Exploratory Data Analysis of Parkinson Disease Progression Prediction

```
In []: import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns

In []: # Import the dataset
train_clinical = pd.read_csv("/Users/louruixin/Downloads/train_clinical_data.csv")
train_peptides = pd.read_csv("/Users/louruixin/Downloads/train_peptides.csv")
train_proteins = pd.read_csv("/Users/louruixin/Downloads/train_proteins.csv")
```

train clinical dataset

The train_clinical sample includes 248 patients; For the dataset, we have 2615 rows and 8 columns

```
In [ ]: train_clinical.head()
Out[]:
           visit_id patient_id visit_month updrs_1 updrs_2 updrs_3 updrs_4 upd23b_clinical_state_on_medication
         0
              55_0
                         55
                                     0
                                           10.0
                                                     6.0
                                                            15.0
                                                                    NaN
                                                                                                     NaN
              55_3
                                            10.0
                                                            25.0
                         55
                                     3
                                                     7.0
                                                                    NaN
                                                                                                     NaN
         2
             55_6
                         55
                                     6
                                            8.0
                                                    10.0
                                                            34.0
                                                                    NaN
                                                                                                     NaN
             55 9
                         55
                                            8.0
                                                     9.0
                                                            30.0
                                                                     0.0
                                                                                                      On
                         55
                                     12
                                                                     0.0
             55_12
                                           10.0
                                                    10.0
                                                            41.0
                                                                                                      On
In [ ]: # check for the number of unique values
         print(f"The number of unique visit month is: {train clinical['visit month'].nunique()}")
         # print each unique value
         print(pd.unique(train_clinical["visit_month"]))
         The number of unique visit month is: 17
                        9 12 18 24 30 36 42 48 54 60 72 84 96 108]
```

```
In []: # check for the number of unique values
    train_clinical["patient_id"].nunique()

Out[]: 248

In []: train_clinical.shape

Out[]: (2615, 8)
```

Missing values check

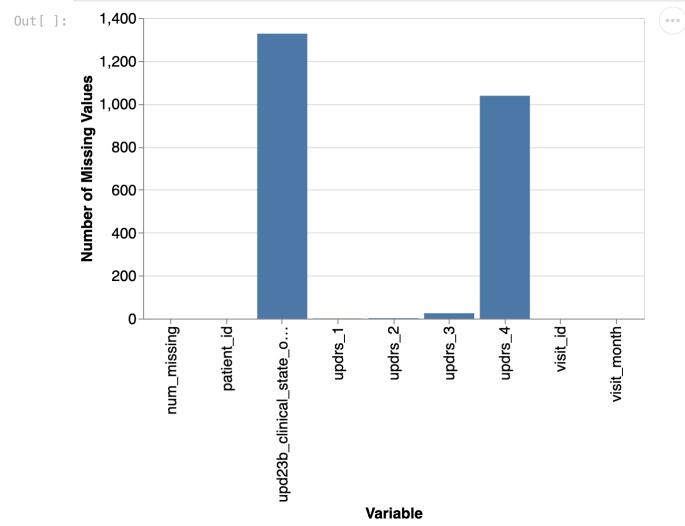
According to the distribution graph, we can see that most of the missing values centered as the variable of "upd23b_clinical_state_on_medication", which explains wheyhrt ot not the patient was taking medication.

updrs_4 also contains a lot of missing values, which account for motor complications in the Parkinson Disease

```
In [ ]: # Check for missing values
        train_clinical.isnull().sum()
Out[]: visit id
                                                   0
        patient id
                                                   0
        visit_month
        updrs 1
                                                   1
        updrs 2
                                                   2
        updrs_3
                                                  25
        updrs 4
                                                1038
        upd23b_clinical_state_on_medication
                                               1327
        dtype: int64
In []: # Count the number of missing values per variable
        missing count = train clinical.isnull().sum()
        # Create a dataframe with the variable names and null counts
        missing count df = pd.DataFrame({'variable': missing count.index, 'missing count': missing count.values})
        # Plot the distribution of missing values per variable
        bars = alt.Chart(missing count df).mark bar().encode(
            x=alt.X('variable:0', axis=alt.Axis(title='Variable')),
            y=alt.Y('null count:Q', axis=alt.Axis(title='Number of Missing Values')),
            tooltip=[alt.Tooltip('variable:0', title='Variable'), alt.Tooltip('missing count:0', title='Missing Count
```

```
).properties(
    width=500,
    height=300
)

# Show the plot
bars.configure_title(fontSize=20).configure_axis(labelFontSize=15, titleFontSize=15)
```



Summary stats

For visit_month, we can see that the maximum number of visiting month is 108;

For updrs_1, we have a mean values of 7.11 and maximum value of 33

For updrs_2, we have a mean values of 6.74 and maximum value of 40

For updrs_3, we have a mean values of 19.42 and maximum value of 86

For updrs_4, we have a mean values of 1.86 and maximum value of 20

Therefore, patients score higher in updrs part 3. While looking at the distribution graph of each updrs score, all of the are right skewed.

For upd23b_clinical_state_on_medication, a slightly higher amount of patients are taking medication. The difference is not large.

