Course Project Report

Parkinson's Disease progress prediction based on Protein and Peptide abundancies in CSF

Submitted By

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as part of the requirements of the course

Data Science (IT258) [Feb - Jun 2023]

in partial fulfillment of the requirements for the award of the degree of

Bachelor of Technology in Artificial Intelligence

under the guidance of

Dr. Sowmya Kamath S, Dept of IT, NITK Surathkal

undergone at

DEPARTMENT OF INFORMATION TECHNOLOGY

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DEPARTMENT OF INFORMATION TECHNOLOGY

National Institute of Technology Karnataka, Surathkal

C E R T I F I C A T E

This is to certify that the Course project Work Report entitled **Parkinson's Disease progress prediction based on Protein and Peptide abundancies in CSF** is submitted by the group mentioned below -

Details of Project Group UPDATE TEAM MEMBER DETAILS

Name of the Student	Register No.	Signature with Date
1. Dhiraj Choudhary Dommalapati	2110129	Dhiraj D 12/6/23.
2. Gummuluri Venkata Ravi Ram	2110502	G V Ravi Ram 12/06/23

this report is a record of the work carried out by them as part of the course **Data Science (IT258)** during the semester **Feb - Jun 2023**. It is accepted as the Course Project Report submission in the partial fulfillment of the requirements for the award of the degree of **Bachelor of Technology in Artificial Intelligence.**

(Name and Signature of Course Instructor)
Dr. Sowmya Kamath S

DECLARATION

We hereby declare that the project report entitled **Parkinson's Disease progress prediction based on Protein and Peptide abundancies in CSF** submitted by us for the course **Data Science (IT258)** during the semester **Feb-Jun 2023**, as part of the partial course requirements for the award of the degree of Bachelor of Technology in Artificial Intelligence at NITK Surathkal is our original work. We declare that the project has not formed the basis for the award of any degree, associateship, fellowship or any other similar titles elsewhere.

Details of Project Group

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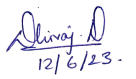
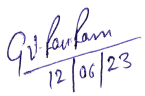
1. Dhiraj Choudhary Dommalapati	2110129	
2. Gummuluri Venkata Ravi Ram	2110502	

Place: NITK, Surathkal
Date: 12/06/23

Parkinson's Disease progress prediction based on Protein and Peptide abundancies in CSF

Team-18

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***Abstract*— This research project focuses on leveraging data science methods to predict Parkinson's disease (PD) progression using protein and peptide levels. By analyzing longitudinal clinical and molecular data from the AMP PD Knowledge Platform, the study aims to identify specific molecular biomarkers associated with PD advancement. Recently several proteins and peptides sem to increase in cerebrospinal fluid in patients suffering from Parkinson's disease. Objective is to gain crucial insights into the underlying molecular changes driving PD progression, facilitating the development of targeted therapies and also trying to automate the monitoring of progress (via predicting UPDRS values) using these biomarkers. Successful outcomes could contribute to earlier diagnosis, personalized interventions, and reduced healthcare costs associated with PD.**

***Keywords:* biomarkers, cerebrospinal fluid, clinical data, data science, molecular data, Parkinson's disease, peptides, proteins, UPDRS**

I. INTRODUCTION

Parkinson's disease (PD) is a debilitating neurodegenerative disorder that affects millions of individuals worldwide, leading to a progressive decline in motor function and overall quality of life. Currently, there is no cure for PD, highlighting the need for innovative approaches to better understand the disease and develop effective treatment strategies. While traditional methods such as gait analysis and speech analysis have been used to assess PD progression, recent research has revealed a promising link between the composition of cerebrospinal fluid (CSF) and PD.

The objective of this research project is to predict the progression of PD by analyzing protein and peptide abundance in CSF and correlating it with Unified Parkinson's Disease Rating Scale (UPDRS) scores. By leveraging data science techniques, including exploratory data analysis, preprocessing, covariance analysis, correlation analysis, feature engineering, dimensionality reduction, and model development, we aim to uncover molecular biomarkers associated with PD progression.

The comprehensive analysis of longitudinal clinical and molecular data from the Accelerating Medicines Partnership® Parkinson's Disease (AMP®PD) Knowledge Platform provides a unique opportunity to investigate the relationship between CSF biomarkers and PD. Through the identification of specific molecular changes associated with disease progression, this research has the potential to significantly enhance our understanding of PD pathology and contribute to the development of improved diagnostic tools and targeted therapies.

