Lithology prediction with Python

Recently, machine learning has increased in popularity in many industries. In the Oil and Gas industry the implementation of data driven methodologies has increased, specially in the Upstream sector, where machine learning models are used to leverage the vast amount of data available for geoscientist although in some circumstances this data is relatively small when compared to the task that must be completed.

The main goal of this project is to build a machine learning model using popular python libraries and datasets available on the FORCE 2020 ML competition Github repository. The datasets available on the official Github repository are the training data, and test data, with the earlier having 29 columns and over one million observations, and the latter with just as many columns but with only around 122,000 examples. The final model will be build gradually, starting from a simple model trained on an imbalanced dataset with only the well logs and the depth as features, and increasing in complexity as we perform different data imputation techniques on the training data to improve its quality and boost learning, and tune the hyperparameters to improve the model performance.

Importing libraries

First, we will import commonly available python libraries. These libraries contain useful classes and functions that allow us to write a few lines of code in order to perform task that otherwise would require a lot of custom written code. Following is a short description of each library:

- **Pandas**: A Python library built over numpy, useful for data analysis tasks. Stores functions that allow us to generate statistics for our data, manipulate the data, and visualize it through wrappers over other libraries such as Matplotllib.
- **Numpy**: A scientific Python library that allows the generation of matrices and vectors, and supports complex operations between such data structures. Numpy also allows for vectorized operations which means that multiple operations are done on a single cpu cycle.
- **Matplotlib**: Maybe Python's most commonly used data visualization library. It is used for visualizing data by generating plots.
- **Seaborn**: A data visualization library that lets us further customize plots and generate more specific plots like violin and linear regression plots, as well as facilitating the generation of conditional plots and pairplots.
- **Scikit-learn**: A popular machine learning library with tools for data processing, building data pipelines, and training, building and evaluating machine learning models.
- **Boruta**: An open source Python library used for feature selection. Commonly used by kagglers on competitions.
- **Umap-learn**: An open source library for Uniform Manifold Approximation and Projection a method for dimensionality reduction commonly preferred over PCA (Principal Component Analysis) and autoencoders because its results are easier to visualize on plots than the results of PCA and it is faster than autoencoders.

In [1]:
```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.model_selection import train_test_split, KFold, cross_val_score
from sklearn.metrics import accuracy_score
from sklearn.neural_network import MLPClassifier
from sklearn.svm import SVC, OneClassSVM
from sklearn.ensemble import RandomForestClassifier
from sklearn.tree import DecisionTreeClassifier
from sklearn.preprocessing import PowerTransformer
from sklearn.compose import ColumnTransformer
from boruta import BorutaPy
import umap
%matplotlib inline
```

For this project we will also use some custom functions, which are commonly stored in python scripts. We can generate folders that store scripts for functions of a similar topic and add such folders to our current python path by using the built-in `sys` python library. This allows us to import this custom functions as if we were importing built-in or commonly available open source libraries.

In [2]:
```
import sys
sys.path.append('formation_evaluation')
```

In [3]:
```
import well_log_display
```

It should be noted that the `well_log_display` function, as well as other functions in the "formation_evaluation" folder, was originally coded by Yohanes Nuwara and is available on his own Github repository.

Loading the data

We will use the pandas library `pd.read_csv()` function to read our dataset, the default separator for csv files is the "," character, however our file uses the ";" character to separate values.

In [4]:
```
logs_data = pd.read_csv('datasets1/log_train.csv', sep=';')
logs_data.head(10)
```

Out[4]:

	WELL	DEPTH_MD	X_LOC	Y_LOC	Z_LOC	GROUP	FORMATION	CALI	RSHA	RMED	...	ROP	DTS	DCA
0	15/9-13	494.528	437641.96875	6470972.5	-469.501831	NORDLAND GP.	NaN	19.480835	NaN	1.611410	...	34.636410	NaN	Na
1	15/9-13	494.680	437641.96875	6470972.5	-469.653809	NORDLAND GP.	NaN	19.468800	NaN	1.618070	...	34.636410	NaN	Na
2	15/9-13	494.832	437641.96875	6470972.5	-469.805786	NORDLAND GP.	NaN	19.468800	NaN	1.626459	...	34.779556	NaN	Na
3	15/9-13	494.984	437641.96875	6470972.5	-469.957794	NORDLAND GP.	NaN	19.459282	NaN	1.621594	...	39.965164	NaN	Na
4	15/9-13	495.136	437641.96875	6470972.5	-470.109772	NORDLAND GP.	NaN	19.453100	NaN	1.602679	...	57.483765	NaN	Na
5	15/9-13	495.288	437641.96875	6470972.5	-470.261780	NORDLAND GP.	NaN	19.453100	NaN	1.585567	...	75.281410	NaN	Na
6	15/9-13	495.440	437641.96875	6470972.5	-470.413788	NORDLAND GP.	NaN	19.462496	NaN	1.576569	...	76.199951	NaN	Na
7	15/9-13	495.592	437641.96875	6470972.5	-470.565796	NORDLAND GP.	NaN	19.468800	NaN	1.587011	...	76.199951	NaN	Na
8	15/9-13	495.744	437641.96875	6470972.5	-470.717773	NORDLAND GP.	NaN	19.468800	NaN	1.613674	...	75.898796	NaN	Na
9	15/9-13	495.896	437641.96875	6470972.5	-470.869782	NORDLAND GP.	NaN	19.468800	NaN	1.634622	...	68.121262	NaN	Na

10 rows × 29 columns

Sometimes our dataset is too big to be completely displayed. We can use the `pd.set_option()` function to specify the maximum number of rows or columns to be displayed.

In [5]:
```
pd.set_option('display.max_columns', None)
logs_data.head(10)
```

Out[5]:

	WELL	DEPTH_MD	X_LOC	Y_LOC	Z_LOC	GROUP	FORMATION	CALI	RSHA	RMED	RDEP	RHOB	
0	15/9-13	494.528	437641.96875	6470972.5	-469.501831	NORDLAND GP.	NaN	19.480835	NaN	1.611410	1.798681	1.884186	80.20
1	15/9-13	494.680	437641.96875	6470972.5	-469.653809	NORDLAND GP.	NaN	19.468800	NaN	1.618070	1.795641	1.889794	79.26
2	15/9-13	494.832	437641.96875	6470972.5	-469.805786	NORDLAND GP.	NaN	19.468800	NaN	1.626459	1.800733	1.896523	74.82
3	15/9-13	494.984	437641.96875	6470972.5	-469.957794	NORDLAND GP.	NaN	19.459282	NaN	1.621594	1.801517	1.891913	72.87
4	15/9-13	495.136	437641.96875	6470972.5	-470.109772	NORDLAND GP.	NaN	19.453100	NaN	1.602679	1.795299	1.880034	71.72
5	15/9-13	495.288	437641.96875	6470972.5	-470.261780	NORDLAND GP.	NaN	19.453100	NaN	1.585567	1.804719	1.879687	72.01
6	15/9-13	495.440	437641.96875	6470972.5	-470.413788	NORDLAND GP.	NaN	19.462496	NaN	1.576569	1.805498	1.878731	72.58
7	15/9-13	495.592	437641.96875	6470972.5	-470.565796	NORDLAND GP.	NaN	19.468800	NaN	1.587011	1.808367	1.867837	71.28
8	15/9-13	495.744	437641.96875	6470972.5	-470.717773	NORDLAND GP.	NaN	19.468800	NaN	1.613674	1.815813	1.847233	69.72
9	15/9-13	495.896	437641.96875	6470972.5	-470.869782	NORDLAND GP.	NaN	19.468800	NaN	1.634622	1.813916	1.836309	66.67

Exploring the data

For quick basic data exploration we can use the `DataFrame.info()` method to display comprehensive information about our dataset like the number of data points(rows), the number of columns, and the name, number of non-null elements and dtype of each column.

In [6]:
```
logs_data.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 1170511 entries, 0 to 1170510
Data columns (total 29 columns):
 #   Column                             Non-Null Count    Dtype
---  ------                             --------------    -----
 0   WELL                               1170511 non-null  object
 1   DEPTH_MD                           1170511 non-null  float64
 2   X_LOC                              1159736 non-null  float64
 3   Y_LOC                              1159736 non-null  float64
 4   Z_LOC                              1159736 non-null  float64
 5   GROUP                              1169233 non-null  object
 6   FORMATION                          1033517 non-null  object
 7   CALI                               1082634 non-null  float64
 8   RSHA                               630650 non-null   float64
 9   RMED                               1131518 non-null  float64
 10  RDEP                               1159496 non-null  float64
 11  RHOB                               1009242 non-null  float64
 12  GR                                 1170511 non-null  float64
 13  SGR                                69353 non-null    float64
 14  NPHI                               765409 non-null   float64
 15  PEF                                671692 non-null   float64
 16  DTC                                1089648 non-null  float64
 17  SP                                 864247 non-null   float64
 18  BS                                 682657 non-null   float64
 19  ROP                                535071 non-null   float64
 20  DTS                                174613 non-null   float64
 21  DCAL                               298833 non-null   float64
 22  DRHO                               987857 non-null   float64
 23  MUDWEIGHT                          316151 non-null   float64
 24  RMIC                               176160 non-null   float64
 25  ROPA                               192325 non-null   float64
 26  RXO                                327427 non-null   float64
 27  FORCE_2020_LITHOFACIES_LITHOLOGY   1170511 non-null  int64
 28  FORCE_2020_LITHOFACIES_CONFIDENCE  1170332 non-null  float64
dtypes: float64(25), int64(1), object(3)
memory usage: 259.0+ MB
```

Dtypes for all columns in our dataframe seem correct, however there is a noticeable amount of missing data in several columns.

Some column names are self explanatory, while others are commonly used log mnemonics. Following is a short list with the mnemonic and what it corresponds to.