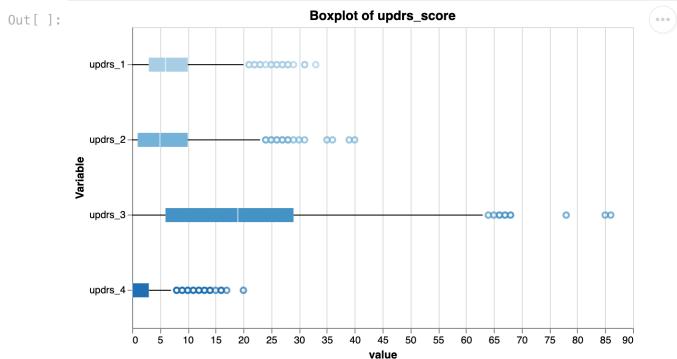
```
Out[]:
                                           std min 25% 50% 75%
                     count
                               mean
                                                                     max
         visit_month 2615.0 31.190822 25.199053 0.0
                                                     10.5
                                                          24.0
                                                               48.0 108.0
            updrs_1 2614.0
                            7.110559
                                     5.525955 0.0
                                                     3.0
                                                           6.0 10.0
                                                                     33.0
            updrs_2 2613.0 6.743590 6.323230 0.0
                                                     1.0
                                                           5.0 10.0
                                                                     40.0
            updrs_3 2590.0 19.421236 15.000289 0.0
                                                          19.0 29.0
                                                     6.0
                                                                     86.0
            updrs_4 1577.0 1.861763
                                      3.022112 0.0
                                                     0.0
                                                           0.0
                                                                3.0
                                                                     20.0
```

```
In []: # Boxplot for the whole dataset

train_clinical_ = train_clinical.dropna()
# Create the boxplot
x = ['updrs_1', 'updrs_2', 'updrs_4']

alt.Chart(train_clinical).mark_boxplot().encode(
    y=alt.Y('variable:0', axis=alt.Axis(title='Variable')),
    x=alt.X('value:0'),
    color=alt.Color('variable:0', legend=None),
).transform_fold(
```

```
x,
    as_=['variable', 'value']
).transform_filter(
    alt.FieldOneOfPredicate(field='variable', oneOf=x)
).properties(
    width=500,
    height=300,
    title='Boxplot of updrs_score'
)
```



```
x=alt.X('value:Q'),
    color=alt.Color('variable:O', legend=None),
).transform_fold(
    X,
        as_=['variable', 'value']
).transform_filter(
        alt.FieldOneOfPredicate(field='variable', oneOf=x)
).properties(
        width=500,
        height=300,
        title='Boxplot of updrs_score while ON medication'
)
```

Boxplot of updrs_score while ON medication Out[]: ... updrs_1 $-\infty$ o updrs_2 Variable updrs_3 ထား တာ တ ∞ updrs_4-0000000 10 15 20 25 30 40 50 55 60 65 70 75 80 35 45

value

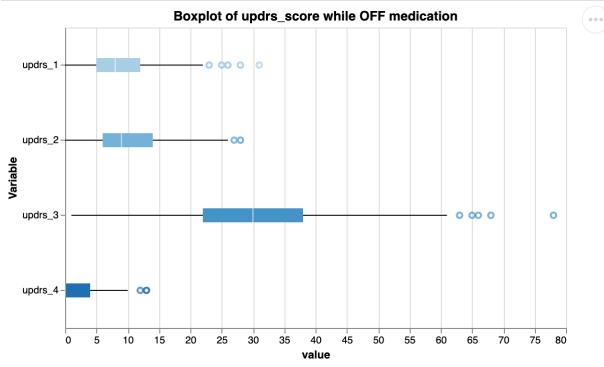
```
In []: # Boxplot for patients who is taking medication
   Off_data = train_clinical[train_clinical["upd23b_clinical_state_on_medication"]=="Off"]

# drop missing values
   Off_data_ = Off_data.dropna()

# Boxplot for the whole dataset
   x = ['updrs_1', 'updrs_2', 'updrs_3', 'updrs_4']
```

```
alt.Chart(Off_data_).mark_boxplot().encode(
    y=alt.Y('variable:0', axis=alt.Axis(title='Variable')),
    x=alt.X('value:0'),
    color=alt.Color('variable:0', legend=None),
).transform_fold(
    x,
    as_=['variable', 'value']
).transform_filter(
    alt.FieldOneOfPredicate(field='variable', oneOf=x)
).properties(
    width=500,
    height=300,
    title='Boxplot of updrs_score while OFF medication'
)
```