The results obtained from this study could have far-reaching implications, including the early detection of PD, personalized treatment approaches, and reduced healthcare costs. By unraveling the complex molecular underpinnings of PD progression, this research aims to pave the way for innovative interventions and ultimately bring us closer to finding a cure or better remedy for Parkinson's disease.

A. *Qualitative explanation of UPDRS-SCALE*

The UPDRS (Unified Parkinson's Disease Rating Scale) is a widely utilized clinical tool used to assess and measure the severity of symptoms in individuals with Parkinson's disease. Developed by the Movement Disorder Society in 1987, it serves as a comprehensive scale for evaluating various aspects of the disease.

The UPDRS comprises different sections, each focusing on specific domains associated with Parkinson's disease. Here is an overview of these sections:

1) UPDRS 1: Mentation, Behavior, and Mood: This section evaluates cognitive and psychiatric symptoms, including mood changes, depression, and cognitive impairment.

2) UPDRS 2: Activities of Daily Living (ADL): ADL assesses the patient's ability to independently perform everyday tasks such as dressing, hygiene, eating, and walking.

3) UPDRS 3: Motor Examination: This section assesses motor symptoms related to Parkinson's disease. It includes several subcategories:

- Speech: Evaluates speech-related symptoms, such as volume, articulation, and clarity.
- Facial Expression: Rates facial expressions for signs of stiffness, reduced mobility, or rigidity.
- Resting Tremor: Measures the severity of tremors when the patient is at rest.
- Action or Postural Tremor: Assesses tremors that occur during voluntary movements or while maintaining a specific posture.
- Rigidity: Evaluates muscle stiffness and resistance to passive movement.
- Finger Taps: Measures the speed and coordination of finger-tapping movements.
- Hand Movements: Assesses rapid alternating movements of the hands.

- Pronation-Supination Movements: Evaluates rotational movements of the hands.
- Leg Agility: Measures the speed and accuracy of leg movements.
- Arising from Chair: Rates the ability to stand up from a chair.
- Gait: Evaluates walking ability, balance, and any abnormalities in the gait pattern.
- Posture: Assesses the patient's ability to maintain an upright posture.

4) UPDRS 4: Hoehn and Yahr Staging: This section assigns a stage to classify the overall severity and progression of Parkinson's disease.

II. Dataset

A. Train Clinical Data

This is the clinical data we got from the Unified Parkinson's Disease Rating Scale (UPDRS) assessments, indicating the severity of PD symptoms. below are the attributes of collected data:

- visit id: An ID code for the visit just represented in the form of patient id underscore visit month
- visit month: The month of the visit after the patient's first visit.
- patient id: An ID code for the patient.
- updrs[1-4]: The patient's score for different parts (1-4) of the UPDRS. Each part covers a distinct category of symptoms, Higher numbers means more severe symptoms.
- upd23b clinical state on medication: shows if the patient is on or off medication during the UPDRS assessment.

B. Supplemental Clinical Data

supplemental clinical data is the record extension of train clinical data hence it has the same attributes as mentioned in train clinical data but the difference lies in the records of patients in supplemental clinical data do not have the protein and peptide data from CSF analysis and hence can be used only for determining trends in UPDRS values.

C. Train Peptide

This is the data of mass spectrometry at the peptide level, giving the composition and abundance of peptides associated with proteins. below are the attributes of collected data:

- visit id: An ID code for the visit just represented in the form of patient id underscore visit month
- visit month: The month of the visit after the patient's first visit.
- patient id: An ID code for the patient.
- UniProt: The UniProt ID code for the associated protein. Multiple peptides may correspond to the same protein.
- Peptide: The sequence of amino acids in the peptide.
- PeptideAbundance: The frequency of the amino acid in the sample, indicating the abundance of the peptide.

D. Train Protein

This is the data of protein expression frequencies clubbed together from the peptide-level data, giving us information about the overall protein abundance patterns.below are the attributes of collected data:

- visit id: An ID code for the visit just represented in the form of patient id underscore visit month
- visit month: The month of the visit after the patient's first visit.
- patient id: An ID code for the patient.
- UniProt: The UniProt ID code for the associated protein. Multiple peptides may correspond to the same protein.
- NPX: Normalized protein expression, representing the frequency of the protein's occurrence in the sample.