- **CALI**: Caliper
- **RSHA**: Shallow resistivity
- **RMED**: Medium resistivity
- **RDEP**: Deep resistivity
- **RHOB**: Bulk resistivity
- **GR**: Gamma Ray
- **SGR**: Spectral Gamma Ray
- **NPHI**: Neutron porosity
- **PEF**: Photo-electric factor
- **DTC**: Density tool compresional wave
- **SP**: Spontaneous potential log
- **BS**: Bit size
- **ROP**: Rate of penetrarion
- **DTS**: Density tool shear wave
- **DCAL**: Differential caliper
- **DRHO**: Bulk density correction
- **MUDWEIGHT**: Density of drilling mud
- **RMIC**: Microresistivity log
- **ROPA**: Electromagnetic propagation log (unsure if this is the correct log)
- **RXO**: Resistivity of flushed zone

Now we will use the `DataFrame.describe()` method to display some basic summary statistics for our datasets. This lets us quickly scan the maximum and minimum values for the data in each column, along with other statistics to see if there is any unusual range or distribution, this is easier on smaller datasets. For datasets with many columns (like our current dataset), visual exploratory data analysis through plots may be preferable.

We can set the `include` parameter to display statistics for columns storing data in numerical or object type.

In [7]:
```
logs_data.describe(include=np.number)
```

Out[7]:

	DEPTH_MD	X_LOC	Y_LOC	Z_LOC	CALI	RSHA	RMED	RDEP	RHOB
count	1.170511e+06	1.159736e+06	1.159736e+06	1.159736e+06	1.082634e+06	630650.000000	1.131518e+06	1.159496e+06	1.009242e+06
mean	2.184087e+03	4.856310e+05	6.681276e+06	-2.138527e+03	1.318568e+01	10.694664	4.986978e+00	1.069103e+01	2.284987e+00
std	9.971821e+02	3.455641e+04	1.281524e+05	9.709426e+02	3.798907e+00	100.642597	5.467269e+01	1.139480e+02	2.532835e-01
min	1.360860e+02	4.268988e+05	6.406641e+06	-5.395563e+03	2.344000e+00	0.000100	-8.418695e-03	3.170056e-02	7.209712e-01
25%	1.418597e+03	4.547996e+05	6.591327e+06	-2.811502e+03	9.429712e+00	0.854120	9.140862e-01	9.102396e-01	2.092203e+00
50%	2.076605e+03	4.769203e+05	6.737311e+06	-2.042785e+03	1.255575e+01	1.399020	1.443584e+00	1.439000e+00	2.321228e+00
75%	2.864393e+03	5.201532e+05	6.784886e+06	-1.391866e+03	1.671075e+01	3.099348	2.680930e+00	2.557220e+00	2.488580e+00
max	5.436632e+03	5.726328e+05	6.856661e+06	-1.110860e+02	2.827900e+01	2193.904541	1.988616e+03	1.999887e+03	3.457820e+00

In [8]:
```
logs_data.describe(include=np.object)
```

Out[8]:

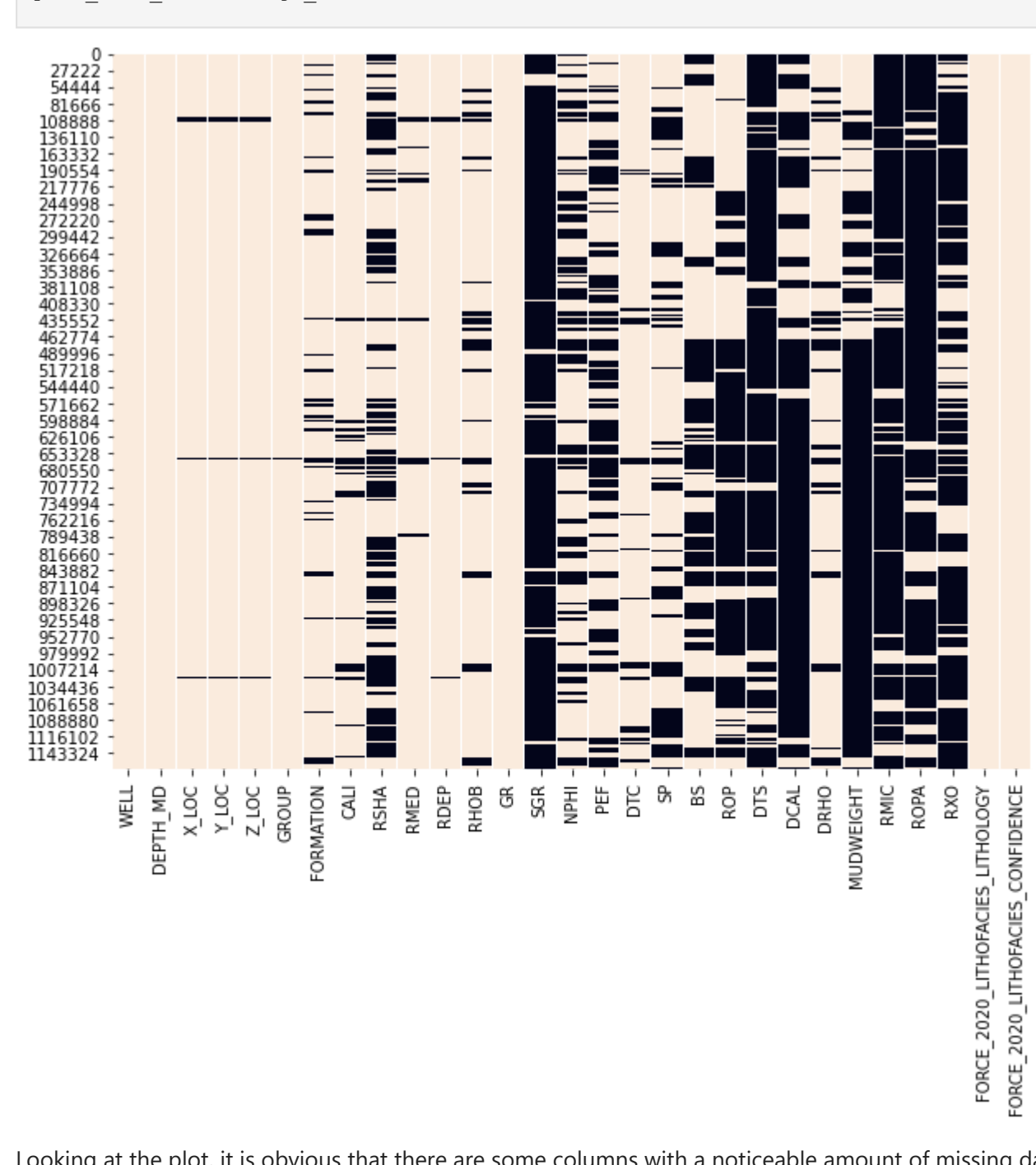
	WELL	GROUP	FORMATION
count	1170511	1169233	1033517
unique	98	14	69
top	25/2-7	HORDALAND GP.	Utsira Fm.
freq	25131	293155	172636

Visual exploratory data analysis

Before we explore each feature, lets first visualize the missing data in our dataset. This way we might focus our analysis in columns that have enough information, or where enough data can be imputed, to be useful for our machine learning algorithm.

In [9]:
```
def plot_null_matrix(df, figsize=(10, 8)):
    plt.figure(figsize=figsize)

    df_null = df.isnull()
    ax = sns.heatmap(~df_null, cbar=False)

    plt.show()
```

In [10]:
```
plot_null_matrix(logs_data)
```



Looking at the plot, it is obvious that there are some columns with a noticeable amount of missing data. We will generate a table with the count of null values and the percentage of the data missing for each column.

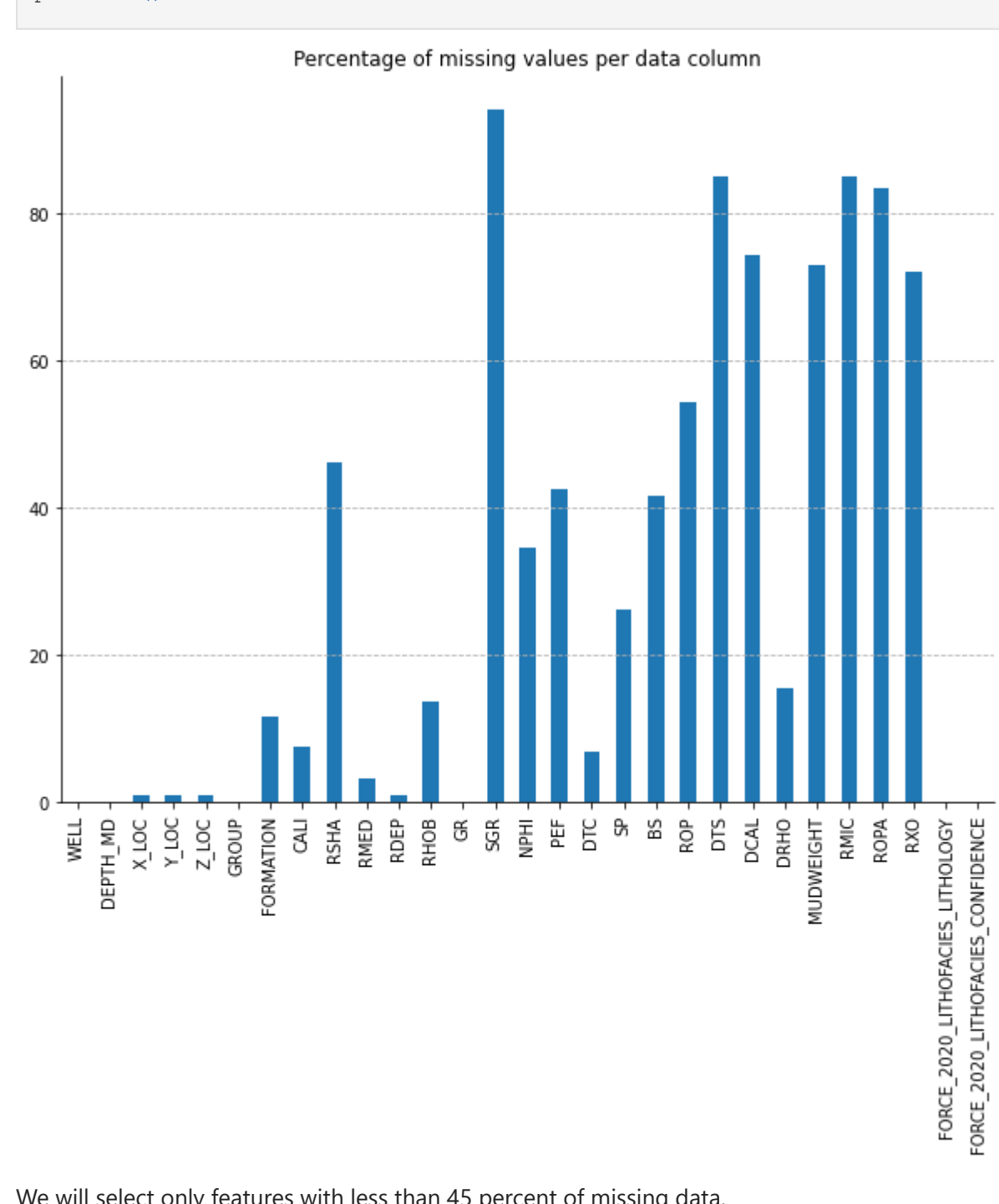
In [11]:
```
null_count = logs_data.isnull().sum()
null_pct = (null_count / logs_data.shape[0]) * 100

null_values = pd.DataFrame({'null_count': null_count,
                            'null_pct': null_pct})
null_values
```