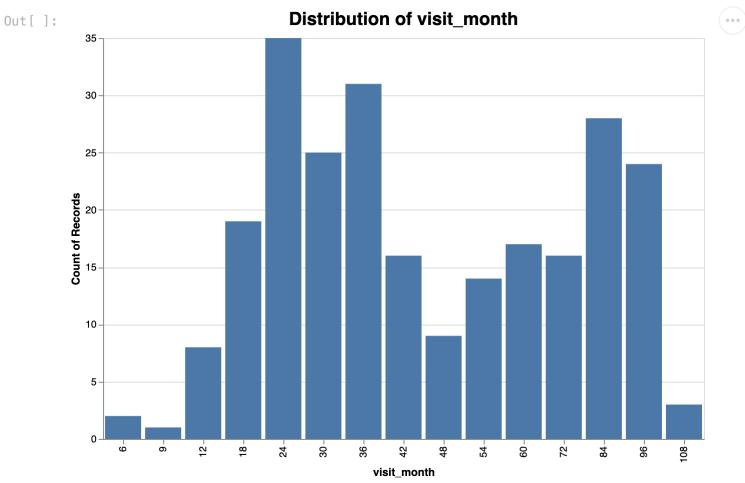
```
In []: # Getting the number of times the patient_id appears, so we will know how many months the patient progress

patient_counts = train_clinical['patient_id'].value_counts().tolist()
visiting_month = []
```

```
for i in range(len(patient_counts)):
            if patient_counts[i] == 1:
                visiting month.append(0)
            elif patient_counts[i] == 2:
                visiting month.append(3)
            elif patient counts[i] == 3:
                visiting month.append(6)
            elif patient counts[i] == 4:
                visiting month.append(9)
            elif patient counts[i] == 5:
                visiting month.append(12)
            elif patient_counts[i] == 6:
                visiting_month.append(18)
            elif patient counts[i] == 7:
                visiting month.append(24)
            elif patient counts[i] == 8:
                visiting month.append(30)
            elif patient_counts[i] == 9:
                visiting month.append(36)
            elif patient_counts[i] == 10:
                visiting month.append(42)
            elif patient_counts[i] == 11:
                visiting month.append(48)
            elif patient_counts[i] == 12:
                visiting month.append(54)
            elif patient counts[i] == 13:
                visiting month.append(60)
            elif patient_counts[i] == 14:
                visiting_month.append(72)
            elif patient counts[i] == 15:
                visiting month.append(84)
            elif patient counts[i] == 16:
                visiting month.append(96)
            elif patient_counts[i] == 17:
                visiting month.append(108)
In [ ]: # Transfer a list object to dataframe
        df visit month = pd.DataFrame(visiting month, columns=['visit month'])
In [ ]: # Create an Altair chart object
        chart = alt.Chart(df visit month).mark bar().encode(
            x=alt.X('visit month:0'),
            y='count()',
```

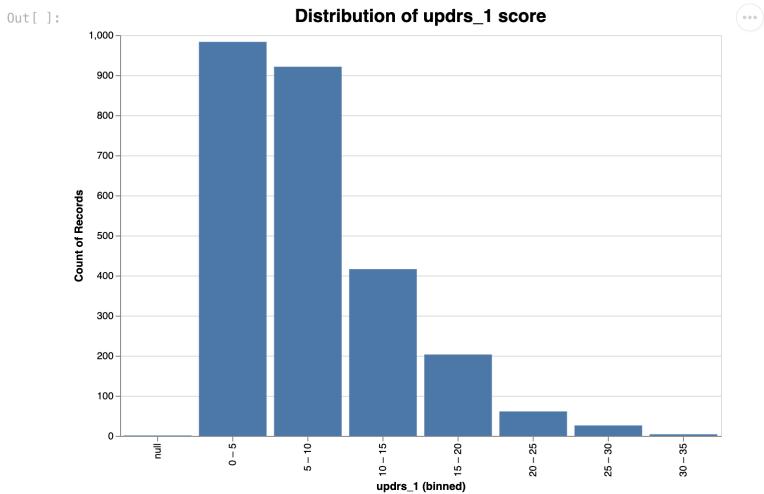
```
# Customize the chart
chart = chart.properties(
    title={
        'text': 'Distribution of visit_month',
        'fontSize': 18,
        'fontWeight': 'bold'
    },
    width=600,
    height=400
)
# Display the chart
chart
```

/opt/miniconda3/lib/python3.10/site-packages/altair/utils/core.py:317: FutureWarning: iteritems is deprecated and will be removed in a future version. Use .items instead. for col_name, dtype in df.dtypes.iteritems():



```
},
width=600,
height=400
)

# Display the chart
chart
```



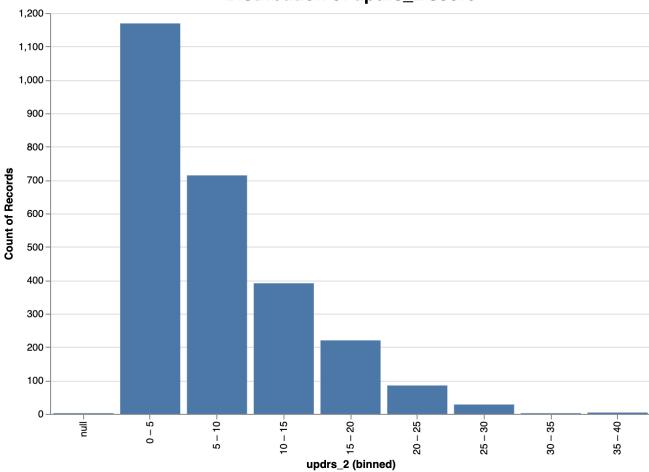
```
# Customize the chart
chart = chart.properties(
    title={
        'text': 'Distribution of updrs_2 score',
        'fontSize': 18,
        'fontWeight': 'bold'
    },
    width=600,
    height=400
)

# Display the chart
chart
```