III. Exploratory Data Analysis (EDA)

A. EDA of clinical data

EDA involves in finding trends in data obtained from the attributes present in the dataset of clinical data first we start with understanding that the data is a timeseries data first we visualize how updrs values vary with number of patients

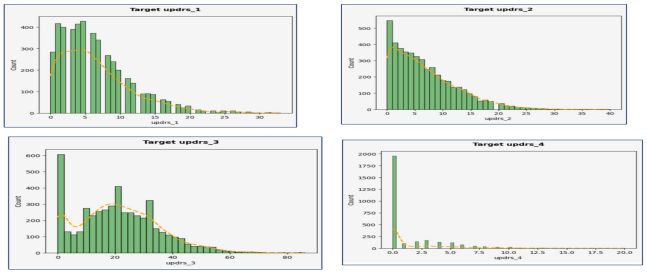

Fig. 1: observe the right skewness of the plots meaning that number of patients having high updrs values are very less

Fig:1 helps visualize the initial data of updrs values that is number of patients having lower updrs value are more than patients having higher updrs value because they are not coming to hospitals once their diseaes is severe or it may mean that the patient has expired.

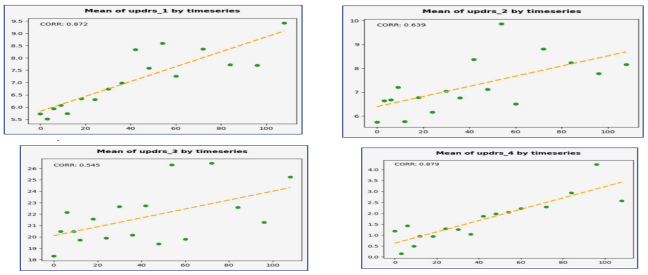

Fig. 2: plot of average updrs values of patients vs visit month

in Fig:2 We see that average values of updrs as time passes is lesser for patients on medication that is slope of the best fit line is lesser than patients off medication

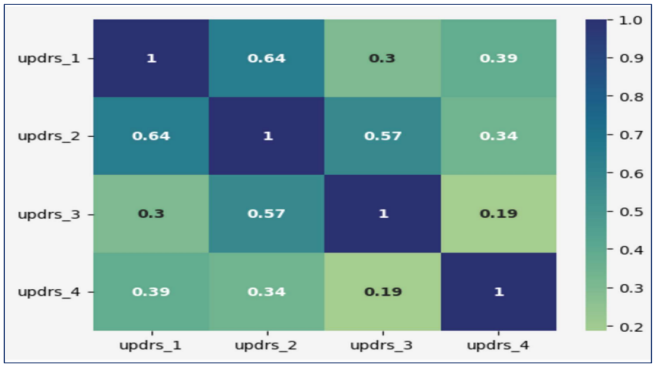

Fig. 3: heatmap of correlation between the updrs values

plotted the correlation matrix to see the relation between features in data in the figure[3].

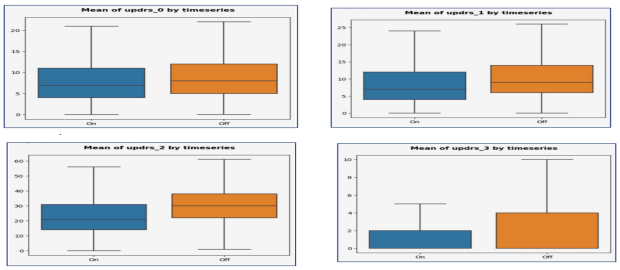

Fig. 4: box plot of the updrs values for patients on and off medication

Medication is effective on reducing the updrs level and patients, with reference to figure[4], so we see that the patients who are on medication their updrs values are increasing at a slower rate than patients who are off medication This matches with the above inferred information from timeseries data Provided original data and additional data statistically has no difference mean in all updrs values

B. EDA of protein data

figure[5] is the correlation matrix to find the relation between features of the protein combined with clinical dataset