Out[11]:

	null_count	null_pct
WELL	0	0.000000
DEPTH_MD	0	0.000000
X_LOC	10775	0.920538
Y_LOC	10775	0.920538
Z_LOC	10775	0.920538
GROUP	1278	0.109183
FORMATION	136994	11.703777
CALI	87877	7.507576
RSHA	539861	46.121822
RMED	38993	3.331280
RDEP	11015	0.941042
RHOB	161269	13.777658
GR	0	0.000000
SGR	1101158	94.074981
NPHI	405102	34.608987
PEF	498819	42.615490
DTC	80863	6.908350
SP	306264	26.164983
BS	487854	41.678720
ROP	635440	54.287401
DTS	995898	85.082327
DCAL	871678	74.469868
DRHO	182654	15.604638
MUDWEIGHT	854360	72.990344
RMIC	994351	84.950163
ROPA	978186	83.569142
RXO	843084	72.027004
FORCE_2020_LITHOFACIES_LITHOLOGY	0	0.000000
FORCE_2020_LITHOFACIES_CONFIDENCE	179	0.015292

Then we can plot these data to visually determine a threshold value for the percentage of missing data we will allow for the features to be used in our machine learning algorithm.

In [12]:
```
null_values['null_pct'].plot(kind='bar', figsize=(10,8), title=
                             'Percentage of missing values per data column')

sns.despine()
plt.grid(axis='y', ls='--')

plt.show()
```



We will select only features with less than 45 percent of missing data.

In [13]:
```
features = null_values[null_values['null_pct'] < 45].index
features
```

Out[13]:
```
Index(['WELL', 'DEPTH_MD', 'X_LOC', 'Y_LOC', 'Z_LOC', 'GROUP', 'FORMATION',
       'CALI', 'RMED', 'RDEP', 'RHOB', 'GR', 'NPHI', 'PEF', 'DTC', 'SP', 'BS',
       'DRHO', 'FORCE_2020_LITHOFACIES_LITHOLOGY',
       'FORCE_2020_LITHOFACIES_CONFIDENCE'],
      dtype='object')
```

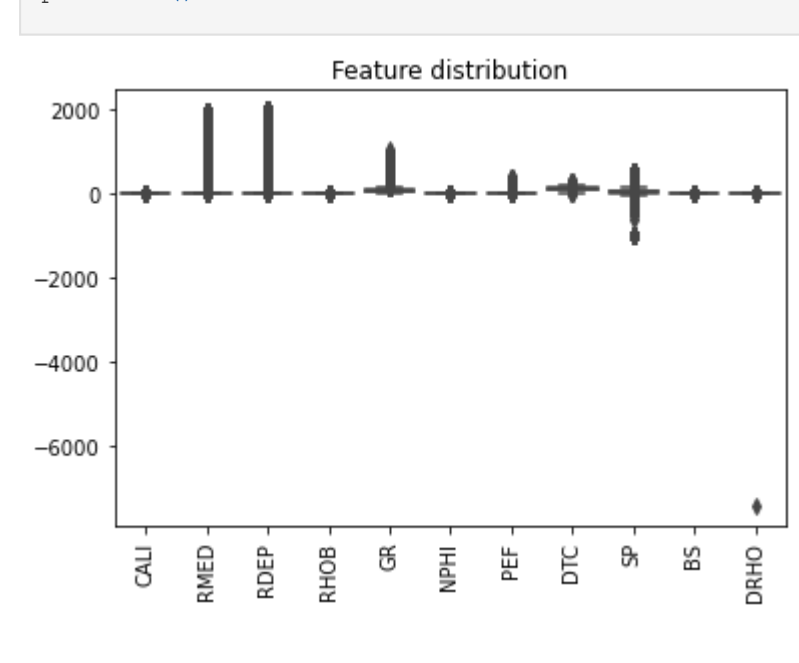
Distribution of values per feature

Now we will explore the feature distribution for each data column. First we will display boxplots to see if there are any outliers.

In [14]:
```
logs_ml = features.drop(['WELL', 'DEPTH_MD', 'X_LOC', 'Y_LOC',
                         'Z_LOC', 'GROUP', 'FORMATION',
                         'FORCE_2020_LITHOFACIES_LITHOLOGY',
                         'FORCE_2020_LITHOFACIES_CONFIDENCE'])

logs_ml
```

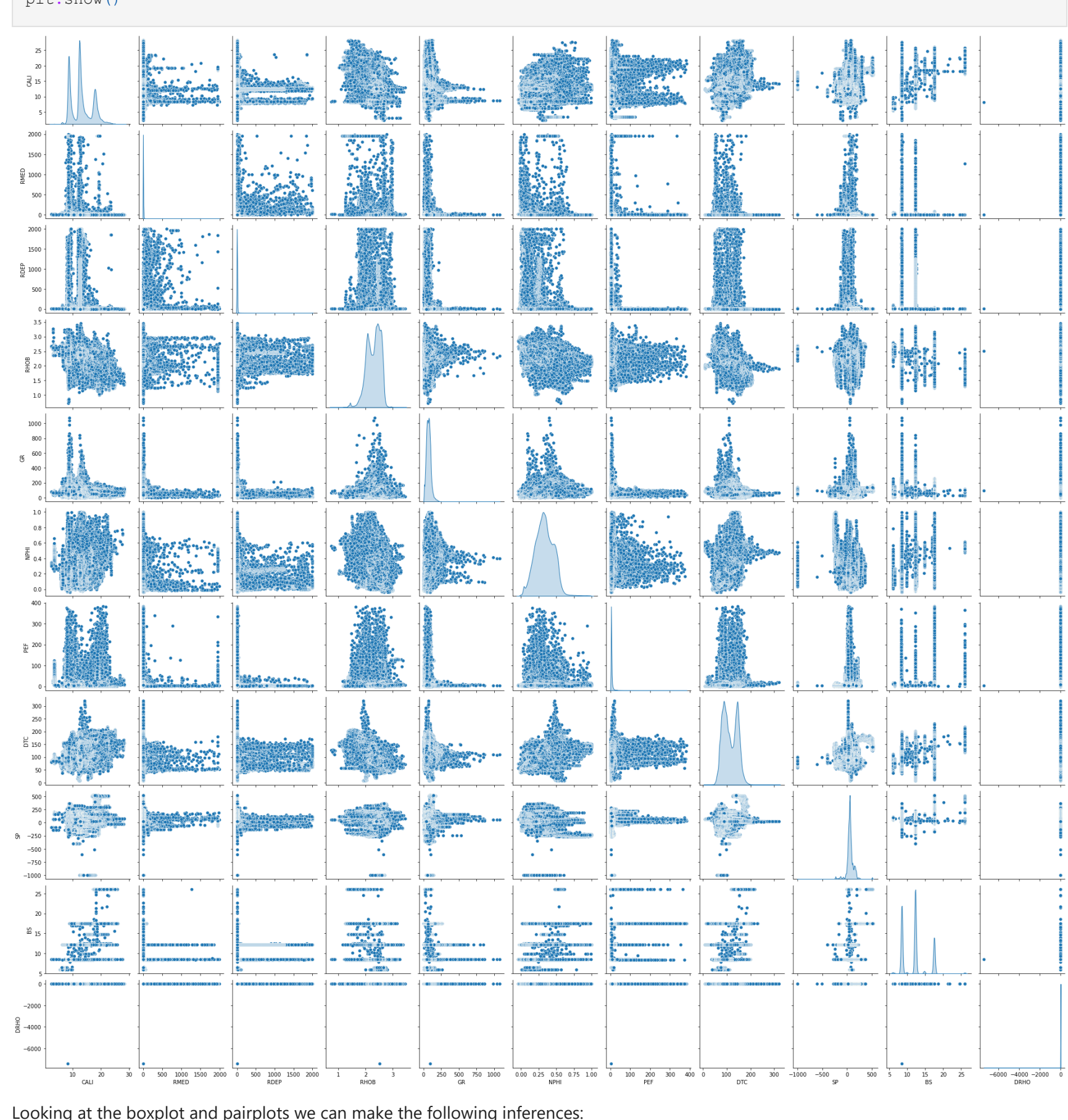
Out[14]:
```
Index(['CALI', 'RMED', 'RDEP', 'RHOB', 'GR', 'NPHI', 'PEF', 'DTC', 'SP', 'BS',
       'DRHO'],
      dtype='object')
```

In [15]:
```
fig, ax = plt.subplots()

ax = sns.boxplot(data=logs_data[logs_ml])
ax.set_title('Feature distribution')
plt.xticks(rotation=90)

plt.show()
```



Pairplots

In [16]:
```
sns.pairplot(logs_data, vars=logs_ml, diag_kind='kde')

plt.show()
```



Looking at the boxplot and pairplots we can make the following inferences:

- Value ranges probably are very different, and thus, some features are outscaled, making it difficult to visualize their distribution.
- The features do contain some outliers. An example of this is the `DRHO` data column, with an outlier that might be the result of an incorrect measurement or a tool error.
- Some features have a distribution that resembles a normal distribution (also known as Gaussian distribution), although skewed, other features have multimodal distributions.

To make the visualization of the feature distributions easier we can normalize the data, a data processing step already required in the machine learning workflow.

Is the dataset balanced?