Distribution of updrs_2 score





```
width=600,
height=400
)

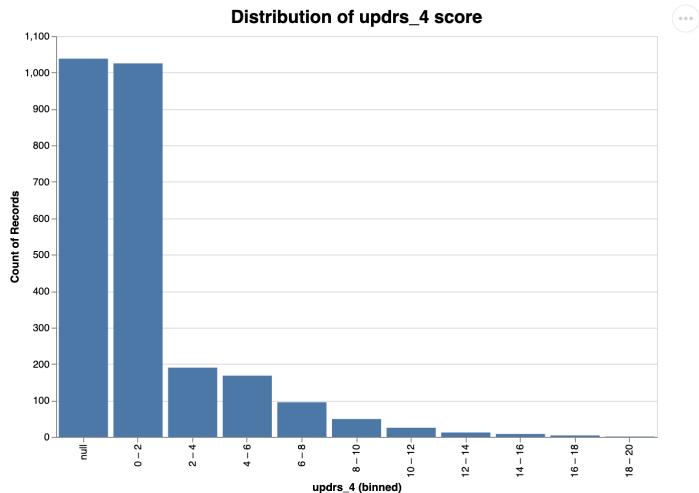
# Display the chart
chart
```

Distribution of updrs_3 score Out[]: ••• 800 700 600 500 **Count of Records** 200 100 40 – 50 -10 – 20 -20 - 30 -09 – 09 updrs_3 (binned)

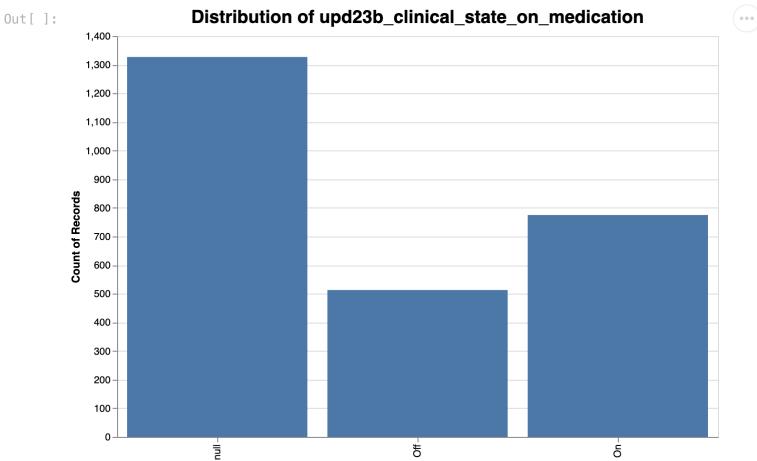
```
# Customize the chart
chart = chart.properties(
    title={
        'text': 'Distribution of updrs_4 score',
            'fontSize': 18,
            'fontWeight': 'bold'
     },
     width=600,
     height=400
)

# Display the chart
chart
```





/opt/miniconda3/lib/python3.10/site-packages/altair/utils/core.py:317: FutureWarning: iteritems is deprecated and will be removed in a future version. Use .items instead. for col_name, dtype in df.dtypes.iteritems():



Correlation map

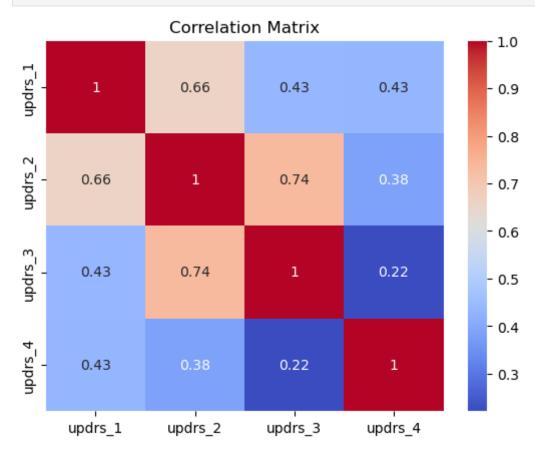
According to the correlation matrix, we can see that updrs_2 and updrs_3 have moderate positive correlation, which is about 0.74; updrs_2 also have moderate positive correlation with updrs_1, which is about 0.66

upd23b_clinical_state_on_medication

```
In []: # Calculate the correlation matrix
    udprs_score = train_clinical[['updrs_1', 'updrs_2', 'updrs_3', 'updrs_4']]
    corr_matrix = udprs_score.corr()

# Create the heatmap using seaborn
    sns.heatmap(corr_matrix, annot=True, cmap='coolwarm')
```

```
# Add title and show the plot
plt.title('Correlation Matrix')
plt.show()
```



Visit_month vs each UPDRS score

We want to see how does time progression has the relationship with each UPDRS score while adjusting for the medication, so I draw a barplot with mean line plot to provide a sense of it.