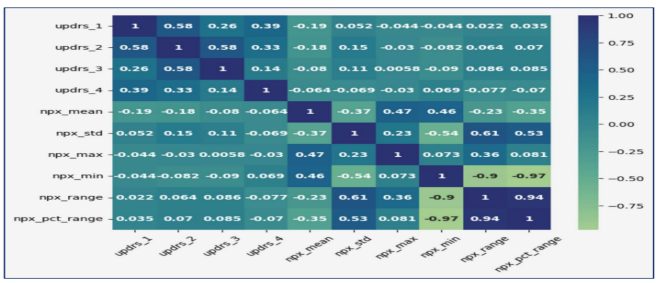

Fig. 5: heatmap of correlation between the updrs including protein data

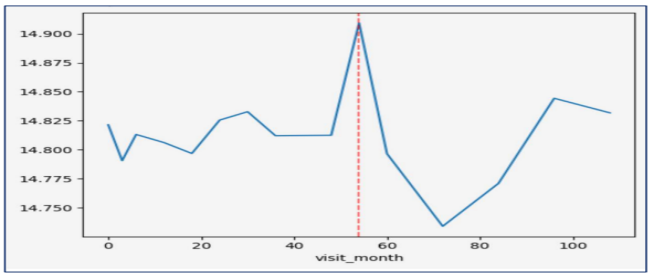

Fig. 6: This plot shows the avg visit month against protein values

We can make the conclusion that at the avg visit month the number of proteins value would be more as the patients would be showing more severe symptoms of parkinson disease

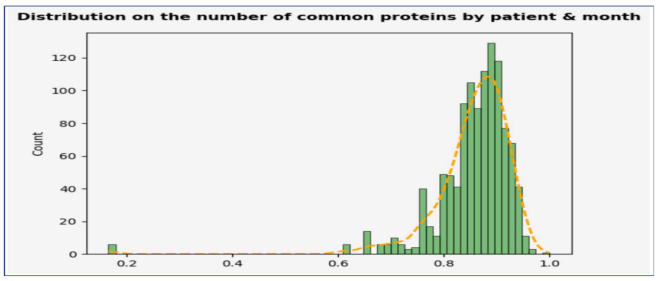

Fig. 7: distribution on the number of common proteins by patient and visit month

We find out that the most common proteins occur in the later stage of the diseases that means they are the protiens that can be used as biomarkers

C. EDA of peptide data

figure[8] is the correlation matrix to find the relation between features of the protein and peptides combined with clinical dataset.

Fig. 8: heatmap of correlation between the updrs including protein and peptide data

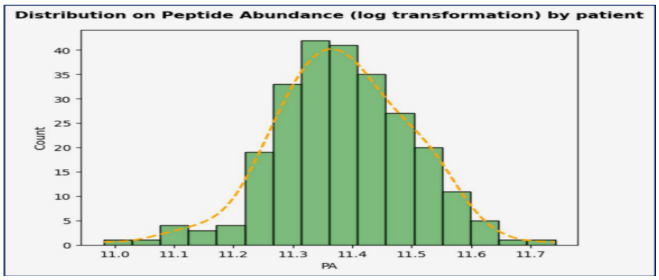

Fig. 9: distribution on peptide abundance

D. Miscellaneous EDA

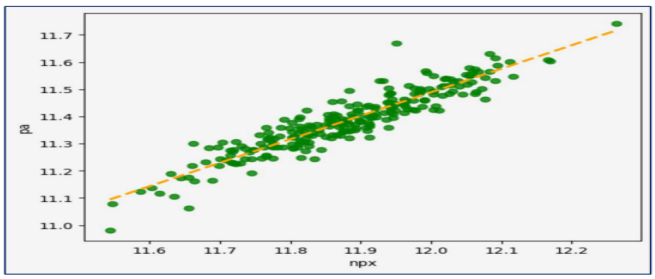

Fig. 10: scatter plot between pa and npx protein values

As observed in the previous heatmap they have a very high positive correlation and all the datapoints are fitting with less error