So far, we have performed EDA (Exploratory Data Analysis) for our features. Now we will explore our target column, which is the `FORCE_2020_LITHOFACIES_LITHOLOGY`. Doing so will also allow us to answer wether our dataset is balanced. A dataset is balanced when it contains an almost equal percentage of examples per class. In the case of a binary classification problem this would mean a distribution of 50% positive class examples and 50% negative class examples, or 60% positive class examples and 40% negative class examples or vice-versa.

First, we will calculate the theoretical relative frequency (the percentage of examples for each class) for our dataset to be balanced.

In [17]:
```
# For readability transform original lithology codes into labels
# (lithology code correspondance was given in the competition starter notebook).
lithology_keys = {30000: 'Sandstone',
                  65030: 'Sandstone/Shale',
                  65000: 'Shale',
                  80000: 'Marl',
                  74000: 'Dolomite',
                  70000: 'Limestone',
                  70032: 'Chalk',
                  88000: 'Halite',
                  86000: 'Anhydrite',
                  99000: 'Tuff',
                  90000: 'Coal',
                  93000: 'Basement'}
```

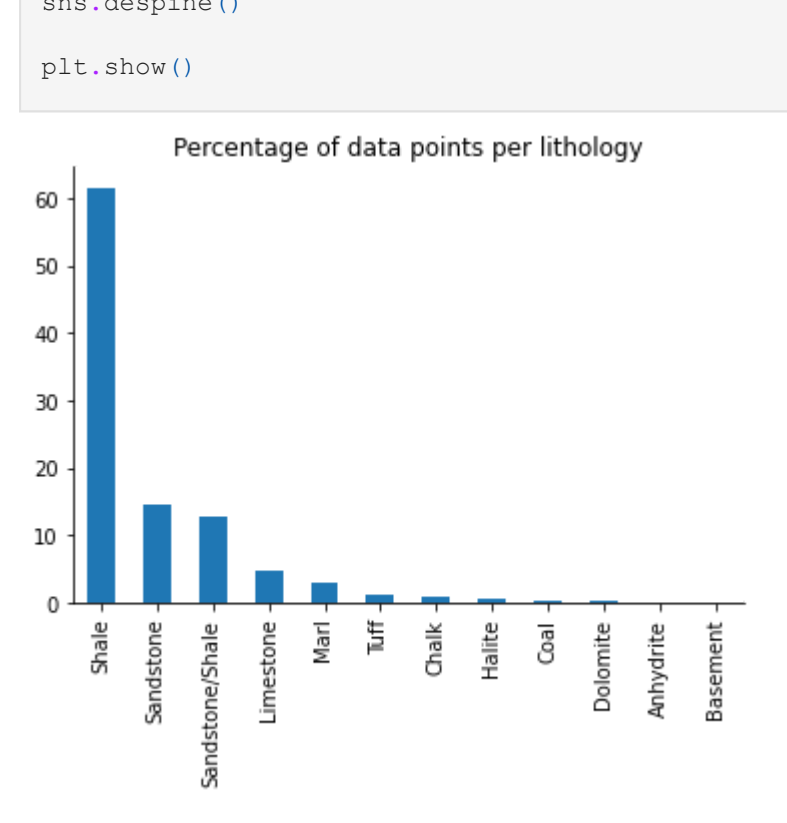
In [18]:
```
label = 'FORCE_2020_LITHOFACIES_LITHOLOGY'

unique_lithologies = logs_data[label].unique()
theoretical_pct_lithology = 100 / unique_lithologies.shape[0]
theoretical_pct_lithology
```

Out[18]:
```
8.333333333333334
```

In [19]:
```
lithologies_labels = logs_data[label].map(lithology_keys)

lithologies_count = lithologies_labels.value_counts(normalize=True) * 100
lithologies_count
```

Out[19]:
```
Shale              61.580199
Sandstone          14.432756
Sandstone/Shale    12.853788
Limestone           4.811574
Marl                2.847389
Tuff                1.302423
Chalk               0.898155
Halite              0.701659
Coal                0.326353
Dolomite            0.144211
Anhydrite           0.092695
Basement            0.008800
Name: FORCE_2020_LITHOFACIES_LITHOLOGY, dtype: float64
```

In [20]:
```
lithologies_count.plot(kind='bar',
                       title='Percentage of data points per lithology')
sns.despine()

plt.show()
```



We can see that the dataset is imbalanced, one class represents over 60 percent of the data points in our dataset. In order to see if our evaluation score for the model improves after balancing the dataset we will first evaluate the model in this imbalanced data.

Data processing

Handling missing data

For simplicity reasons, we will perform data imputation on the numerical columns by replacing the missing values with the mean of each column. We will also work with a subset of our original dataset, which will drop columns like `DEPTH_MD`, `X_LOC`, `Y_LOC`, and `FORCE_2020_LITHOFACIES_CONFIDENCE`.

In [21]:
```
columns = features.drop(['DEPTH_MD', 'X_LOC', 'Y_LOC',
                         'FORCE_2020_LITHOFACIES_CONFIDENCE'])
columns
```

Out[21]:
```
Index(['WELL', 'Z_LOC', 'GROUP', 'FORMATION', 'CALI', 'RMED', 'RDEP', 'RHOB',
       'GR', 'NPHI', 'PEF', 'DTC', 'SP', 'BS', 'DRHO',
       'FORCE_2020_LITHOFACIES_LITHOLOGY'],
      dtype='object')
```

In [22]:
```
ml_data = logs_data[columns]
ml_data
```

Out[22]:

	WELL	Z_LOC	GROUP	FORMATION	CALI	RMED	RDEP	RHOB	GR	NPHI	PEF	DTC
0	15/9-13	-469.501831	NORDLAND GP.	NaN	19.480835	1.611410	1.798681	1.884186	80.200851	NaN	20.915468	161.131180
1	15/9-13	-469.653809	NORDLAND GP.	NaN	19.468800	1.618070	1.795641	1.889794	79.262886	NaN	19.383013	160.603470
2	15/9-13	-469.805786	NORDLAND GP.	NaN	19.468800	1.626459	1.800733	1.896523	74.821999	NaN	22.591518	160.173615
3	15/9-13	-469.957794	NORDLAND GP.	NaN	19.459282	1.621594	1.801517	1.891913	72.878922	NaN	32.191910	160.149429
4	15/9-13	-470.109772	NORDLAND GP.	NaN	19.453100	1.602679	1.795299	1.880034	71.729141	NaN	38.495632	160.128342
...	...	...	...	...	...	...	...	...	...	...	...	...
1170506	7/1-2 S	NaN	VESTLAND GP.	Bryne Fm.	8.423170	NaN	NaN	2.527984	77.654900	NaN	4.586425	NaN
1170507	7/1-2 S	NaN	VESTLAND GP.	Bryne Fm.	8.379244	NaN	NaN	2.537613	75.363937	NaN	7.019858	NaN
1170508	7/1-2 S	NaN	VESTLAND GP.	Bryne Fm.	8.350248	NaN	NaN	2.491860	66.452843	NaN	9.049782	NaN
1170509	7/1-2 S	NaN	VESTLAND GP.	Bryne Fm.	8.313779	NaN	NaN	2.447539	55.784817	NaN	8.903917	NaN
1170510	7/1-2 S	NaN	VESTLAND GP.	Bryne Fm.	8.294910	NaN	NaN	2.430716	48.432129	NaN	9.150043	NaN

1170511 rows × 16 columns

In [23]:
```
ml_data_num = ml_data.select_dtypes(include=np.number).drop(label, axis=1)
print(ml_data_num.columns)

ml_data_num = ml_data_num.fillna(ml_data_num.mean())
ml_data_num.isnull().sum()
```

```
Index(['Z_LOC', 'CALI', 'RMED', 'RDEP', 'RHOB', 'GR', 'NPHI', 'PEF', 'DTC',
       'SP', 'BS', 'DRHO'],
      dtype='object')
```

Out[23]:
```
Z_LOC    0
CALI     0
RMED     0
RDEP     0
RHOB     0
GR       0
NPHI     0
PEF      0
DTC      0
SP       0
BS       0
DRHO     0
dtype: int64
```

For the categorical data, replacing null values with an specific lithology would imply thorough geological analysis. For simplicity we will replace null values with the string `Unknown`.

In [24]:
```
ml_data_categorical = ml_data.select_dtypes(include=np.object)

ml_data_categorical = ml_data_categorical.fillna('Unknown')
ml_data_categorical.isnull().sum()
```

Out[24]:
```
WELL         0
GROUP        0
FORMATION    0
dtype: int64
```

In [25]:
```
ml_data_clean = pd.concat([ml_data_categorical, ml_data_num], axis=1)
ml_data_clean
```

Out[25]:

	WELL	GROUP	FORMATION	Z_LOC	CALI	RMED	RDEP	RHOB	GR	NPHI	PEF	DT
0	15/9-13	NORDLAND GP.	Unknown	-469.501831	19.480835	1.611410	1.798681	1.884186	80.200851	0.331966	20.915468	161.13118
1	15/9-13	NORDLAND GP.	Unknown	-469.653809	19.468800	1.618070	1.795641	1.889794	79.262886	0.331966	19.383013	160.60347
2	15/9-13	NORDLAND GP.	Unknown	-469.805786	19.468800	1.626459	1.800733	1.896523	74.821999	0.331966	22.591518	160.17361
3	15/9-13	NORDLAND GP.	Unknown	-469.957794	19.459282	1.621594	1.801517	1.891913	72.878922	0.331966	32.191910	160.14942
4	15/9-13	NORDLAND GP.	Unknown	-470.109772	19.453100	1.602679	1.795299	1.880034	71.729141	0.331966	38.495632	160.12834
...	...	...	...	...	...	...	...	...	...	...	...	...
1170506	7/1-2 S	VESTLAND GP.	Bryne Fm.	-2138.527143	8.423170	4.986978	10.691026	2.527984	77.654900	0.331966	4.586425	113.35808
1170507	7/1-2 S	VESTLAND GP.	Bryne Fm.	-2138.527143	8.379244	4.986978	10.691026	2.537613	75.363937	0.331966	7.019858	113.35808
1170508	7/1-2 S	VESTLAND GP.	Bryne Fm.	-2138.527143	8.350248	4.986978	10.691026	2.491860	66.452843	0.331966	9.049782	113.35808
1170509	7/1-2 S	VESTLAND GP.	Bryne Fm.	-2138.527143	8.313779	4.986978	10.691026	2.447539	55.784817	0.331966	8.903917	113.35808
1170510	7/1-2 S	VESTLAND GP.	Bryne Fm.	-2138.527143	8.294910	4.986978	10.691026	2.430716	48.432129	0.331966	9.150043	113.35808

1170511 rows × 15 columns

In [26]:
```
ml_data_clean['LITHOLOGY'] = ml_data[label].map(lithology_keys)
ml_data_clean.isnull().sum()
```

Out[26]:
```
WELL         0
GROUP        0
FORMATION    0
Z_LOC        0
CALI         0
RMED         0
RDEP         0
RHOB         0
GR           0
NPHI         0
PEF          0
DTC          0
SP           0
BS           0
DRHO         0
LITHOLOGY    0
dtype: int64
```

Scaling the data

As mentioned earlier in the notebook, the value ranges for the features are very different, with some having maximum values that are in a different order of magnitude. We will scale the data so that the features are not outscaled.

