

Assignment – E11

DS- 203 program

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Data

- Daily averaged values of observations of some parameters at a chemical processing plant
- 240 columns and 1025 rows. Each row corresponds to data for the date given in column c1
- Rest of the columns represent can be grouped into operating and controllable parameters
- Controllable parameters: c26, c27, c28, c29, c30, c31, c32, c33, c39, c139, c142, c143, c155, c156, c157, c158, c160, c161, c162, c163

Objectives

- c 51, c52, c53, c54 represent vibrations: need to be kept in limit
- c241 is specific energy or i.e. energy consumption per unit output: should be as minimum as possible
- All of them are non-controllable parameters i.e. can't control them directly
- Have to control them using controllable parameters

Our Job

Task 1: Reducing the vibrations

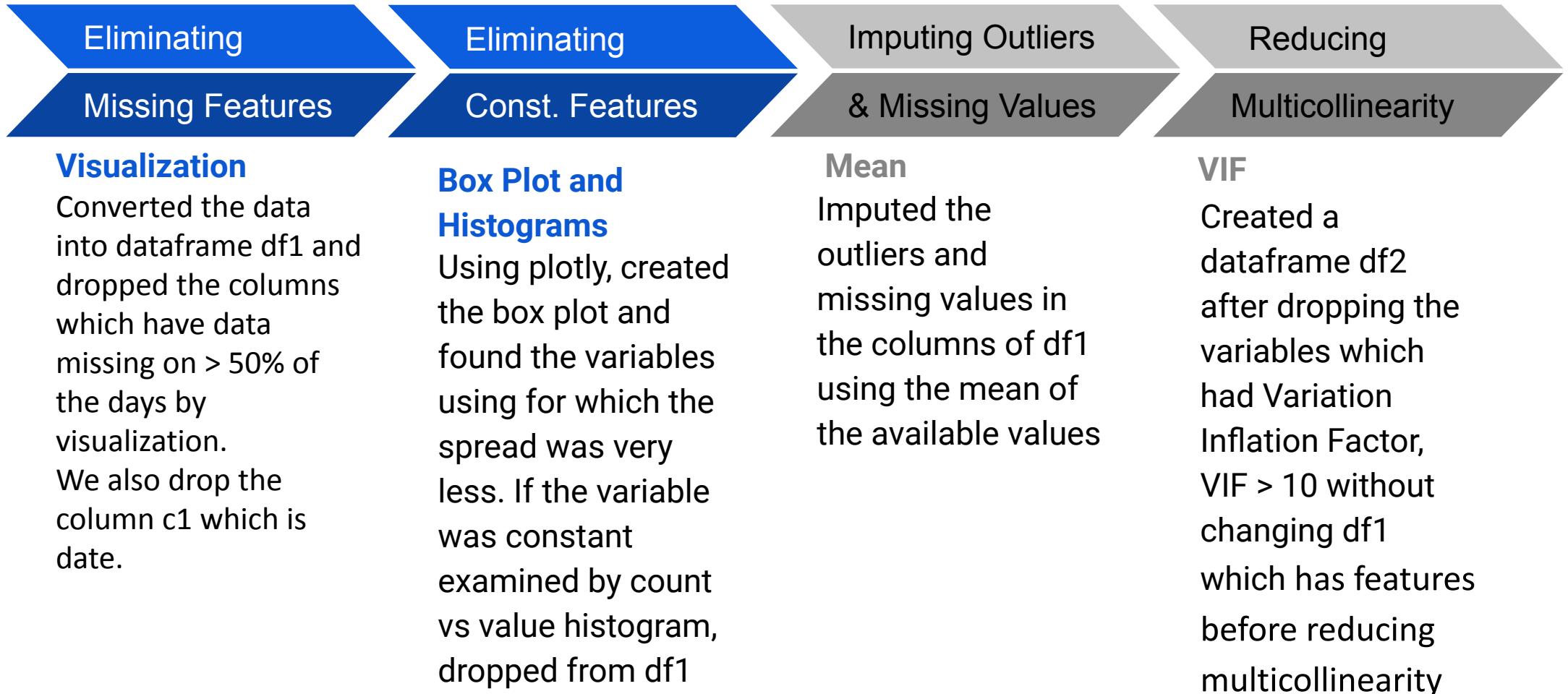
- Task 1.1 :
 - Create an ML model with operating + controllable parameters to predict HIGH and CRITICAL vibrations (c51, c52, c53, c54)
 - This model can be used to raise alerts and alarms
- Task 1.2:
 - Create an ML model with controllable parameters for c51, c52, c53, c54
 - From the model create a list of most important parameters to reduce vibrations

Task 2: Reducing the specific energy

- Task 2.1 :
 - Creating an ML model with operating + controllable parameters to predict specific energy, c241
 - From the mode, create a list of most important parameters to reduce the energy consumption
- Task 2.2:
 - Find the minimum number of independent variables which can predict the energy consumption
 - Create an ML model with those variables