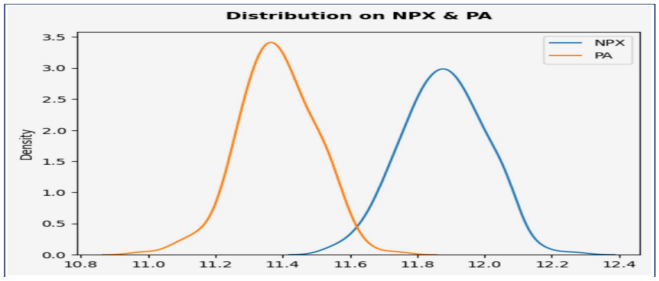

Fig. 11: distribution on npx values and peptide abundance

This data is nothing but the representation of the peptides that are building blocks of the most abundant proteins found hence giving similar curves but have different values as a protein is made up of many peptides

IV. Advanced Processing

A. Correlation Analysis

Correlation analysis helps to understand the pattern of relationship between variables and provides insights into how changes in one variable might affect another. It is widely applied in various fields, including economics, social sciences, and data analysis, to explore connections, make predictions, and uncover meaningful patterns in data.

1) Correlation between UPDRS: Initially, the correlation between updrs values was calculated In order to observe how strongly change in one variable alters change in the other.Initially, the correlation between updrs values was calculated In order to observe how strongly change in one variable alters change in the other.

TABLE I: Correlation matrix for UPDRS values

	UPDRS-1	**UPDRS-2**	**UPDRS-3**
UPDRS-1	1	0.61	0.25
UPDRS-2	0.61	1	0.53
UPDRS-3	0.25	0.53	1

Clearly this correlation analysis emphasizes the same as we observed in the EDA phase; updrs_2 is co-related to updrs_1 and updrs_3 wheras, updrs_1 and updrs_3 are too weakly correlated.

2) Correlation between Protein/Peptide abundancy v/s updrs values: Though there are several proteins and peptide, not all of them act as potential biomarkers. Correlation analysis of updrs with respective abundancies would provide a statistical measure to how far each protein/peptide (an amino acid constitute) impacts updrs values thereby signifying parkinson's disease.
Clearly from correlation heat map in figure [13] we can infer that seeveral peptides like O00533, O14498, O15240, O15394, O43505, O60888, P00738, P01034, P01042, P01717, P02452, P02649, P02751, P02753, P02787, P04075, P04156 etc are having very weak correlation with updrs values. From here we infer that the peptides and proteins corresponding to forementioned UniProt values are statistically least significant for determining target values (updrs).

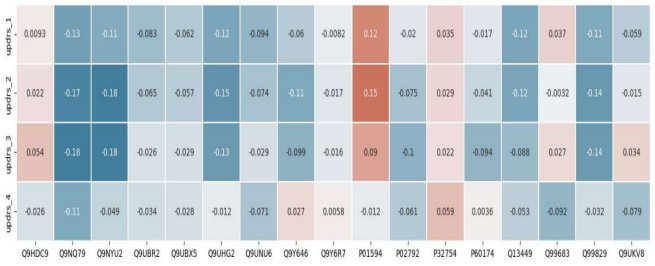

Fig. 12: correlation heatmap of updrs values and PA

B. Covariance Analysis

Covariance of Updrs values (except updrs_4) is analyzed which reveals that updrs_2 has higher covariance with other two. (refer table 1:) variables.

updrs_2 signifying disturbances in motor abilities like chewing, swallowing, handwriting etc, implies more lack in sleep, pain etc which are reflected by updrs_1 values. While these develop or gain severity, the freezing of gait, lack of speech etc also occur which are reflected by updrs_3 scores.

This qualitatively exlpains the observation

TABLE II: Co-variance matrix for UPDRS values

	UPDRS-1	**UPDRS-2**	**UPDRS-3**
UPDRS-1	31.134	20.215	17.969
UPDRS-2	20.215	35	39.672
UPDRS-3	17.969	39.672	159.937

C. Feature Engineering

Feature engineering is a critical process in machine learning that involves transforming and selecting relevant features from raw data to improve the performance and efficiency of models. Feature selection, a key component of feature engineering, aims to identify the most informative and discriminative features that contribute the most to the target variable while discarding irrelevant or redundant ones.

Various feature selection techniques exist, including filter methods that evaluate features based on statistical measures, wrapper methods that utilize the performance of a specific model, and embedded methods that incorporate feature selection within the model training process.

Feature Selection: We implemented Univariate feature selection and Recursive feature elimination and compared wit absence of feature selection to understand which updrs values are being affected truly by outliers. We are using Linear regression Model as experimental setup.