Data scaling is also considered a best practice for machine learning workflows, since it decreases training time, avoids the algorithm to show some "preference" to columns with higher magnitudes, and prevents problems such as numerical overflow. There are two widely used data scaling techniques:

- Min-max normalization: Values are scaled to a range from 0 to 1, by using the formula:

- Standardization (Z-score normalization): Values are scaled so that their distribution is described in terms of how much they deviate from the mean of the distribution.

For our data we will use another scaling strategy, we will use the `PowerTransformer()` class to build a scaler that uses a power transform (specifically, the "yeo-johnson" method) to scale our data and make the distribution of features more Gaussian-like, which in some cases helps in making training the modeling algorithm easier.

However, before doing so, we will transform some of the data with large ranges into logarithmic scale. Through a quick search on the internet or using domain knowledge, you can find that there are two features in our dataset that are normally plotted in logarithmic scale due to their large value ranges. These features are the resisitivity logs.

In [27]:
```
# transform resisitivity logs into logarithmic scale
ml_data_clean['RMED'] = np.log10(ml_data_clean['RMED'])
ml_data_clean['RMED'] = np.log10(ml_data_clean['RDEP'])
```

```
C:\Users\Angel\anaconda3\lib\site-packages\pandas\core\series.py:726: RuntimeWarning: invalid value encountered in log10
  result = getattr(ufunc, method)(*inputs, **kwargs)
```

In [28]:
```
# generate PowerTransfomer instance
scaler = PowerTransformer(method='yeo-johnson')

# initialize ColumnTransformer instance
ct = ColumnTransformer([('scaler', scaler, logs_ml)],
```

```
                    remainder='passthrough')

ml_data_norm = ct.fit_transform(ml_data_clean)
ml_data_norm
```

Out[28]:
```
array([[1.5689912275097166, 0.2486494060957612, 0.20783885430564225, ...,
        'Unknown', -469.50183110000006, 'Shale'],
       [1.5666240027409932, 0.24676390577291818, 0.2055382336439452, ...,
        'Unknown', -469.6538086, 'Shale'],
       [1.5666240027409932, 0.24991934300156396, 0.2093888463955194, ...,
        'Unknown', -469.80578610000003, 'Shale'],
       ...,
       [-1.4722701998916912, 1.6346457776087622, 1.8002290920693833, ...,
        'Bryne Fm.', -2138.5271425447368, 'Sandstone/Shale'],
       [-1.4868594357887681, 1.6346457776087622, 1.8002290920693833, ...,
        'Bryne Fm.', -2138.5271425447368, 'Sandstone/Shale'],
       [-1.4944278375104374, 1.6346457776087622, 1.8002290920693833, ...,
        'Bryne Fm.', -2138.5271425447368, 'Sandstone/Shale']],
      dtype=object)
```

In [29]:
```
df_cols = np.append(logs_ml, ['WELL', 'GROUP', 'FORMATION', 'Z_LOC',
                               'LITHOLOGY'])
ml_data_norm = pd.DataFrame(ml_data_norm, columns=df_cols)
ml_data_norm
```

Out[29]:

	CALI	RMED	RDEP	RHOB	GR	NPHI	PEF	DTC	SP	BS	DRHO	WELL	G
0	1.56899	0.248649	0.207839	-1.59668	0.39483	0.0327833	2.57258	1.56265	-0.653382	0.115317	-1.78822	15/9-13	NORD
1	1.56662	0.246764	0.205538	-1.57899	0.368797	0.0327833	2.46553	1.54731	-0.664776	0.115317	-1.77586	15/9-13	NORD
2	1.56662	0.249919	0.209389	-1.55765	0.24323	0.0327833	2.67732	1.53479	-0.664446	0.115317	-1.78644	15/9-13	NORD
3	1.56475	0.250404	0.20998	-1.57228	0.18703	0.0327833	3.11326	1.53408	-0.666393	0.115317	-1.81786	15/9-13	NORD
4	1.56353	0.246551	0.205279	-1.60972	0.153395	0.0327833	3.30713	1.53347	-0.661464	0.115317	-1.84792	15/9-13	NORD
...	...	...	...	...	...	...	...	...	...	...	...	...	
1170506	-1.44325	1.63465	1.80023	1.08109	0.323779	0.0327833	-0.318391	0.0606547	-0.0661068	-1.5483	-0.0968679	7/1-2 S	VEST
1170507	-1.46071	1.63465	1.80023	1.13215	0.258765	0.0327833	0.656712	0.0606547	-0.0661068	-1.5483	-0.1166	7/1-2 S	VEST
1170508	-1.47227	1.63465	1.80023	0.892694	-0.0048011	0.0327833	1.17817	0.0606547	-0.0661068	-1.5483	-0.15259	7/1-2 S	VEST
1170509	-1.48686	1.63465	1.80023	0.668305	-0.346688	0.0327833	1.14621	0.0606547	-0.0661068	-1.5483	-0.129537	7/1-2 S	VEST
1170510	-1.49443	1.63465	1.80023	0.585053	-0.603234	0.0327833	1.19973	0.0606547	-0.0661068	-1.5483	-0.129404	7/1-2 S	VEST

1170511 rows × 16 columns

The `fit_transform()` method not only removed the column names, but also stored all information as object dtype.

In [30]:
```
ml_data_norm.dtypes
```

Out[30]:
```
CALI         object
RMED         object
RDEP         object
RHOB         object
GR           object
NPHI         object
PEF          object
DTC          object
SP           object
BS           object
DRHO         object
WELL         object
GROUP        object
FORMATION    object
Z_LOC        object
LITHOLOGY    object
dtype: object
```

In [31]:
```
ml_data_norm[logs_ml] = ml_data_norm[logs_ml].astype(float)
ml_data_norm['Z_LOC'] = ml_data_norm['Z_LOC'].astype(float)
ml_data_norm.dtypes
```

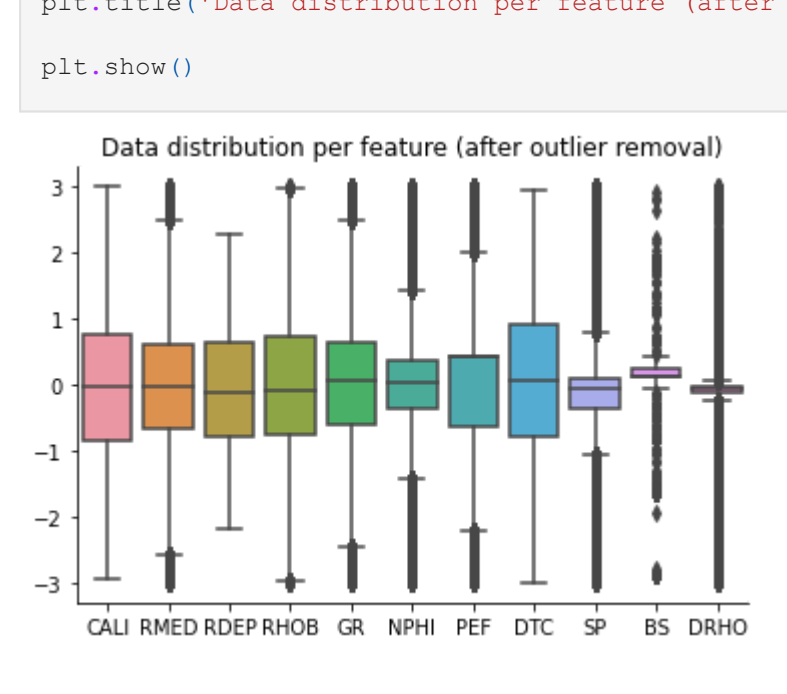
Out[31]:
```
CALI         float64
RMED         float64
RDEP         float64
RHOB         float64
GR           float64
NPHI         float64
PEF          float64
DTC          float64
SP           float64
BS           float64
DRHO         float64
WELL          object
GROUP         object
FORMATION     object
Z_LOC        float64
LITHOLOGY     object
dtype: object
```

Outlier removal

There are many techniques for outlier removal. Perhaps the most widely known is the standard deviation method, where we compute the absolute value of the difference between each feature example and its mean and keep only those examples where the difference is less than or equal to three times the standard deviation of the feature. There are other statistical techniques, but for now we will use the standard deviation method.

In [32]:
```
ml_features = ml_data_norm[logs_ml].copy()

ml_train_std = ml_features[np.abs(ml_features - ml_features.mean()) <=
                           (3 * ml_features.std())]

ml_train_std = ml_train_std.dropna()
train_norm = ml_data_norm.loc[ml_train_std.index]
```

In [33]:
```
sns.boxplot(data=ml_train_std)

sns.despine()
plt.title('Data distribution per feature (after outlier removal)')

plt.show()
```



Encoding target and categorical features

Some machine learning algorithms, like decision trees and random forest can work with categorical features in string format, most of them require the target and the features to be of a numeric data type. We can use pandas methods to transform columns to categorical type and access the integer used to code them.

In practice, One-Hot encoding often yields better results. This encoding consists of generating one column per unique value of each categorical feature, which will store the number one if the feature is present for the data example and a zero otherwise.

Note: For our dataframe this step is done merely as an example, as we already know we are not going to use the categorical feature columns.

