree Regressor with accuracy (cv mean) of 0.9650901083151113 for prediction without aquifer thickness



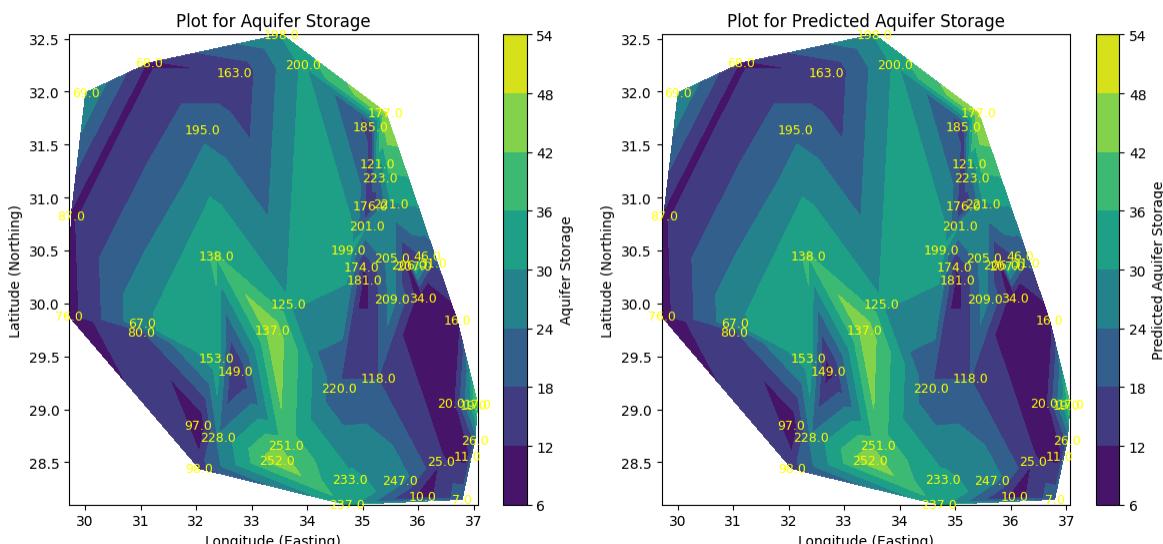
```
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/metrics/_regression.py:483: FutureWarning: 'squared' is deprecated in version 1.4 and will be removed in 1.6. To calculate the root mean squared error, use the function 'root_mean_squared_error'.
warnings.warn(
```

Random Forest Regressor with accuracy (cv mean) of 0.9787459006913878 for prediction without aquifer thickness



```
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/metrics/_regression.py:483: FutureWarning: 'squared' is deprecated in version 1.4 and will be removed in 1.6. To calculate the root mean squared error, use the function 'root_mean_squared_error'.
    warnings.warn(
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `auto` in 1.5. Set the value of `dual` explicitly to suppress the warning.
    warnings.warn(
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `auto` in 1.5. Set the value of `dual` explicitly to suppress the warning.
    warnings.warn(
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `auto` in 1.5. Set the value of `dual` explicitly to suppress the warning.
    warnings.warn(
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `auto` in 1.5. Set the value of `dual` explicitly to suppress the warning.
    warnings.warn(
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `auto` in 1.5. Set the value of `dual` explicitly to suppress the warning.
    warnings.warn(
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `auto` in 1.5. Set the value of `dual` explicitly to suppress the warning.
    warnings.warn(
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `auto` in 1.5. Set the value of `dual` explicitly to suppress the warning.
    warnings.warn(
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/svm/_classes.py:31: FutureWarning: The default value of `dual` will change from `True` to `auto` in 1.5. Set the value of `dual` explicitly to suppress the warning.
```

Linear SVR with accuracy (cv mean) of 0.9973595779820302 for prediction without aquifer thickness