- Univariate feature Selection :
  This method selects the features with the highest correlation with the target variable using statistical tests like chi-squared test, ANOVA F-test, mutual information, etc. We considered F-test scores to select features.
- Recursive feature elimination:
  This method recursively removes features which contribute the least from the dataset and selects(retains) the features that contribute the most to the model's accuracy.

Comparative Analysis: From the results given in tables [III] [IV] [V] we can observe the following :

- In Univariate Feature Selection, except SMAPE in case of updrs_4 remaining all showed significant increase in remaining accuracy metrics than those without features selection..
- Using RFE the results are similar to that of Univariate Feature Selection.

From above observations we can infer that clearly more important features are having greater impact on judgement. Hence we will be considering only few features for final model to predict updrs values.

TABLE III: Results without feature selection

TARGET	**MSE**	**MAE**	**R-2**	**SMAPE**
UPDRS-1	185.35	8.97	-7.24	123.67
UPDRS-2	141.03	7.71	-2.96	119.03
UPDRS-3	886.74	21.08	-2.56	115.79
UPDRS-4	11.08	2.38	-0.50	122.63

TABLE IV: Results with univariate feature selection

TARGET	**MSE**	**MAE**	**R-2**	**SMAPE**
UPDRS-1	22.05	3.90	-0.002	74.35
UPDRS-2	34.64	4.73	0.02	101.98
UPDRS-3	237.37	12.83	0.04	96.61
UPDRS-4	7.90	2.16	-0.07	148

TABLE V: Results with recursive feature elimination

TARGET	**MSE**	**MAE**	**R-2**	**SMAPE**
UPDRS-1	21.97	3.89	0.001	74.14
UPDRS-2	35.08	4.76	0.01	102.20
UPDRS-3	235.83	12.76	0.05	96.05
UPDRS-4	7.94	2.15	-0.07	148.73

TABLE VI: Results with univariate feature selection and PCA

TARGET	**MSE**	**MAE**	**R-2**	**SMAPE**
UPDRS-1	22.68	3.97	-0.03	75.10
UPDRS-2	34.69	4.72	0.02	103.52
UPDRS-3	244.65	13.01	0.01	96
UPDRS-4	6.71	2.09	0.09	122.63

D. Dimensionality Reduction

Dimensionality reduction is a technique used to reduce the number of features or variables in a dataset while preserving the most relevant information.

Popular approaches for dimensionality reduction include Principal Component Analysis (PCA), which transforms the data into a new set of uncorrelated variables called principal components, and t-SNE (t-distributed Stochastic Neighbor Embedding), which maps high-dimensional data into a lower dimensional space while preserving local structure.

We applied PCA to the selected features using UFS and w.r.t. F-score identified top 10 Principal Components. We used same experimental setup to evaluate it and clearly the observations shown in table[VI] shows that there has not been much improvement in accuracy metrics compared to UFS. The visualization in figure[13] clearly shows that Principal Components obtained are good fit for data due to which there is not much difference in accuracy when compared to UFS.

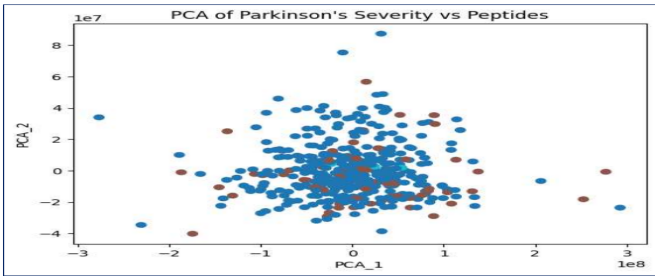

Fig. 13: PCA-1 vs PCA-2 for dataframe components as disease severity

V. Data Modelling

We have 4 datasets train protiens , train peptides , train clinical and supplemental clinical data. Based on all above inferences now we will be creating the final dataframe and model to predict updrs values based on peptide abundancy values in CSF.

A. Cleaning and preparing clinical data

- Supplement clinical data can only be used to make trend observations but only clinical data can be used for prediction.
- As we observed linear relation in updrs values as time-series, we use linear interpolation to fill in missing values of updrs_1, updrs_2, and updrs_3.
- Owing to more than 80% of zeroes in updrs_4, we can impute zeroes in missing values.