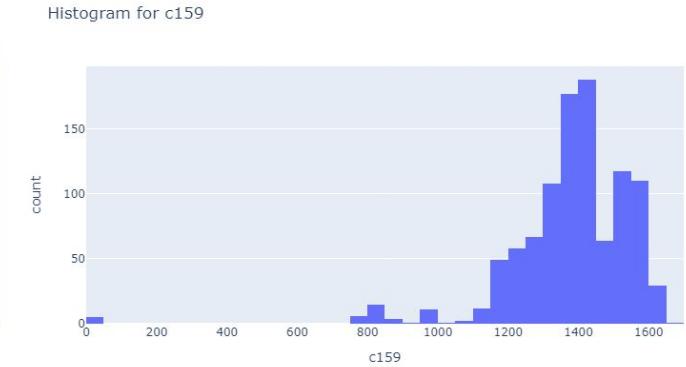
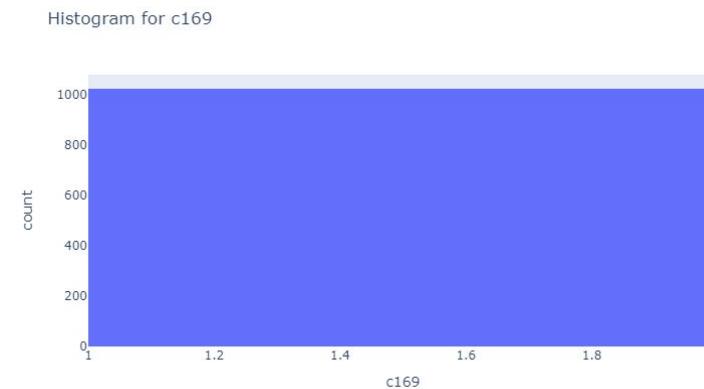
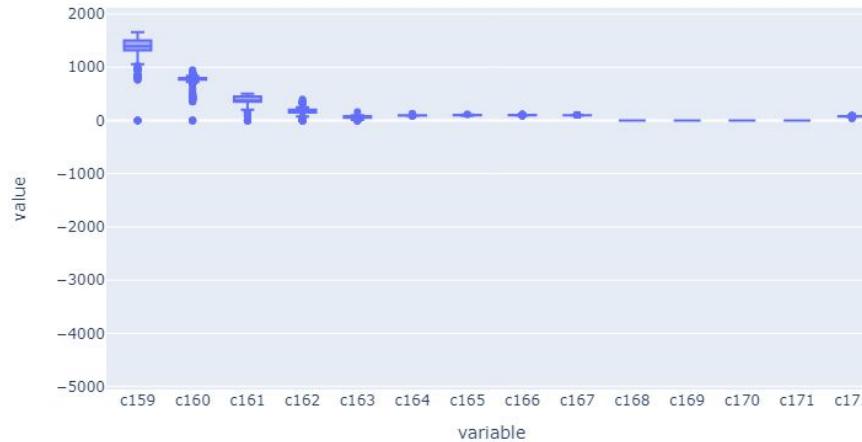
Data Pre-processing

While eliminating features, we take care not to drop the vibration, specific energy & controllable parameter



Data Pre-processing: Eliminating Constant Features

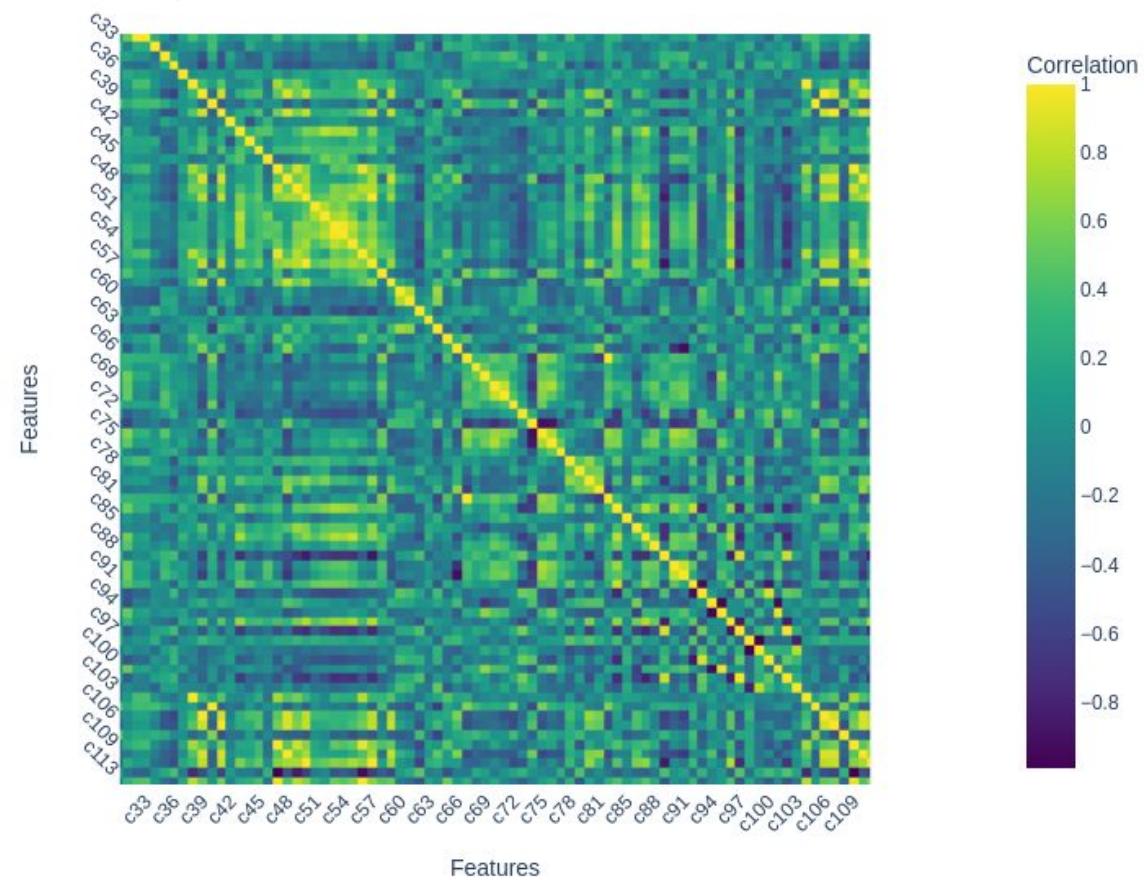
- A section of box plots for all variables



- c168, c169, c170, c171 look constant and on plotting histograms of such variables we find it to be the case and we such variables
- count vs value histogram of non-constant variables like c159 looks like the third figure and we keep such variables

Data Pre-processing: Reducing Multicollinearity

- Visualization using heat maps: In a section of heat map presented below, it can be seen that there is high collinearity between some variables as indicated by bright yellow and dark green squares, off the diagonal.