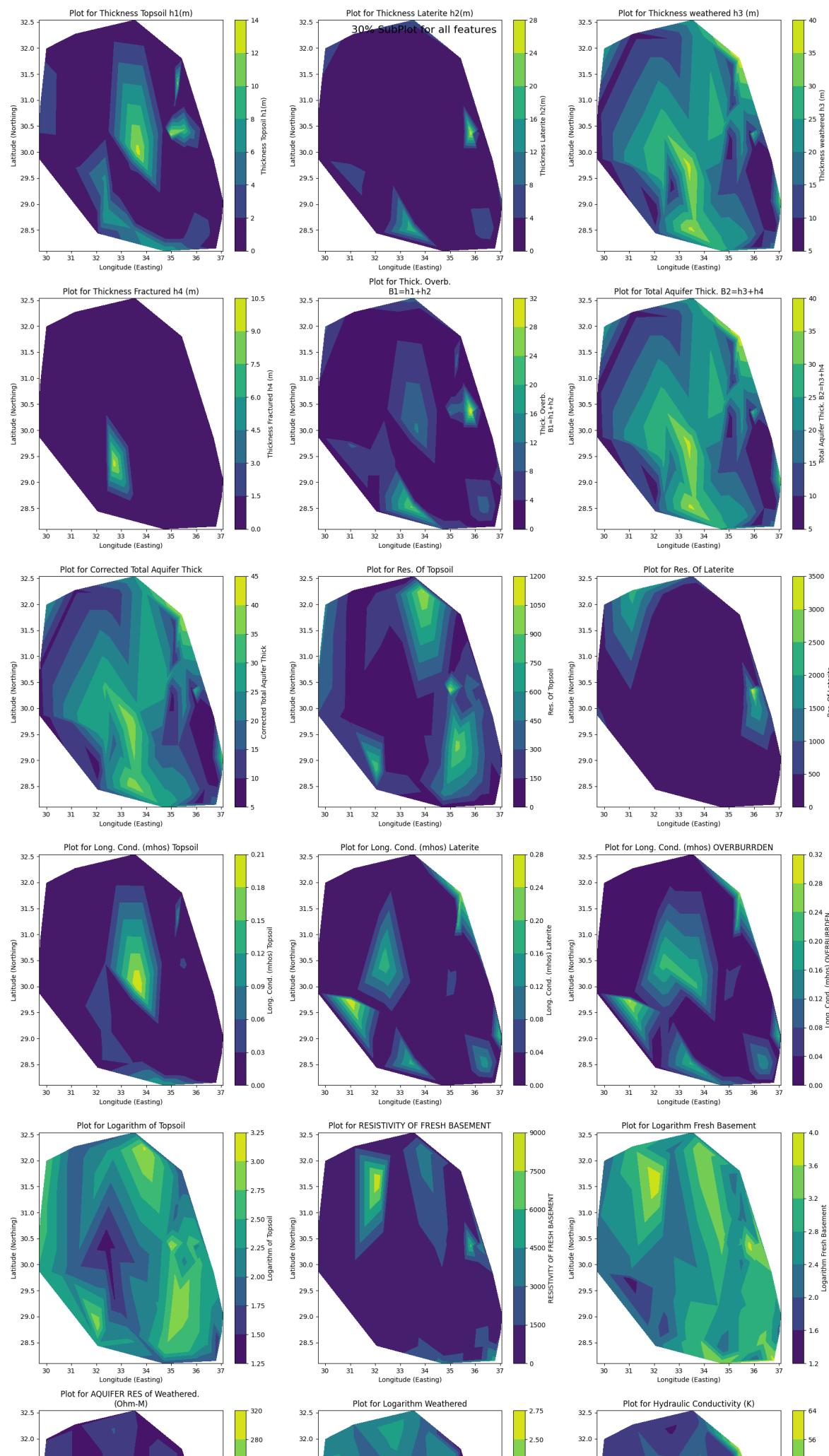
LinearSVR() is the best model with a CV mean score / accuracy score of 0.9973595779820302.

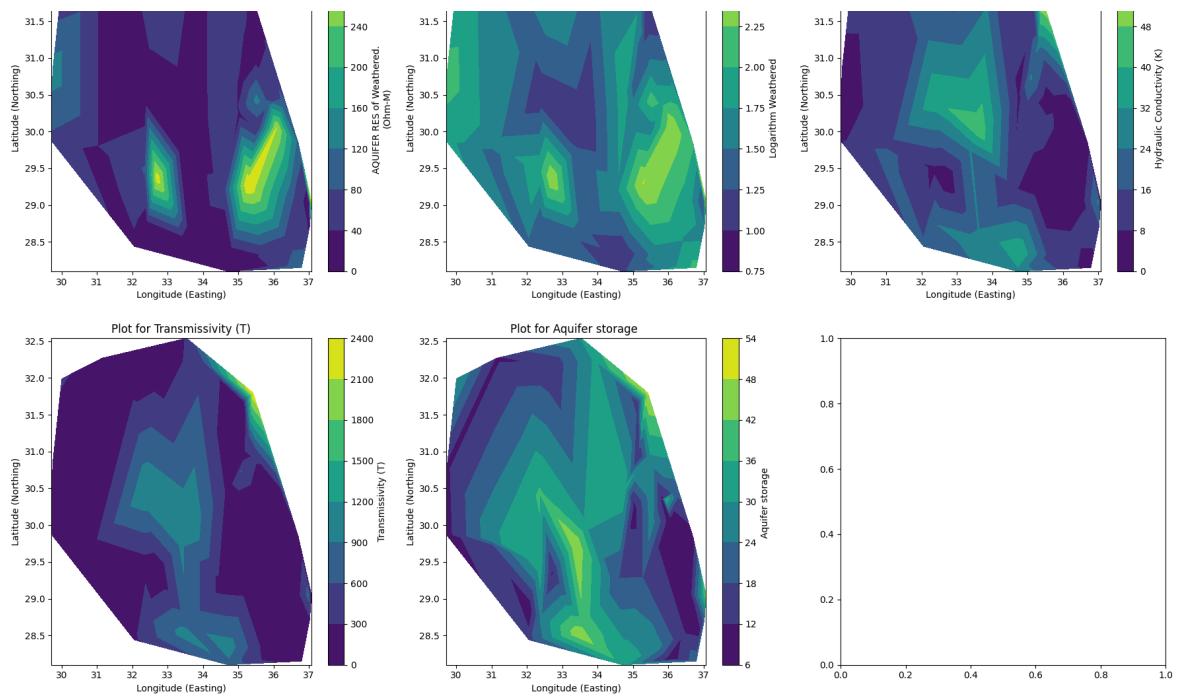
```
/Users/ayomide/Work/ML/AquiferStorage/env/lib/python3.9/site-packages/sklearn/metrics/_regression.py:483: FutureWarning: 'squared' is deprecated in version 1.4 and will be removed in 1.6. To calculate the root mean squared error, use the function 'root_mean_squared_error'.
    warnings.warn(
```