B. Merging protein and peptide datasets

- both train_proteins and train_peptides are grouped by 'visit_id' and a specific column ('UniProt' for proteins and 'Peptide' for peptides) and then averaged and generated two new DataFrames.
- Both generated dataframes are now merged pivoted at Visit_ID.

C. Final Dataframe Preperation

- The proteins' features merged DataFrame is merged with the clinical DataFrame based on the 'visit_id' column of train clinical data and the index of proteins features. This merge adds the protein features as additional columns to clinical data.
- Hence we obtained the dataframe ready to be used for purpose of training.

VI. Building the Model

- The core of the model involves estimating the relationship between the target variable (UPDRS score) and the predicted months. The model fits a trend or pattern to this relationship using a linear or quadratic equation. The coefficients of the trend equation are determined by minimizing an evaluation metric called symmetric mean absolute percentage error (sMAPE). The sMAPE measures the accuracy of the predicted values compared to the true values.
- sMAPE is chosen as metric as this was the metric chosen for evaluating in the Kaggle competition.
- The model considers multiple target variables, namely UPDRS_1, UPDRS_2, UPDRS_3, and UPDRS_4, which represent different aspects of Parkinson's Disease progression. For each target variable, the model calculates a trend specific to that variable.
- To make predictions, the model takes the predicted months, trend coefficients, and target variable as inputs. It uses these inputs to calculate the predicted values using the trend equation. The model also accounts for specific constraints on the predicted values for certain target variables.
- This is a kind of linear regression based on Time series tailored for updrs_1 ,updrs_2, updrs_4 and quadratic regression for updrs_3 owing to its higher deviation when fit under straight line which is evident from Tables [III] [IV] [V] in context of MAE, MSE.
- Also owing to anamolous behaviour of updrs_4 values, we have seen that most of updrs_4 values have been reported after 54 months. Hence to obtain proper results, pred_month is clipped to 54 while predicting updrs_4.

VII. Result Analysis

In this section we disclose all the important observations in trends as well as highlight the important biomarkers of Parkinson's disease in CSF obtained from Data Analysis.

A. Relation between various symptoms

- updrs_2 value reflecting motor abilities involved in daily activities is closely related to general motor abilities tested for updrs_3 values.
- All first 3 stages of symtoms are closely related except for updrs_4 which has several unreported values or either zero due to which we couldnt conclude much about its relationship.
- Taking medicine has been effective in providing relief. Amongst all symptoms, the motor abilities were most impacted by medication. (corresponding to updrs 3 and updrs 2)

B. Biomarkers impacting the symptoms

- The peptides having less than or equal to 0.1 correlation are more likely noise in the data and are least important biomarkers for PD.
- Not all proteins and peptides are present in all patients. And hence we cant assure that less correlation (around 0.5)implies less effect due to which we have taken 0.1 as treshold.
- There are several peptides that may not be so significant for regression viz; O14498, O43505, P01717,P02649, O60888, P01034, P01042 etc.
- Some proteins have weak correlation with only updrs_4 and hence must not be considered only in its prediction.viz; P02749, P04217, P20774, P02774, P06681 etc

C. Result of Model

The model resulted in sMAPE score of 56.1 on test file provided by Kaggle which is far impressive than when we directly conduct regression on the updrs values without considering other analytic factors.

D. Kaggle competetion submission details

The best score in our competetion submission is as given below : private score: 69.837(sMape) public score: 56.169(sMape) For consice submission, all tools used for EDA and preprocessing aren't included in Kaggle notebook. instead few necessary for model building are included for further details see **Our kaggle submission notebook**

VIII. CONCLUSIONS

By focusing on illness progression instead than merely categorization, our work adds to the expanding body of knowledge on Parkinson's disease prediction. Our machine learning (ML) model has shown results for offering insightful information about the long-term course of the disease, eventually assisting physicians in making well-informed decisions about treatment strategies and treatments. We can open up new avenues for Parkinson's disease early diagnosis and better care by continuing to enhance and validate these models.

But it's important to recognise the constraints on our study. Even though our model produced encouraging findings, more testing and improvement are required to guarantee its applicability to a range of patient groups. Furthermore, given the dynamic nature of Parkinson's disease, future research should include longitudinal data and clinical indicators to improve the model's prediction capabilities.

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APPENDIX

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