Data Pre-processing: Reducing Multicollinearity using VIF

VIF

Determining High VIF features Deleting features

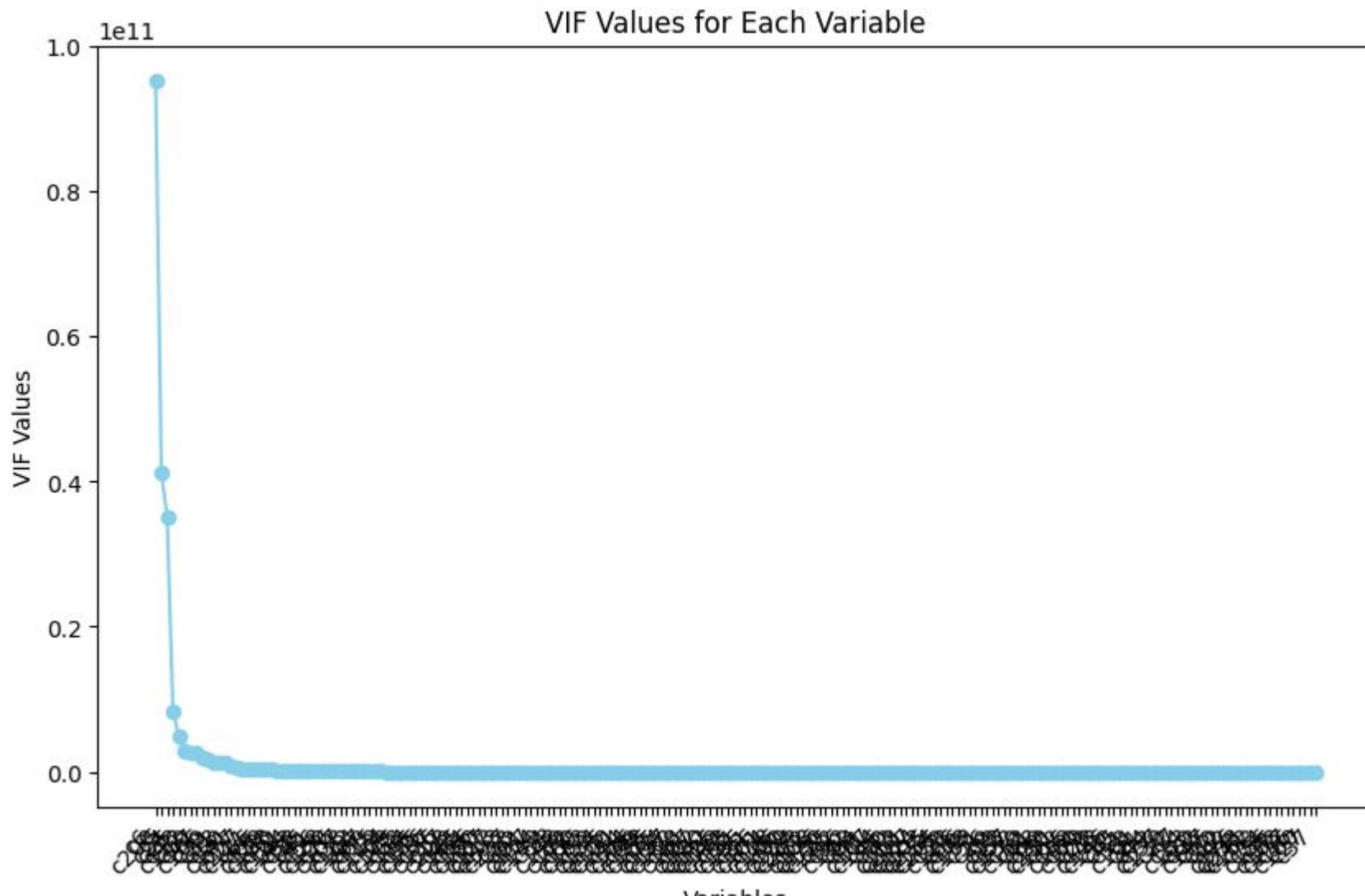
Variance inflation factor of all variables were checked

Features with VIF higher than 10 identified

High VIF features deleted after checking if they were either 'controllable parameters' or 'target variables' in which case they were retained

Now we create a new df, df2 which has 53 columns after dropping hgh VIF features as opposed to df1 which has 202 columns after dropping redundant variables

Data Pre-processing: Plot showing VIF



Task 1: Reducing the vibrations

Task 1.1: Implementing ML to predict High and Critical Vibration Levels

- Creating model using df1 which contains variables with multicollinearity as well

Feature Transformation	Label Encoding	Splitting Data & Normalization	Creating ML Model
We created a new target variable 'overall risk' using columns c51, c52, c53 & c54. 'overall_risk' takes values CRITICAL, HIGH, MODERATE, SAFE if any of the values from c51, c52, c53, c54 satisfy the criteria with 'CRITICAL>HIGH>MODERATE>SAFE.'	We label encode overall_risk i.e. CRITICAL = 0 HIGH = 1 MODERATE = 2 SAFE = 3 Interestingly, we don't find any SAFE Our input features are features in df1 other than c51, c52, c53 & c54 and target is overall_risk	We split the data into train and test with 80:20 ratio and then normalize them separately using min-max scaling. It is necessary to normalize the data after splitting so as to ensure the independence of training and test data.	This is a classification problem so we used Logistic Regression model as our baseline model which we trained on both dfs with high VIF features and without. We did not see much difference in the outputs. We also used a more sophisticated ML model which is SVM on df1 as models such as SVM automatically take care of multicolinearity

Task 1.1: Implementing ML to predict High and Critical Vibration Levels - Logistic Regression on unfiltered df1

Initial Model Accuracy: 0.9414634146341463

Confusion Matrix:

```
[[19  0  0]
 [ 1 88  5]
 [ 0  6 86]]
```

Classification Report:

	precision	recall	f1-score	support
CRITICAL	0.95	1.00	0.97	19
HIGH	0.94	0.94	0.94	94
MODERATE	0.95	0.93	0.94	92
accuracy			0.94	205
macro avg	0.94	0.96	0.95	205
weighted avg	0.94	0.94	0.94	205

Task 1.1: Implementing ML to predict High and Critical Vibration Levels

Logistic Regression on filtered data that is without features with High VIF

```
New Model Accuracy: 0.9121951219512195
```

```
Confusion Matrix:
```

```
[[19  0  0]
 [ 1 80 13]
 [ 0  4 88]]
```

```
Classification Report:
```

	precision	recall	f1-score	support
CRITICAL	0.95	1.00	0.97	19
HIGH	0.95	0.85	0.90	94
MODERATE	0.87	0.96	0.91	92
accuracy			0.91	205
macro avg	0.92	0.94	0.93	205
weighted avg	0.92	0.91	0.91	205

Alternative ML Model: SVM

There are some machine learning models which take care of the multicollinearity of the features by using certain methods like regularization and can give good results with the right hyper parameter tuning even without using tools like VIF.