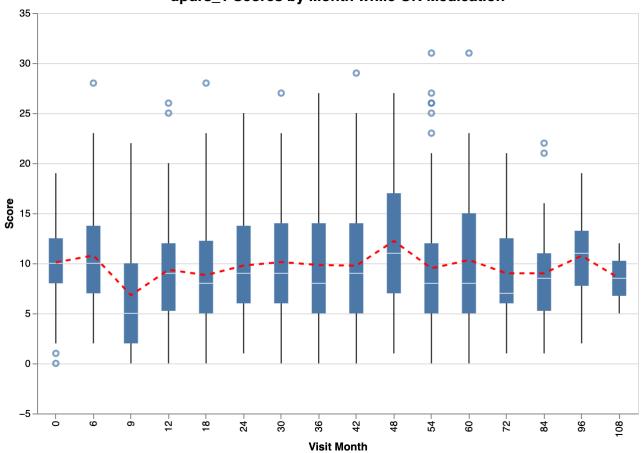
While the patient is taking the medication, the trend lines are pretty flat for UPDRS Parts 1, 2, and 4. However, for part 3, it shows a slight increase trend, which indicate a time progression.

While the patient is not taking the medication, the trend lines are increasing for all UPDRS Parts, 1, 2, 3, and 4, which are all responsible for time progression.

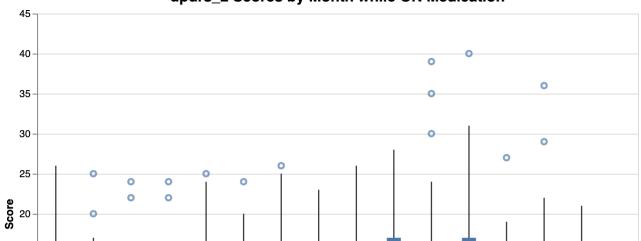
```
In [ ]: # Filter the data for only ON medication
        On_data = train_clinical[train_clinical["upd23b_clinical_state_on_medication"]=="0n"]
        # Define the chart object
        base = alt.Chart(On_data).properties(
            width=600,
            height=400
        # Loop through each UPDRS feature and create a box plot and mean line plot
        charts = []
        for i, feature in enumerate(["updrs_1", "updrs_2", "updrs_3", "updrs_4"]):
            # Create the box plot
            box_plot = base.mark_boxplot().encode(
                x=alt.X('visit_month:0', title='Visit Month'),
                y=alt.Y(feature, title='Score', scale=alt.Scale(zero=False, padding=1))
            ).properties(
                title={"text": f"{feature} Scores by Month while ON Medication", "fontSize": 15},
            # Create the mean line plot
            mean_line = base.mark_line(color='red', strokeDash=[5, 5]).encode(
                x=alt.X('visit_month:0', title='Visit Month'),
                y=alt.Y(f"mean({feature})", scale=alt.Scale(zero=False, padding=1))
            # Combine the plots into one chart
            chart = (box_plot + mean_line).resolve_scale(y='shared')
            # Add the chart to the list of charts
            charts.append(chart)
        # Display the charts
        alt.vconcat(*charts)
```