In [34]:
```
train_norm.info()
```

```
<class 'pandas.core.frame.DataFrame'>
Int64Index: 1096326 entries, 0 to 1170510
Data columns (total 16 columns):
 #   Column     Non-Null Count    Dtype  
---  ------     --------------    -----  
 0   CALI       1096326 non-null  float64
 1   RMED       1096326 non-null  float64
 2   RDEP       1096326 non-null  float64
 3   RHOB       1096326 non-null  float64
 4   GR         1096326 non-null  float64
 5   NPHI       1096326 non-null  float64
 6   PEF        1096326 non-null  float64
 7   DTC        1096326 non-null  float64
 8   SP         1096326 non-null  float64
 9   BS         1096326 non-null  float64
 10  DRHO       1096326 non-null  float64
 11  WELL       1096326 non-null  object 
 12  GROUP      1096326 non-null  object 
 13  FORMATION  1096326 non-null  object 
 14  Z_LOC      1096326 non-null  float64
 15  LITHOLOGY  1096326 non-null  object 
dtypes: float64(12), object(4)
memory usage: 142.2+ MB
```

In [35]:
```
categorical_labels = ['WELL', 'GROUP', 'FORMATION']
target = 'LITHOLOGY'

train_norm[categorical_labels] = train_norm[categorical_labels]\
.astype('category')
train_norm[target] = train_norm[target].astype('category')

train_norm.dtypes
```

Out[35]:
```
CALI          float64
RMED          float64
RDEP          float64
RHOB          float64
GR            float64
NPHI          float64
PEF           float64
DTC           float64
SP            float64
BS            float64
DRHO          float64
WELL         category
GROUP        category
FORMATION    category
Z_LOC         float64
LITHOLOGY    category
dtype: object
```

Now we are going to explore the categorical features to see how many unique values each one has.

In [36]:
```
train_norm[categorical_labels].describe()
```

Out[36]:

	WELL	GROUP	FORMATION
count	1096326	1096326	1096326
unique	98	15	70
top	34/2-4	HORDALAND GP.	Utsira Fm.
freq	23224	278449	160838

We can see that there many unique wells and formations. One-Hot encoding would result in a dataframe with a much higher dimensionality. This would limit the options of machine learning algorithms that we can use.

In [37]:
```
dummy_cols = pd.get_dummies(train_norm[categorical_labels])
dummy_cols
```

Out[37]:

	WELL_15/9-13	WELL_15/9-15	WELL_15/9-17	WELL_16/1-2	WELL_16/1-6 A	WELL_16/10-1	WELL_16/10-2	WELL_16/10-3	WELL_16/10-5	WELL_16 1
0	1	0	0	0	0	0	0	0	0	
1	1	0	0	0	0	0	0	0	0	
2	1	0	0	0	0	0	0	0	0	
31	1	0	0	0	0	0	0	0	0	
38	1	0	0	0	0	0	0	0	0	
...	...	...	...	...	...	...	...	...	...	
1170506	0	0	0	0	0	0	0	0	0	
1170507	0	0	0	0	0	0	0	0	0	
1170508	0	0	0	0	0	0	0	0	0	
1170509	0	0	0	0	0	0	0	0	0	
1170510	0	0	0	0	0	0	0	0	0	

1096326 rows × 183 columns

In [38]:
```
train_norm = train_norm.drop(['WELL', 'GROUP', 'FORMATION'], axis=1)
train_coded = pd.concat([train_norm, dummy_cols], axis=1)
train_coded
```

Out[38]:

	CALI	RMED	RDEP	RHOB	GR	NPHI	PEF	DTC	SP	BS	DRHO	Z_LOC
0	1.568991	0.248649	0.207839	-1.596682	0.394830	0.032783	2.572578	1.562651	-0.653382	0.115317	-1.788225	-469.501831
1	1.566624	0.246764	0.205538	-1.578992	0.368797	0.032783	2.465534	1.547306	-0.664776	0.115317	-1.775855	-469.653809
2	1.566624	0.249919	0.209389	-1.557648	0.243230	0.032783	2.677322	1.534790	-0.664446	0.115317	-1.786445	-469.805786
31	1.569893	0.272831	0.237415	-1.698926	0.202743	0.032783	2.868035	1.523600	-0.662652	0.115317	-1.965463	-474.213715
38	1.572758	0.268708	0.232364	-1.716231	0.204041	0.032783	2.895321	1.524977	-0.663457	0.115317	-2.005383	-475.277679
...	...	...	...	...	...	...	...	...	...	...	...	...
1170506	-1.443252	1.634646	1.800229	1.081085	0.323779	0.032783	-0.318391	0.060655	-0.066107	-1.548304	-0.096868	-2138.527143
1170507	-1.460707	1.634646	1.800229	1.132149	0.258765	0.032783	0.656712	0.060655	-0.066107	-1.548304	-0.116600	-2138.527143
1170508	-1.472270	1.634646	1.800229	0.892694	-0.004801	0.032783	1.178166	0.060655	-0.066107	-1.548304	-0.152590	-2138.527143
1170509	-1.486859	1.634646	1.800229	0.668305	-0.346688	0.032783	1.146207	0.060655	-0.066107	-1.548304	-0.129537	-2138.527143
1170510	-1.494428	1.634646	1.800229	0.585053	-0.603234	0.032783	1.199726	0.060655	-0.066107	-1.548304	-0.129404	-2138.527143

1096326 rows × 196 columns

In [39]:
```
sorted_cols = np.append(logs_ml, dummy_cols.columns)
sorted_cols = np.append(sorted_cols, ['Z_LOC', 'LITHOLOGY'])

train_coded = train_coded[sorted_cols].copy()
train_coded
```

Out[39]:

	CALI	RMED	RDEP	RHOB	GR	NPHI	PEF	DTC	SP	BS	DRHO	WELL_15/9-13
0	1.568991	0.248649	0.207839	-1.596682	0.394830	0.032783	2.572578	1.562651	-0.653382	0.115317	-1.788225	1
1	1.566624	0.246764	0.205538	-1.578992	0.368797	0.032783	2.465534	1.547306	-0.664776	0.115317	-1.775855	1
2	1.566624	0.249919	0.209389	-1.557648	0.243230	0.032783	2.677322	1.534790	-0.664446	0.115317	-1.786445	1
31	1.569893	0.272831	0.237415	-1.698926	0.202743	0.032783	2.868035	1.523600	-0.662652	0.115317	-1.965463	1
38	1.572758	0.268708	0.232364	-1.716231	0.204041	0.032783	2.895321	1.524977	-0.663457	0.115317	-2.005383	1
...	...	...	...	...	...	...	...	...	...	...	...	...
1170506	-1.443252	1.634646	1.800229	1.081085	0.323779	0.032783	-0.318391	0.060655	-0.066107	-1.548304	-0.096868	0
1170507	-1.460707	1.634646	1.800229	1.132149	0.258765	0.032783	0.656712	0.060655	-0.066107	-1.548304	-0.116600	0
1170508	-1.472270	1.634646	1.800229	0.892694	-0.004801	0.032783	1.178166	0.060655	-0.066107	-1.548304	-0.152590	0
1170509	-1.486859	1.634646	1.800229	0.668305	-0.346688	0.032783	1.146207	0.060655	-0.066107	-1.548304	-0.129537	0
1170510	-1.494428	1.634646	1.800229	0.585053	-0.603234	0.032783	1.199726	0.060655	-0.066107	-1.548304	-0.129404	0

1096326 rows × 196 columns

For the target column, we will use pandas `Series.cat` accesor and the `series.cat.codes` attribute to assign the integer for each category to the target colum. Before doing so we will generate a dictionary with the category codes as keys and the lithology label as the value, this will be useful to transform the code to label.

In [40]:
```
code_lithology = dict(enumerate(train_coded['LITHOLOGY'].cat.categories))
code_lithology
```

Out[40]:
```
{0: 'Anhydrite',
 1: 'Basement',
 2: 'Chalk',
 3: 'Coal',
 4: 'Dolomite',
 5: 'Halite',
 6: 'Limestone',
 7: 'Marl',
 8: 'Sandstone',
 9: 'Sandstone/Shale',
 10: 'Shale',
 11: 'Tuff'}
```

In [41]:
```
train_coded['LITHOLOGY'] = train_coded['LITHOLOGY'].cat.codes
train_coded
```

Out[41]:

	CALI	RMED	RDEP	RHOB	GR	NPHI	PEF	DTC	SP	BS	DRHO	WELL_15/9-13
0	1.568991	0.248649	0.207839	-1.596682	0.394830	0.032783	2.572578	1.562651	-0.653382	0.115317	-1.788225	1
1	1.566624	0.246764	0.205538	-1.578992	0.368797	0.032783	2.465534	1.547306	-0.664776	0.115317	-1.775855	1
2	1.566624	0.249919	0.209389	-1.557648	0.243230	0.032783	2.677322	1.534790	-0.664446	0.115317	-1.786445	1
31	1.569893	0.272831	0.237415	-1.698926	0.202743	0.032783	2.868035	1.523600	-0.662652	0.115317	-1.965463	1
38	1.572758	0.268708	0.232364	-1.716231	0.204041	0.032783	2.895321	1.524977	-0.663457	0.115317	-2.005383	1
...	...	...	...	...	...	...	...	...	...	...	...	...
1170506	-1.443252	1.634646	1.800229	1.081085	0.323779	0.032783	-0.318391	0.060655	-0.066107	-1.548304	-0.096868	0
1170507	-1.460707	1.634646	1.800229	1.132149	0.258765	0.032783	0.656712	0.060655	-0.066107	-1.548304	-0.116600	0
1170508	-1.472270	1.634646	1.800229	0.892694	-0.004801	0.032783	1.178166	0.060655	-0.066107	-1.548304	-0.152590	0
1170509	-1.486859	1.634646	1.800229	0.668305	-0.346688	0.032783	1.146207	0.060655	-0.066107	-1.548304	-0.129537	0
1170510	-1.494428	1.634646	1.800229	0.585053	-0.603234	0.032783	1.199726	0.060655	-0.066107	-1.548304	-0.129404	0

1096326 rows × 196 columns

Defining baseline model performance

Baseline model performance is the minimum score that our model must obtain, to consider that said model actually add value or performs better than non-machine learning approaches. We will define our baseline model performance using the "zero rule" algorithm, which assigns the majority value to the target column.

In the case of our example, we know that the majority value for our target column is "Shale"(10), which represents over 60 percent of our data. This means that if we assigned "shale" as the label for our label. we would achieve an accuracy of over 60 percent in our training data.