We demonstrate the use of one such ML model which Support Vector Classifier

Results of SVM

```
Best Parameters: {'C': 0.1, 'gamma': 'scale', 'kernel': 'poly'}
Best Score: 0.9597560975609755
Best Parameters: {'C': 0.1, 'gamma': 'scale', 'kernel': 'poly'}
Best Accuracy: 0.9597560975609755
Test Accuracy SVM: 0.975609756097561
```

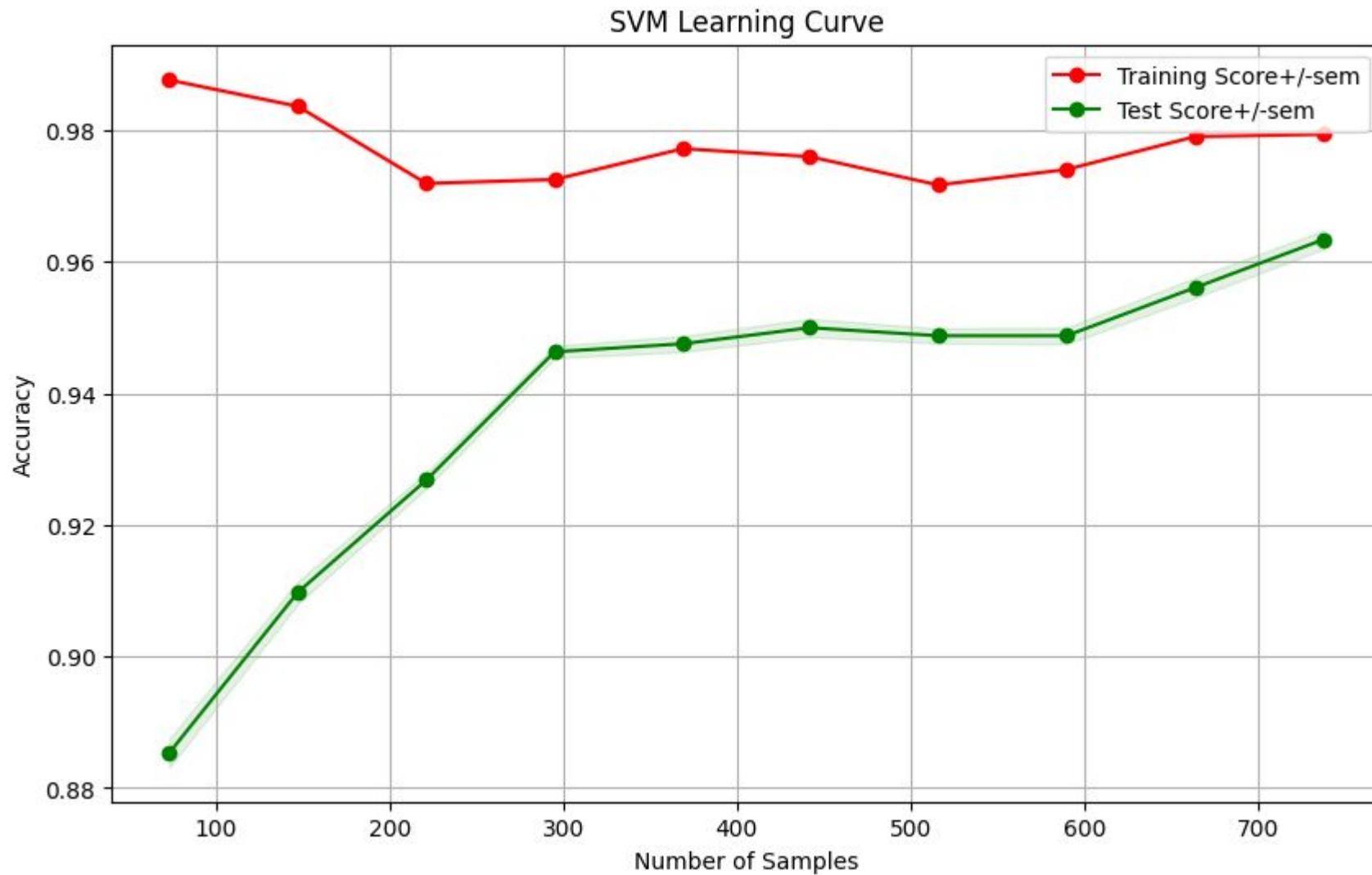
Confusion Matrix SVM:

```
[[19  0  0]
 [ 1 91  2]
 [ 0  2 90]]
```

Classification Report SVM:

	precision	recall	f1-score	support
CRITICAL	0.95	1.00	0.97	19
HIGH	0.98	0.97	0.97	94
MODERATE	0.98	0.98	0.98	92
accuracy			0.98	205
macro avg	0.97	0.98	0.98	205
weighted avg	0.98	0.98	0.98	205

Learning Curves of SVM



Task 1.1: Implementing ML to predict High and Critical Vibration Levels

As we can see SVM gave us better results, this could be due to the inherent features of sophisticated ML models such as SVM which take care of factors like multicollinearity.