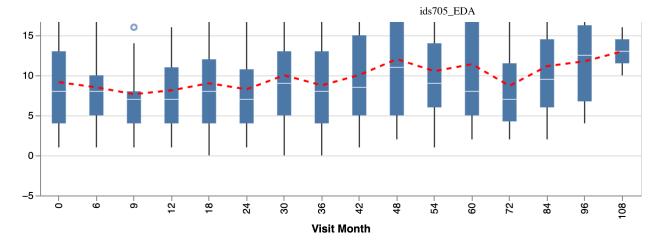


updrs_1 Scores by Month while ON Medication

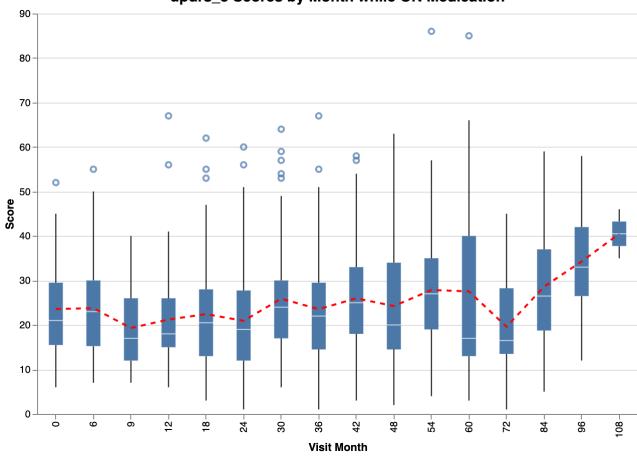


updrs_2 Scores by Month while ON Medication

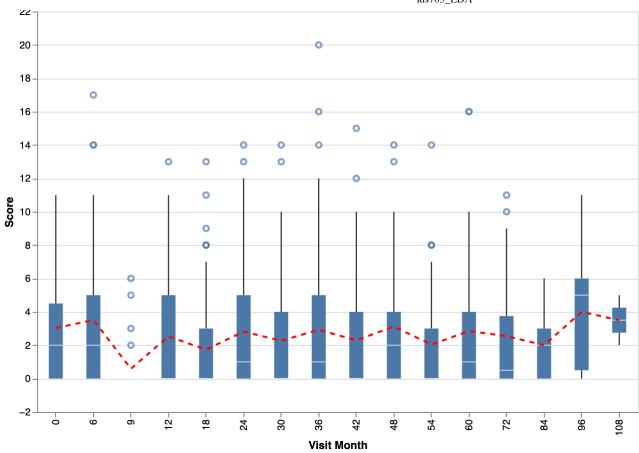




updrs_3 Scores by Month while ON Medication



updrs_4 Scores by Month while ON Medication



```
y=alt.Y(feature, title='Score', scale=alt.Scale(zero=False, padding=1))
).properties(
    title={"text": f"{feature} Scores by Month while OFF Medication", "fontSize": 15},
)

# Create the mean line plot
mean_line = base.mark_line(color='red', strokeDash=[5, 5]).encode(
    x=alt.X('visit_month:0', title='Visit Month'),
    y=alt.Y(f"mean({feature})", scale=alt.Scale(zero=False, padding=1))
)

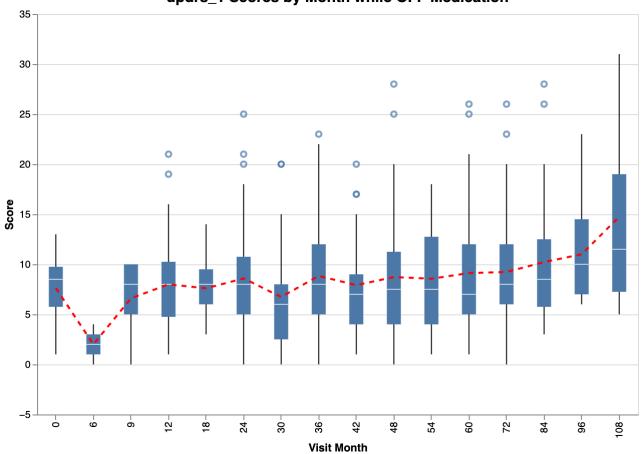
# Combine the plots into one chart
    chart = (box_plot + mean_line).resolve_scale(y='shared')

# Add the chart to the list of charts
    charts.append(chart)

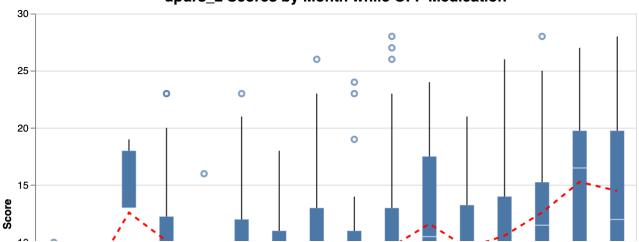
# Display the charts
alt.vconcat(*charts)
```

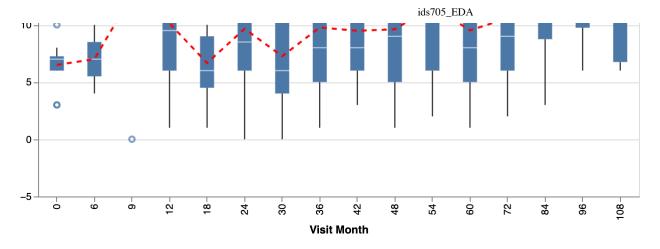


updrs_1 Scores by Month while OFF Medication

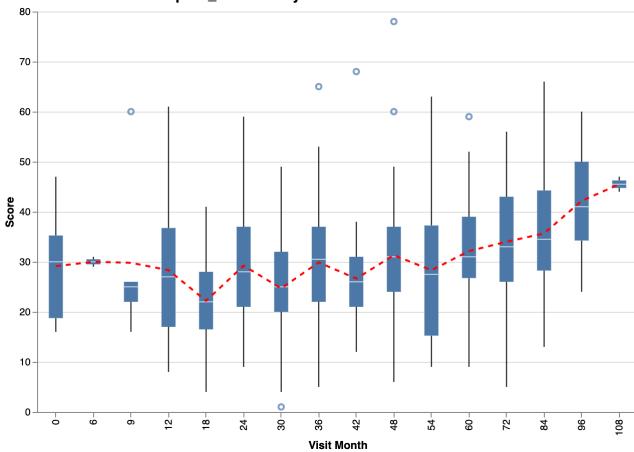


updrs_2 Scores by Month while OFF Medication

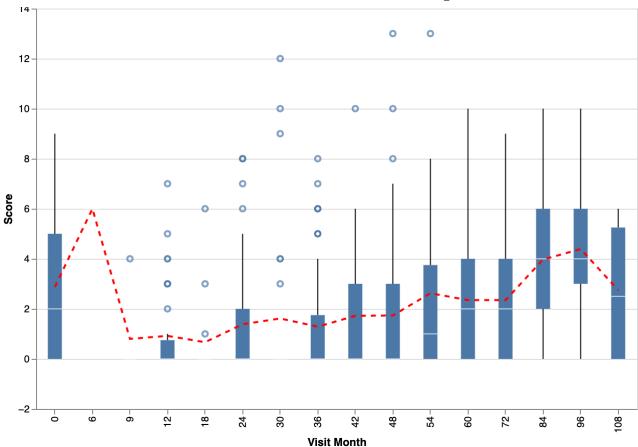








updrs_4 Scores by Month while OFF Medication



Visit_month vs Sum of UPDRS score

While summing all the category and patient is not taking the medication, we can see there is a clear increasing trend which shows the disease progression is occurring.