In [42]:
```
df = train_coded.copy()

# assign features and target
X_train = df.drop(['LITHOLOGY', 'Z_LOC'], axis=1)
y_train = df['LITHOLOGY']

# generate synthetic prediction using zero rule algorithm
y_zr = pd.Series(np.full(y_train.shape[0], 10))

baseline_accuracy_training = accuracy_score(y_train, y_zr)
baseline_accuracy_training
```

Out[42]: 0.623314598030148

Selecting features

Some readers may have already noticed that there is something off with our dataframe. So far we have worked under the assumption that we were going to use all features remaining after we dropped columns with a fraction of missing data above some threshold, and dropping the `X_LOC`, `Y_LOC`, and `DEPTH_MD` data columns.

The selection of features to use four our model depends, among other things, in the amount of data available for each feature (which was the criterion we used when dropping columns with more than a certain amount of data missing), the predictive power of each feature, and in a certain way what the goal of the model is.

We must also avoid training the model using data that will be available only after the predictions are generated and thus won't be availabe for data the model has never seen. This phenomena is known as data leakage, and it can actually happen at several stages of workflow. For example, if we calculated the mean of the features and imputed missing values before splitting the dataset into train, validation and test sets, then our training data would be contaminated because in some way the mean contains information about the distribution of the test data, and our model will overperform in our train and test data but may underperform when deployed.

For our example, suppose we are building our model specifically for a well characterized field, and will be used after drilling to reduce the amount of time spent by a dedicated geosciences team to determine lithologies, in such case the `GROUP` and `FORMATION` columns could be used because it is very likely that seismic markers exist for these formations and we can be confident of their quality. However, is the aim of the model is such that it needs to predict lithology with information available inmediately on the field, then we could only use information suchs as the well logs to train our model.

If we suppose that our model is also going to be used for other fields, away from the wells from which the data was obtained, there may be no use for including information regarding the well name and coordinates. In fact, doing so may affect negatively affect model performance.

Another consideration is training and prediction time. Models using more features generally take longer to train, if the model response must be quicker then we must reduce the number of features while maintaining acceptable performance.

For our model, we will drop the binary columns obtained from the `WELL`, `GROUP`, and `FORMATION` data columns. When generating this columns, Pandas, by default, generates the column labels by adding the original column name as a suffix. We will take advantage of Python regex to select only column with labels that contain the substrings `WELL`, `GROUP`, or `FORMATION`. The `|` character is an special character in regex that means "or".

In [43]:
```
# select appropiate subset of dataframe
well_labels = df.columns[df.columns.str.contains('WELL|GROUP|FORMATION')]

df_ml = df.drop(well_labels, axis=1)
df_ml.columns
```

Out[43]:
```
Index(['CALI', 'RMED', 'RDEP', 'RHOB', 'GR', 'NPHI', 'PEF', 'DTC', 'SP', 'BS',
       'DRHO', 'Z_LOC', 'LITHOLOGY'],
      dtype='object')
```

Building the model

We will start by shuffling our training dataset. This can be done easily using the `DataFrame.sample()` method and setting the `frac` parameter to one. This method returns a random sample with n specified rows, setting the parameter to one means that it will return the entire dataframe. For reproducibility purposes we will set the `random state` parameter to one.

In [44]:
```
df_shuffled = df_ml.sample(frac=1, random_state=1).copy()
```

Now we will generate two arrays, one with only the features and another with the values in the target column. This arrays will be used to fit the model. Then we will initialize our model with default hyperparameter values, the parameters `random_state`, and `n_jobs` are meant for reproducibility and workload distribution among cpu cores, respectively, while the `verbose` parameter allows us to monitor the progress of training our model.

In [45]:
```
# generate arrays
X_train = df_shuffled.drop('LITHOLOGY', axis=1)
y_train = df_shuffled['LITHOLOGY']

# initalize model instance with default values
rfc = RandomForestClassifier(random_state=1, n_jobs=6, verbose=3)

# train the model
rfc.fit(X_train.values, y_train.values)

# generate predictions and calculate accuracy
y_pred = rfc.predict(X_train.values)
rfc_accuracy_training = accuracy_score(y_train, y_pred)
rfc_accuracy_training
```

```
[Parallel(n_jobs=6)]: Using backend ThreadingBackend with 6 concurrent workers.
building tree 1 of 100building tree 2 of 100

building tree 3 of 100
building tree 4 of 100
building tree 5 of 100
building tree 6 of 100
building tree 7 of 100
building tree 8 of 100
building tree 9 of 100
building tree 10 of 100
building tree 11 of 100
building tree 12 of 100
building tree 13 of 100
building tree 14 of 100
building tree 15 of 100
building tree 16 of 100
building tree 17 of 100
building tree 18 of 100
building tree 19 of 100
building tree 20 of 100
building tree 21 of 100
building tree 22 of 100
building tree 23 of 100
building tree 24 of 100
building tree 25 of 100
building tree 26 of 100
building tree 27 of 100
[Parallel(n_jobs=6)]: Done  20 tasks      | elapsed:   36.1s
building tree 28 of 100
building tree 29 of 100
building tree 30 of 100
building tree 31 of 100
building tree 32 of 100
building tree 33 of 100
building tree 34 of 100
building tree 35 of 100
building tree 36 of 100
building tree 37 of 100
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building tree 92 of 100
building tree 93 of 100
building tree 94 of 100
building tree 95 of 100
building tree 96 of 100
building tree 97 of 100
building tree 98 of 100
building tree 99 of 100
building tree 100 of 100
[Parallel(n_jobs=6)]: Done 100 out of 100 | elapsed:  2.4min finished
[Parallel(n_jobs=6)]: Using backend ThreadingBackend with 6 concurrent workers.
[Parallel(n_jobs=6)]: Done  20 tasks      | elapsed:    3.3s
[Parallel(n_jobs=6)]: Done 100 out of 100 | elapsed:   14.8s finished
```

Out[45]: 0.9999981757251036

Evaluating model performance in the training set is done to see how well the model fits the data, and to compare this training score performance with the score in the test set. If performance on the training data is considerably better than in the test data, then our model is overfitting, this means that the model is very sensible to small changes in the feature values and has poor generalization. We aim to achieve similar performance on both datasets, to do so we may try to simplify our model by selecting less features, keeping the ones with higher correlation with our target or in other words, features with high predictive power; or choose a different learning algorithm.

Note: There are several reasons for model underfitting and overfitting, I don't mention them all. Further research is suggested. There probably are many articles in websites like "Towards Data Science" or "Stack Data Science", describing these and several other machine learning concepts.

Generating test set

To generate the test set used for our machine learning algorithm, we will read the file containing the data not used to train the model. Then we must preprocess the data, applying the same data processing steps used in the training set and only for the same columns.

In [46]:
```
test_df = pd.read_csv('datasets1/log_official_test.csv', sep=';')
test_df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 122397 entries, 0 to 122396
Data columns (total 29 columns):
 #   Column                             Non-Null Count   Dtype  
---  ------                             --------------   -----  
 0   WELL                               122397 non-null  object 
 1   DEPTH_MD                           122397 non-null  float64
 2   X_LOC                              122386 non-null  float64
 3   Y_LOC                              122386 non-null  float64
 4   Z_LOC                              122386 non-null  float64
 5   GROUP                              122397 non-null  object 
 6   FORMATION                          114248 non-null  object 
 7   CALI                               118954 non-null  float64
 8   RSHA                               25683 non-null   float64
 9   RMED                               112580 non-null  float64
 10  RDEP                               122386 non-null  float64
 11  RHOB                               112869 non-null  float64
 12  GR                                 122397 non-null  float64
 13  SGR                                1139 non-null    float64
 14  NPHI                               96560 non-null   float64
 15  PEF                                100439 non-null  float64
 16  DTC                                118291 non-null  float64
 17  SP                                 46725 non-null   float64
 18  BS                                 74489 non-null   float64
 19  ROP                                91150 non-null   float64
 20  DTS                                72871 non-null   float64
 21  DCAL                               43104 non-null   float64
 22  DRHO                               112267 non-null  float64
 23  MUDWEIGHT                          0 non-null       float64
 24  RMIC                               15181 non-null   float64
 25  ROPA                               64221 non-null   float64
 26  RXO                                8894 non-null    float64
 27  FORCE_2020_LITHOFACIES_LITHOLOGY   122397 non-null  int64  
 28  FORCE_2020_LITHOFACIES_CONFIDENCE  122377 non-null  float64
dtypes: float64(25), int64(1), object(3)
memory usage: 27.1+ MB
```

Assign labels to the lithology column

In [47]:
```
label = 'FORCE_2020_LITHOFACIES_LITHOLOGY'

test_df['LITHOLOGY'] = test_df[label].map(lithology_keys)
```

In [48]:
```
test_df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 122397 entries, 0 to 122396
Data columns (total 30 columns):
 #   Column                             Non-Null Count   Dtype  
---  ------                             --------------   -----  
 0   WELL                               122397 non-null  object 
 1   DEPTH_MD                           122397 non-null  float64
 2   X_LOC                              122386 non-null  float64
 3   Y_LOC                              122386 non-null  float64
 4   Z_LOC                              122386 non-null  float64
 5   GROUP                              122397 non-null  object 
 6   FORMATION                          114248 non-null  object 
 7   CALI                               118954 non-null  float64
 8   RSHA                               25683 non-null   float64
 9   RMED                               112580 non-null  float64
 10  RDEP                               122386 non-null  float64
 11  RHOB                               112869 non-null  float64
 12  GR                                 122397 non-null  float64
 13  SGR                                1139 non-null    float64
 14  NPHI                               96560 non-null   float64
 15  PEF                                100439 non-null  float64
 16  DTC                                118291 non-null  float64
 17  SP                                 46725 non-null   float64
 18  BS                                 74489 non-null   float64
 19  ROP                                91150 non-null   float64
 20  DTS                                72871 non-null   float64
 21  DCAL                               43104 non-null   float64
 22  DRHO                               112267 non-null  float64
 23  MUDWEIGHT                          0 non-null       float64
 24  RMIC                               15181 non-null   float64
 25  ROPA                               64221 non-null   float64
 26  RXO                                8894 non-null    float64
 27  FORCE_2020_LITHOFACIES_LITHOLOGY   122397 non-null  int64  
 28  FORCE_2020_LITHOFACIES_CONFIDENCE  122377 non-null  float64
 29  LITHOLOGY                          122397 non-null  object 
dtypes: float64(25), int64(1), object(4)
memory usage: 28.0+ MB
```