ML Model for Controllable Parameters only

Task 1.2: Implementing ML to find Important Controllable Parameters

- We take the controllable parameters as x variables and 'overall_risk' as the y variable
- We then split the x variables into train and test data 80:20 and normalize using min-max scaling
- We train our model using Random Forest Classifier which has built-in feature importance function
- On fitting we find our performance of the model as follows:

Accuracy RF: 0.9560975609756097

Classification Report RF:

	precision	recall	f1-score	support
CRITICAL	0.95	1.00	0.97	19
HIGH	0.95	0.96	0.95	94
MODERATE	0.97	0.95	0.96	92
accuracy			0.96	205
macro avg	0.95	0.97	0.96	205
weighted avg	0.96	0.96	0.96	205

Task: List Important Features

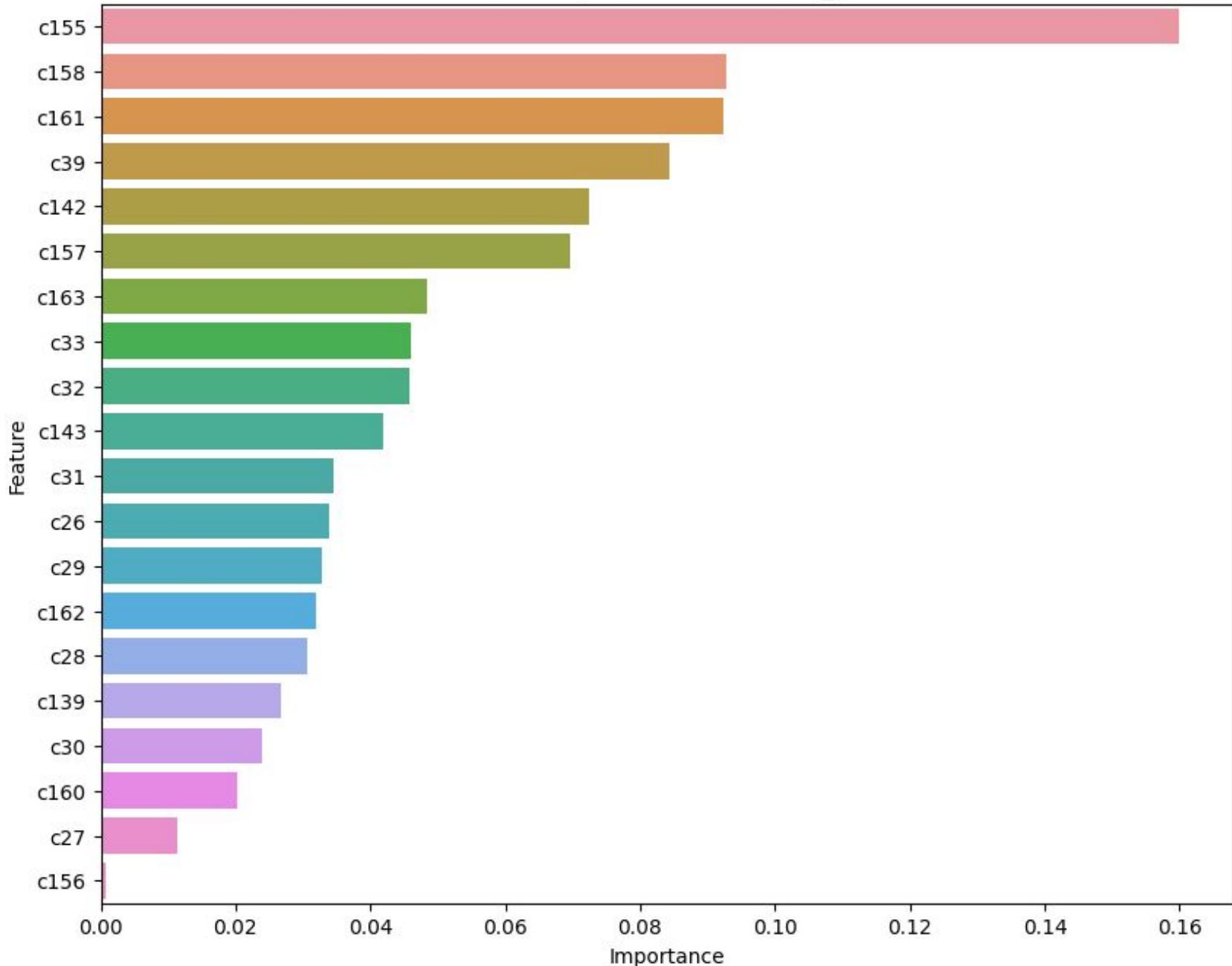
Two Approaches

**Inherent
Feature
Importance
of Random
Forest
Classifier**

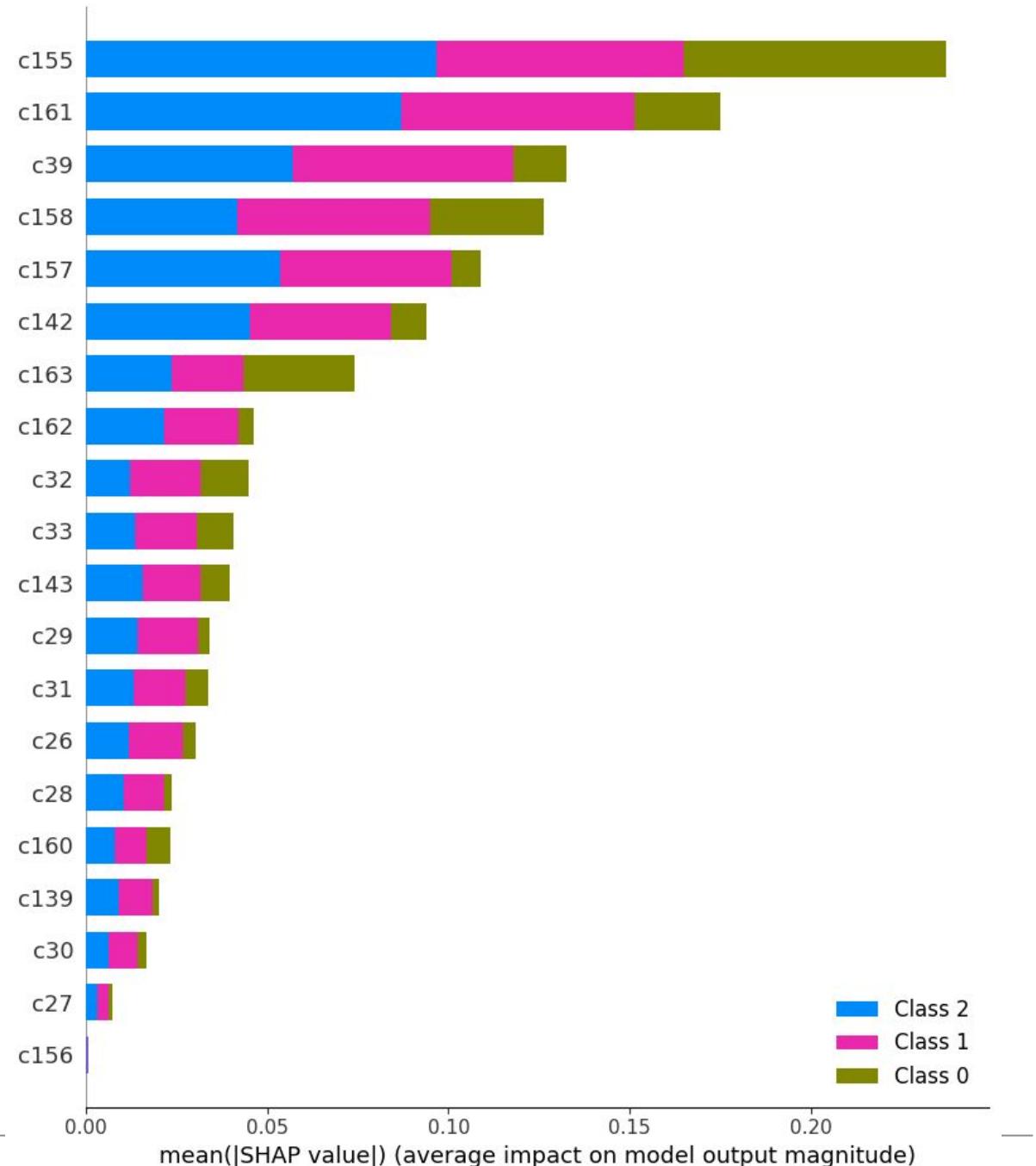
**Model
Agnostic
feature
Importance
Method Such
as SHapley
Additive
exPlanations**

Feature importance using Random Forest Classifier

Feature Importance for Overall_Risk



Class wise Feature Importance using SHAP



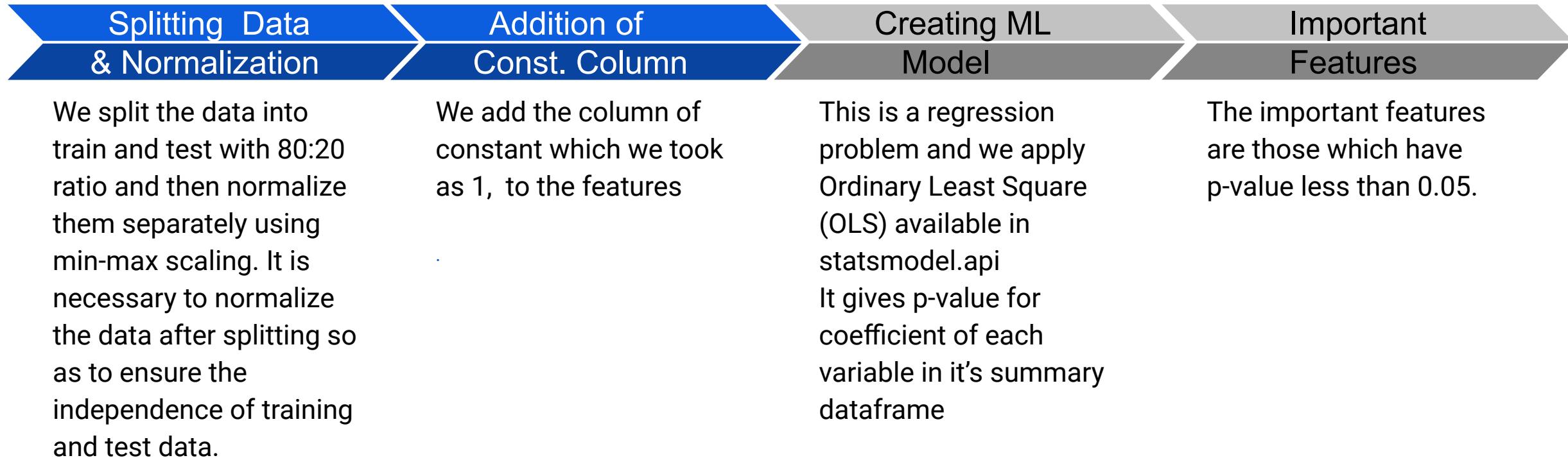
Task 1.2: Important Features