While summing all the category and patient is taking the medication, the trend is not clear before month 72. After 72 months, the disease progression begins.

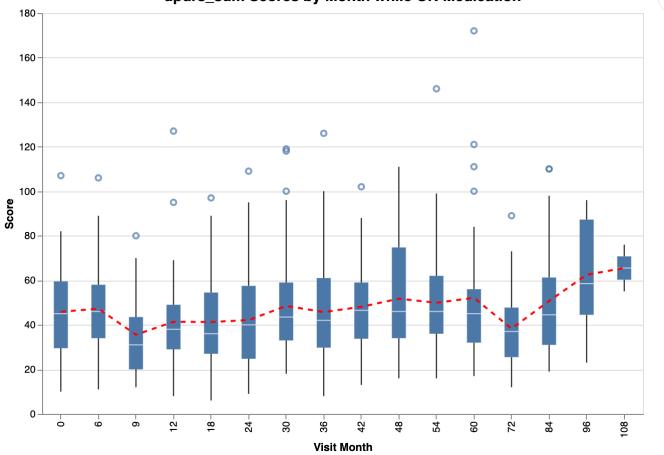
```
In []: # create a new variable which sums the updrs
On_data.loc[:, "updrs_sum"] = On_data["updrs_1"] + On_data["updrs_2"] + On_data["updrs_3"] + On_data["updrs_4"]
# Define the chart object
base = alt.Chart(On_data).properties(
    width=600,
```

```
height=400
# Create the box plot
box_plot = base.mark_boxplot().encode(
   x=alt.X('visit_month:0', title='Visit Month'),
   y=alt.Y('updrs_sum:Q', title='Score', scale=alt.Scale(zero=False, padding=1))
).properties(
   title={"text": "updrs_sum Scores by Month while ON Medication", "fontSize": 15},
# Create the mean line plot
mean_line = base.mark_line(color='red', strokeDash=[5, 5]).encode(
   x=alt.X('visit_month:0', title='Visit Month'),
   y=alt.Y(f"mean(updrs sum):0", scale=alt.Scale(zero=False, padding=1))
# Combine the plots into one chart
chart = (box_plot + mean_line).resolve_scale(y='shared')
# Display the charts
chart
/var/folders/92/6467ymq56qn8qy3v68tsr84r0000gn/T/ipykernel_74699/762108245.py:2: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead
See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#r
eturning-a-view-versus-a-copy
/opt/miniconda3/lib/python3.10/site-packages/altair/utils/core.py:317: FutureWarning:
iteritems is deprecated and will be removed in a future version. Use .items instead.
```

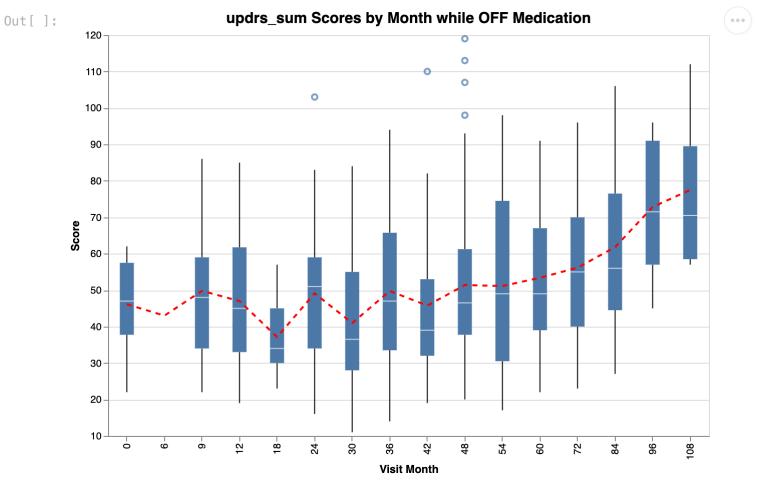


updrs_sum Scores by Month while ON Medication





```
title={"text": "updrs_sum Scores by Month while OFF Medication", "fontSize": 15},
# Create the mean line plot
mean_line = base.mark_line(color='red', strokeDash=[5, 5]).encode(
   x=alt.X('visit_month:0', title='Visit Month'),
   y=alt.Y(f"mean(updrs_sum):Q", scale=alt.Scale(zero=False, padding=1))
# Combine the plots into one chart
chart = (box_plot + mean_line).resolve_scale(y='shared')
# Display the charts
chart
/var/folders/92/6467ymq56qn8qy3v68tsr84r0000gn/T/ipykernel_74699/4106097603.py:2: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead
See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html#r
eturning-a-view-versus-a-copy
/opt/miniconda3/lib/python3.10/site-packages/altair/utils/core.py:317: FutureWarning:
iteritems is deprecated and will be removed in a future version. Use .items instead.
```



train_peptides dataset

The train_peptides sample includes 248 patients. The dataset contains 981834 rows and 6 columns.