A plot showing the 30% subset of values we have

```
In [ ]: filtered_df = df_1[df_1['VES S/N'].isin(df_pred_wat['VES S/N'])]
```

```
In [ ]: plot_features(filtered_df, cols_to_plot, False)
```





Key Insights and Conclusion

The evaluation of the project on developing a machine learning model to predict aquifer storage capacity has yielded several important insights. A data split of 30:70 (test:training) was employed, and multiple models were trained to identify the one best suited for predicting aquifer storage. The models were evaluated across different feature groups, highlighting the significance of feature selection in machine learning. Below are the key insights derived from testing these feature groups:

- **All Selected Features:**

- **Features:** Thickness Topsoil h1(m), Thickness weathered h3 (m), Thick. Overb.
 $B1=h1+h2$, Total Aquifer Thick. $B2=h3+h4$, Long. Cond. (mhos)
OVERBURRDEN, Long. Cond. (mhos) Topsoil, Transmissivity (T).
- **Result:** Linear Regression emerged as the best model with a cross-validation (CV) mean score of 1.0. This indicates a potentially perfect prediction, suggesting a linear relationship between these features and the target variable.

- **Features Without High Correlation:**

- **Features:** Excluding the two highest correlators (with correlation scores of 0.98 and above), the features used were Thickness Topsoil h1(m), Thick. Overb.
 $B1=h1+h2$, Long. Cond. (mhos) Topsoil, Long. Cond. (mhos)
OVERBURRDEN, Transmissivity (T).
- **Result:** RandomForestRegressor was the best model with a CV mean score of 0.239. The drop in CV score compared to the all features model suggests that the excluded features were significant predictors of aquifer storage.

- **Features Without Weathered Thickness:**

- **Features:** After removing one of the highest correlators, the selected features included Thickness Topsoil h1(m), Thick. Overb.
 $B1=h1+h2$, Total

Aquifer Thick. B2=h3+h4, Long. Cond. (mhos) OVERBURRDEN, Long. Cond. (mhos) Topsoil, Transmissivity (T).

- **Result:** Linear Regression again proved to be the best model with a CV mean score of 0.9109, highlighting its robustness in capturing the relationship between the selected features and the target variable even after the exclusion of a significant predictor.
- **Features Without Aquifer Thickness:**
 - **Features:** By excluding one of the highest correlators, the remaining features were Thickness Topsoil h1(m), Thickness weathered h3 (m), Thick. Overb.
B1=h1+h2, Long. Cond. (mhos) OVERBURRDEN, Long. Cond. (mhos) Topsoil, Transmissivity (T).
 - **Result:** LinearSVR emerged as the best model with a CV mean score of 0.9974, indicating excellent performance and suggesting that the remaining features still capture significant predictive power.

Conclusion

The evaluation across different feature groups has shown that careful feature selection is paramount in developing predictive models. While Linear Regression showed outstanding performance in two of the feature groupings, suggesting a strong linear relationship, RandomForestRegressor and LinearSVR's best performances in other groupings indicate the complexity and non-linear nature of the relationships in groundwater potential prediction. This analysis underscores the necessity of experimenting with both feature selection and various modeling approaches to identify the best predictor of aquifer storage.

References

- Raji, W.O., Abdulkadir, K.A. Evaluation of groundwater potential of bedrock aquifers in Geological Sheet 223 Ilorin, Nigeria, using geo-electric sounding. Appl Water Sci 10, 220 (2020). <https://doi.org/10.1007/s13201-020-01303-2>