Note that the important features remain the same, but SHAP gives us added information of class wise feature importance.

Task 2: Reducing Specific Energy

Task 2.1: Implementing ML to Find Significant Features for Specific Energy Prediction

- We create a model using df2 which has no feature with high VIF
- Our target is c241 and the independent variables are all features in df2 other than c241



Task 2.1: Implementing ML to Find Significant Features for Specific Energy Prediction

- Truncated OLS results

OLS Regression Results												
Dep. Variable:		c241	R-squared:		0.258							
Model:		OLS	Adj. R-squared:		0.218							
Method:		Least Squares	F-statistic:		6.494							
Date:		Sun, 12 Nov 2023	Prob (F-statistic):		4.70e-36							
Time:		02:31:40	Log-Likelihood:		-981.61							
No. Observations:		1025	AIC:		2069.							
Df Residuals:		972	BIC:		2331.							
Df Model:		52										
Covariance Type:												
nonrobust												
	coef	std err	t	P> t	[0.025	0.975]						
const	4.0180	0.487	8.242	0.000	3.061	4.975						
c7	0.5587	0.158	3.526	0.000	0.248	0.870						
	0.0711	0.001	0.010	0.700	0.170	0.200						

Omnibus:	2471.438	Durbin-Watson:	1.682
Prob(Omnibus):	0.000	Jarque-Bera (JB):	18573182.518
Skew:	23.022	Prob(JB):	0.00
Kurtosis:	660.848	Cond. No.	284.