Select only the columns used in the training data

In [49]:
```
test_df1 = test_df[df_ml.columns].copy()
test_df1.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 122397 entries, 0 to 122396
Data columns (total 13 columns):
 #   Column     Non-Null Count   Dtype  
---  ------     --------------   -----  
 0   CALI       118954 non-null  float64
 1   RMED       112580 non-null  float64
 2   RDEP       122386 non-null  float64
 3   RHOB       112869 non-null  float64
 4   GR         122397 non-null  float64
 5   NPHI       96560 non-null   float64
 6   PEF        100439 non-null  float64
 7   DTC        118291 non-null  float64
 8   SP         46725 non-null   float64
 9   BS         74489 non-null   float64
 10  DRHO       112267 non-null  float64
 11  Z_LOC      122386 non-null  float64
 12  LITHOLOGY  122397 non-null  object 
dtypes: float64(12), object(1)
memory usage: 12.1+ MB
```

Replace missing data with the mean value of each feature

In [50]:
```
num_cols = test_df1.select_dtypes(include=np.number)
categorical_cols = test_df1.select_dtypes(include=np.object)
```

In [51]:
```
num_cols_clean = num_cols.fillna(num_cols.mean())
num_cols_clean.isnull().sum()
```

Out[51]:
```
CALI     0
RMED     0
RDEP     0
RHOB     0
GR       0
NPHI     0
PEF      0
DTC      0
SP       0
BS       0
DRHO     0
Z_LOC    0
dtype: int64
```

In [52]:
```
categorical_cols_clean = categorical_cols.fillna('Unknown')
categorical_cols_clean.isnull().sum()
```

Out[52]:
```
LITHOLOGY    0
dtype: int64
```

In [53]:
```
test_df_clean = pd.concat([num_cols_clean, categorical_cols_clean], axis=1)
test_df_clean.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 122397 entries, 0 to 122396
Data columns (total 13 columns):
 #   Column     Non-Null Count   Dtype  
---  ------     --------------   -----  
 0   CALI       122397 non-null  float64
 1   RMED       122397 non-null  float64
 2   RDEP       122397 non-null  float64
 3   RHOB       122397 non-null  float64
 4   GR         122397 non-null  float64
 5   NPHI       122397 non-null  float64
 6   PEF        122397 non-null  float64
 7   DTC        122397 non-null  float64
 8   SP         122397 non-null  float64
 9   BS         122397 non-null  float64
 10  DRHO       122397 non-null  float64
 11  Z_LOC      122397 non-null  float64
 12  LITHOLOGY  122397 non-null  object 
dtypes: float64(12), object(1)
memory usage: 12.1+ MB
```

Scaling the data

In [54]:
```
# transform resistivity logs to logarithmic scale
test_df_clean['RMED'] = np.log10(test_df_clean['RMED'])
test_df_clean['RDEP'] = np.log10(test_df_clean['RDEP'])
```

In [55]:
```
# select labels of columns to apply power transformer
columns_scale = test_df_clean.columns[:11].copy()

# initialize PowerTransformer instance
scaler = PowerTransformer()

# initialize ColumnTransformer instance
ct = ColumnTransformer([('scaler', scaler, columns_scale)],
                       remainder='passthrough')

test_ml_norm = ct.fit_transform(test_df_clean)

# assign back column labels and transform numerical columns back to float
test_ml_norm = pd.DataFrame(test_ml_norm, columns=test_df_clean.columns)
test_ml_norm[columns_scale] = test_ml_norm[columns_scale].astype(float)
test_ml_norm.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 122397 entries, 0 to 122396
Data columns (total 13 columns):
 #   Column     Non-Null Count   Dtype  
---  ------     --------------   -----  
 0   CALI       122397 non-null  float64
 1   RMED       122397 non-null  float64
 2   RDEP       122397 non-null  float64
 3   RHOB       122397 non-null  float64
 4   GR         122397 non-null  float64
 5   NPHI       122397 non-null  float64
 6   PEF        122397 non-null  float64
 7   DTC        122397 non-null  float64
 8   SP         122397 non-null  float64
 9   BS         122397 non-null  float64
 10  DRHO       122397 non-null  float64
 11  Z_LOC      122397 non-null  object 
 12  LITHOLOGY  122397 non-null  object 
dtypes: float64(11), object(2)
memory usage: 12.1+ MB
```

Outlier removal

In [56]:
```
# remove outliers with standard deviation method
ml_features = test_ml_norm[columns_scale].copy()

ml_test_std = ml_features[np.abs(ml_features - ml_features.mean()) <=
                          (3 * ml_features.std())]

ml_test_std = ml_test_std.dropna().copy()
test_norm = test_ml_norm.loc[ml_test_std.index]
```

In [57]:
```
test_norm.info()
```

```
<class 'pandas.core.frame.DataFrame'>
Int64Index: 116251 entries, 45 to 122395
Data columns (total 13 columns):
 #   Column     Non-Null Count   Dtype  
---  ------     --------------   -----  
 0   CALI       116251 non-null  float64
 1   RMED       116251 non-null  float64
 2   RDEP       116251 non-null  float64
 3   RHOB       116251 non-null  float64
 4   GR         116251 non-null  float64
 5   NPHI       116251 non-null  float64
 6   PEF        116251 non-null  float64
 7   DTC        116251 non-null  float64
 8   SP         116251 non-null  float64
 9   BS         116251 non-null  float64
 10  DRHO       116251 non-null  float64
 11  Z_LOC      116251 non-null  object 
 12  LITHOLOGY  116251 non-null  object 
dtypes: float64(11), object(2)
memory usage: 12.4+ MB
```

Assign codes to each lithology label

To ensure that we assign the same code to each lithology as in the training data we will use the dictionary `code_lithology`, that we previously generated, to obtain a dictionary to use with the `Series.map()` function.

In [58]:
```
code_lithology
```

Out[58]:
```
{0: 'Anhydrite',
 1: 'Basement',
 2: 'Chalk',
 3: 'Coal',
 4: 'Dolomite',
 5: 'Halite',
 6: 'Limestone',
 7: 'Marl',
 8: 'Sandstone',
 9: 'Sandstone/Shale',
 10: 'Shale',
 11: 'Tuff'}
```

In [59]:
```
lithology_code = dict()

for code, lithology in code_lithology.items():
    if lithology not in lithology_code:
        lithology_code[lithology] = code

lithology_code
```

Out[59]:
```
{'Anhydrite': 0,
 'Basement': 1,
```

```
 'Chalk': 2,
 'Coal': 3,
 'Dolomite': 4,
 'Halite': 5,
 'Limestone': 6,
 'Marl': 7,
 'Sandstone': 8,
 'Sandstone/Shale': 9,
 'Shale': 10,
 'Tuff': 11}
```

In [60]:
```
test_norm['LITHOLOGY'] = test_norm['LITHOLOGY'].map(lithology_code)
```

In [61]:
```
test_norm.columns
```

Out[61]:
```
Index(['CALI', 'RMED', 'RDEP', 'RHOB', 'GR', 'NPHI', 'PEF', 'DTC', 'SP', 'BS',
       'DRHO', 'Z_LOC', 'LITHOLOGY'],
      dtype='object')
```

In [62]:
```
test_data = test_norm.copy()
```

Model performance on test data

Now we will first evaluate baseline performance on the test data with the "zero rule" algorithm, and then use the model we built to predict the lithologies for the test data, and use our score function to evaluate its performace.

In [63]:
```
# specify features and target arrays

X_test = test_data.drop('LITHOLOGY', axis=1)
y_test = test_data['LITHOLOGY']

# predict labels
yzr_pred = np.full(y_test.shape[0], 10)
y_pred = rfc.predict(X_test.values)

# calculate accuracy
baseline_accuracy_test = accuracy_score(y_test.values, yzr_pred)
rfc_accuracy_test = accuracy_score(y_test.values, y_pred)
```

```
[Parallel(n_jobs=6)]: Using backend ThreadingBackend with 6 concurrent workers.
[Parallel(n_jobs=6)]: Done  20 tasks      | elapsed:    0.0s
[Parallel(n_jobs=6)]: Done 100 out of 100 | elapsed:    0.6s finished
```

In [64]:
```
models_summary = dict()

yzr_summary = {'Accuracy_training': baseline_accuracy_training,
               'Accuracy_test': baseline_accuracy_test}

rfc_summary = {'Accuracy_training': rfc_accuracy_training,
               'Accuracy_test': rfc_accuracy_test}

models_summary['Zero rule algorithm'] = yzr_summary
models_summary['Random Forest Classifier'] = rfc_summary

models_summary_df = pd.DataFrame.from_dict(models_summary, orient='index')
models_summary_df
```

Out[64]:

	Accuracy_training	Accuracy_test
Zero rule algorithm	0.623315	0.600279
Random Forest Classifier	0.999998	0.717929

Conclusion

We managed to generate a simple model that performed better than the baseline model in both, the training and test data, without taking into account geolocation data (except for the `Z_LOC` column), and with default hyperparameters, although the model shows overfitting.

Future improvements

- Application of techniques to handle imbalanced datasets, both, before model training (oversampling and undersampling), and during model training (for machine learning algorithms that support this functionality).
- Extensive feature engineering and feature selection techniques.
- Try other data imputation techniques.
- Compare performance of other algorithms like Multilayer Perceptron Classifier or KNeighbors Classifier.
- Combine the predictions of different models to see if there is any improvement in accuracy.
- Build a confusion matrix to see if there are any patterns in the misclassification.

Also, in other notebooks, regarding the prediction of well log curves, the columns describing the depth at which the measurement was recorded is not scaled. It would be interesting to scale this column to see if there is any improvement on model performance. As far as I understand, there might be because this column outscales other features.

References

- Burkov, A. (2020).*Machine Learning Engineering*(1st ed.). True Positive Inc.
- Nuwara, Y. (2020,October 27).*A Demo on P-Sonic Log Prediction using Machine Learning in the Volve Field Dataset* https://github.com/yohanesnuwara/volve-machine-learning/blob/main/notebook/demo_volve_soniclog_prediction.ipynb