Notes:

[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.

- 19 Significant Features

	p_val
const	5.431615e-16
c155	3.699908e-14
c39	1.810322e-09
c22	6.204579e-05
c143	1.191433e-04
c139	3.987530e-04
c7	4.415969e-04
c42	8.409049e-04
c137	9.382014e-04
c72	2.067982e-03
c26	2.498036e-03
c147	4.441144e-03
c21	5.471427e-03
c14	1.016282e-02
c157	1.216262e-02
c158	1.468552e-02
c73	2.464412e-02
c20	2.534467e-02
c28	3.119151e-02

Task 2.2: Determining ‘minimum set’ of ‘independent feature’ utilized to only ‘predict not control’ c241

- Here our approach will be to use PCA with the original data set with all features (even ones with high VIF). The reasoning for this as follows:
 - PCA will help us identify those minimum number of components which explain the maximum variance in the dataset.
 - PCA makes us loose feature importance, so we know the principal components but we don’t know which features contributed to these principal components.
 - However, since our purpose is to only ‘predict’ and ‘not control’ the target, we can afford to loose explainability in lieu of better predictions.
 - Use of original df even with high VIF features is justified and PCA itself takes multicollinearity of the data set into consideration.

Task 2.2: Determining ‘minimum set’ of ‘independent feature’ utilized to only ‘predict not control’ c241

- Our approach:

Splitting Data & Normalization

We split the data into train and test with 80:20 ratio and then normalize them separately using min-max scaling. It is necessary to normalize the data after splitting so as to ensure the independence of training and test data.

Performing PCA

We implement PCA such that number of components are enough to explain at least 90% of the variance of the dataset.

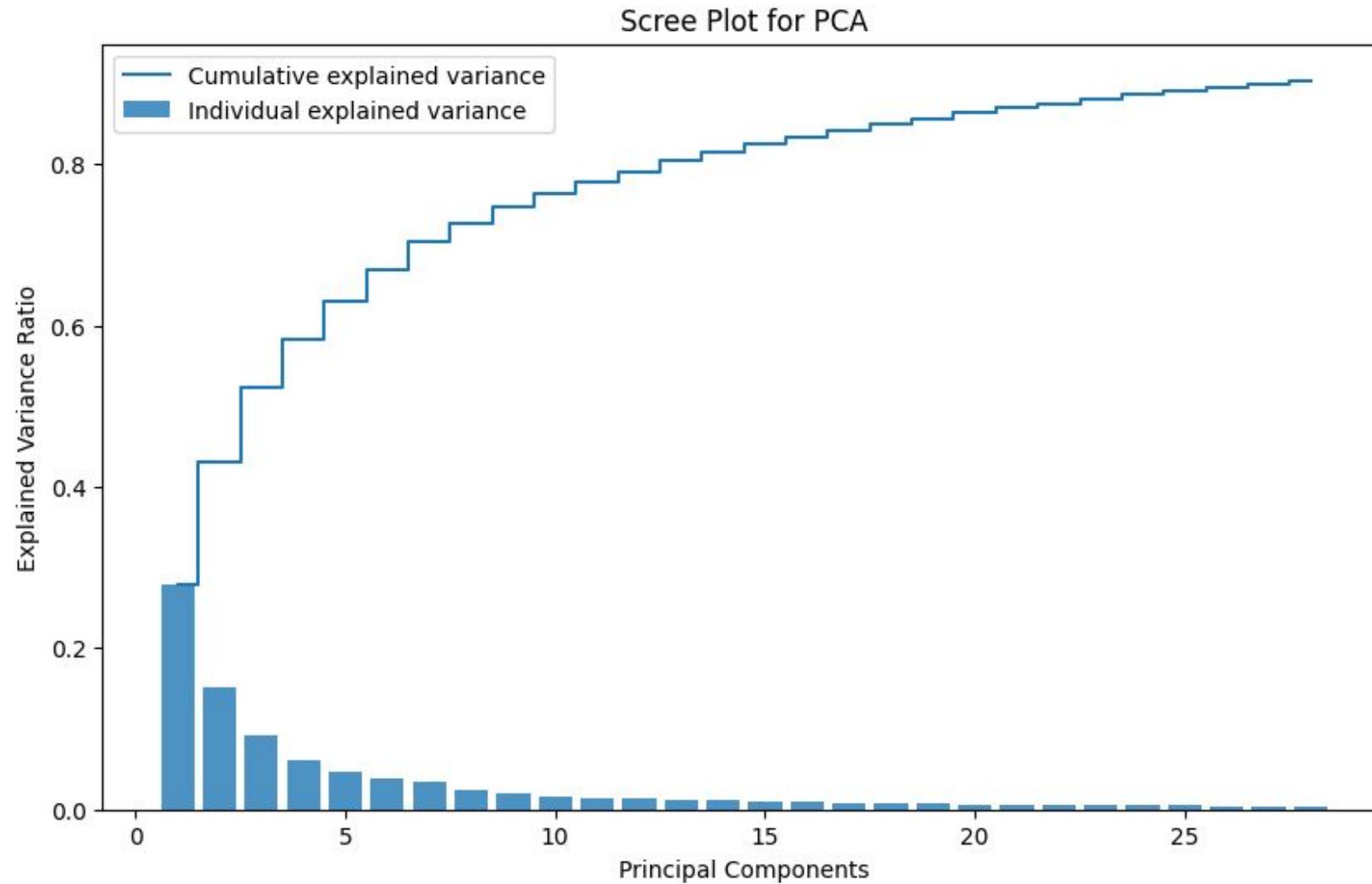
We plot the Scree plot and a scatter plot to visualise this output

Creating ML Model

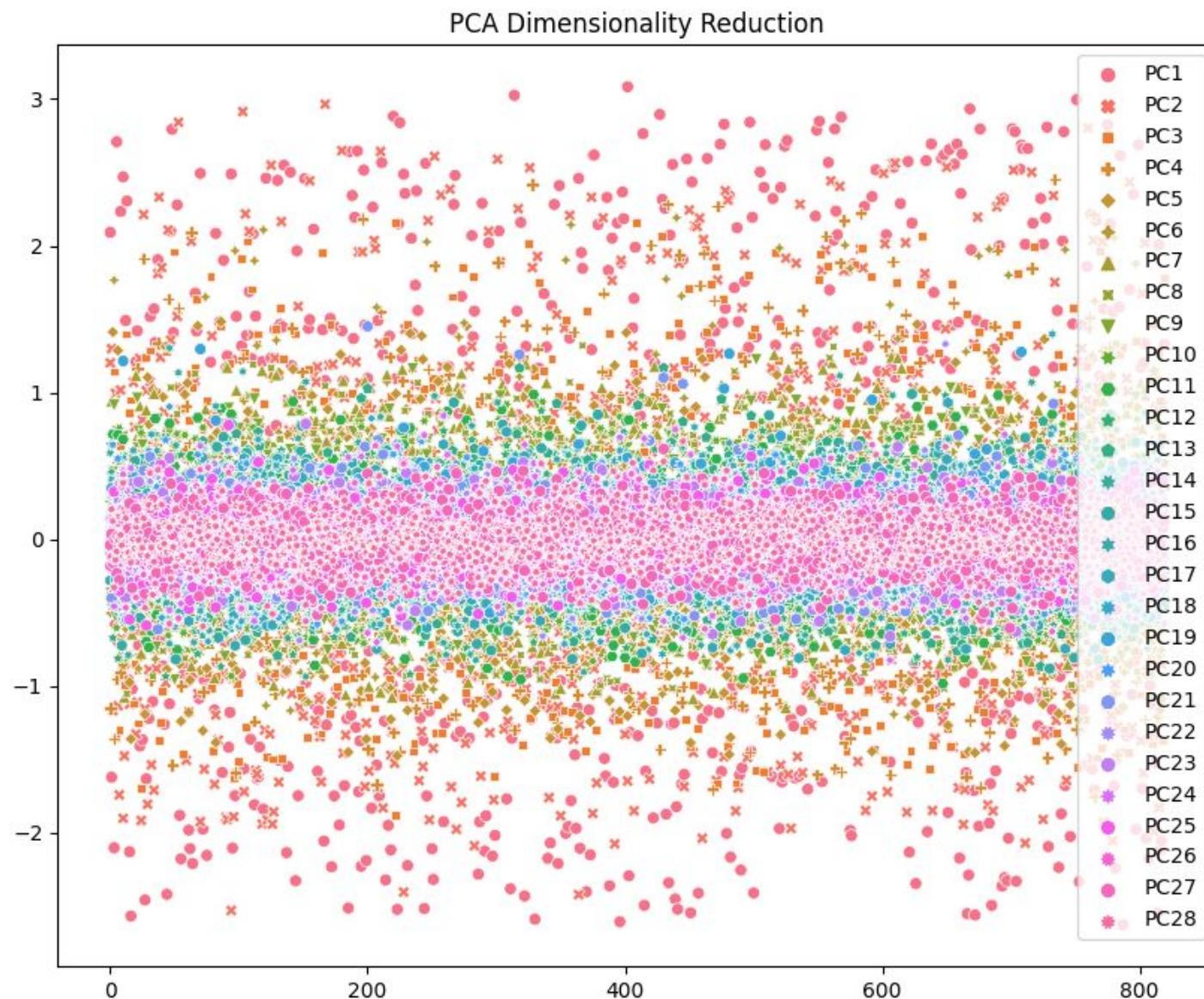
We use the Principal components in the ML model (we used random forest regressor, we tried others too but rf gave the best results).

We used the functions fit_transform for training set and only transform for test set.

Scree plot for PCA



Scatter Plot of PCA components



Results of Random Forest Model using PCA

Training MSE PCA RF: 0.093

Training R2 PCA RF: 0.861

Testing MSE PCA RF: 0.002

Testing R2 PCA RF: 0.847

Key Achievements

- We employed multiple methods of data pre processing for different problems in the data set.
 - Feature binning: For largely missing/ constant variables
 - Data imputation
 - Identifying outliers using IQR
 - Imputing outliers
 - Identifying multicollinearity in the data set and filtering the data set accordingly
- We were successfully able to build machine learning models for the various tasks while taking care of the problems in the dataset.
- For task 1 we created a single ML model and not multiple for c51, c52, c53, c54, by creating a new variable which depended on these four. We could do this as the purpose was to raise an alert if ‘any’ of these were off.
- For the feature importance task from among the controllable parameters we used ‘SHAP’ which goes a step ahead and gives us class wise feature importance, thus determining which features contribute heavily to predicting ‘CRITICAL’ level.

Challenges

- Deciding which machine learning algorithm is the best to use can be a challenge, we had to try multiple ones in our effort and then report the one with best results.
- Data being noisy was a challenge, which we tackled with a series of pre processing steps.

Recommendations

- Machine learning models thus created can be deployed to raise alerts/ alarms when levels reach High/ Critical accordingly.
- Important controllable features identified can be monitored more closely for better outcomes
- In task 2.1 we identified ‘significant features’ responsible for the outcome ‘energy consumption’ these features can be adjusted when a rise in energy consumption is seen
- Finally a simple model created using only principal components can help predict/identify changes in energy consumption with even slight change in input variable.

Thank You