In []: train_peptides.head()

t[]:	visit_id	visit_month	patient_id	UniProt	Peptide	PeptideAbundance
0	55_0	0	55	000391	NEQEQPLGQWHLS	11254.3
1	55_0	0	55	000533	GNPEPTFSWTK	102060.0
2	55_0	0	55	000533	IEIPSSVQQVPTIIK	174185.0
3	55_0	0	55	000533	KPQSAVYSTGSNGILLC(UniMod_4)EAEGEPQPTIK	27278.9
4	55_0	0	55	000533	SMEQNGPGLEYR	30838.7
Th	he number 0 3	r of unique 6 12 18	e values i 3 24 30	s: 15 36 48	54 60 72 84 96 108]	
[]: #	0 3	6 12 18	3 24 30 Der of union	36 48 que valu	ies	
pr	rint(f"Th	ne number d	of unique	values c	of patient_id is: {train_peptides['pat of UniProt is: {train_peptides['UniPro of Peptide is: {train_peptides['Peptid	<pre>ot'].nunique()}")</pre>
Tł	ne numbe	r of unique r of unique r of unique	values o	f UniPro		
]: tr	rain_pep	tides.shape	2			
[]: (9	981834, 6	5)				

Missing values check

No missing values for the train_peptides dataset

```
In []: # Check for missing values
    train_peptides.isnull().sum()
```

```
Out[]: visit_id
                            0
        visit month
        patient id
        UniProt
        Peptide
        PeptideAbundance
        dtype: int64
In [ ]: uniprot_counts_high_pep = train_peptides['UniProt'].value_counts().head(10).to_dict()
        uniprot_counts_low_pep = train_peptides['UniProt'].value_counts().sort_values(ascending=True).head(10).to_dic
        print(f'Top 10 most frequent UniProt IDs: {uniprot_counts_high_pep.keys()}')
        print(f'Top 10 least frequent UniProt IDs: {uniprot_counts_low_pep.keys()}')
        Top 10 most frequent UniProt IDs: dict_keys(['P02787', 'P02768', 'P01024', 'P02751', 'P02649', 'P02774', 'P01
        009', 'P02647', 'P08603', 'P10909'])
        Top 10 least frequent UniProt IDs: dict_keys(['Q99829', 'Q99832', 'Q562R1', 'P01780', 'Q6UX71', '075326', 'P0
        6310', 'P19827', 'P36980', 'P02655'])
```

Summary stats

The mean value of peptide abundance is about 642890.25; The maximum value is 178752000, and the minimum value is about 11. The variation is very large.

train_proteins dataset

The train_proteins sample includes 248 patients. The dataset contains 232741 rows and 5 columns.

```
In [ ]: train_proteins.head()
```

visit_id visit_month patient_id UniProt

```
0
             55_0
                          0
                                   55 000391
                                               11254.3
                                   55 000533 732430.0
             55_0
        1
        2
             55_0
                          0
                                   55 000584
                                              39585.8
                          0
                                   55 014498
        3
             55_0
                                              41526.9
                          0
        4
             55_0
                                   55 014773
                                              31238.0
In [ ]: # check for the number of unique values
        print(f"The number of unique visit month is: {train_proteins['visit_month'].nunique()}")
        # print each unique value
        print(pd.unique(train_proteins["visit_month"]))
        The number of unique visit month is: 15
              3 6 12 18 24 30 36 48 54 60 72 84 96 108]
In [ ]: # check for the number of unique values
        print(f"The number of unique values of patient_id is: {train_proteins['patient_id'].nunique()}")
        print(f"The number of unique values of UniProt is: {train proteins['UniProt'].nunique()}")
        The number of unique values of patient id is: 248
```

NPX

```
In [ ]: train_proteins.shape
```

Out[]: (232741, 5)

Out[]:

Missing values check

no missing values for the train_proteins dataset

The number of unique values of UniProt is: 227

```
In []: # Check for missing values
    train_proteins.isnull().sum()
```

0

```
visit month
                       0
        patient id
                       0
        UniProt
        NPX
        dtype: int64
In [ ]:
       uniprot_counts_high_pep = train_peptides['UniProt'].value_counts().head(10).to_dict()
        uniprot_counts_low_pep = train_peptides['UniProt'].value_counts().sort_values(ascending=True).head(10).to_dic
        print(f'Top 10 most frequent UniProt IDs: {uniprot_counts_high_pep.keys()}')
        print(f'Top 10 least frequent UniProt IDs: {uniprot_counts_low_pep.keys()}')
        Top 10 most frequent UniProt IDs: dict_keys(['P02787', 'P02768', 'P01024', 'P02751', 'P02649', 'P02774', 'P01
        009', 'P02647', 'P08603', 'P10909'])
        Top 10 least frequent UniProt IDs: dict_keys(['Q99829', 'Q99832', 'Q562R1', 'P01780', 'Q6UX71', '075326', 'P0
        6310', 'P19827', 'P36980', 'P02655'])
In []: uniprot counts high = train proteins['UniProt'].value counts().head(10).to dict()
        uniprot_counts_low = train_proteins['UniProt'].value_counts().sort_values(ascending=True).head(10).to_dict()
        print(f'Top 10 most frequent UniProt IDs: {uniprot counts high.keys()}')
        print(f'Top 10 least frequent UniProt IDs: {uniprot counts low.keys()}')
        Top 10 most frequent UniProt IDs: dict_keys(['P01024', 'P05090', 'P01011', 'P01023', 'Q92520', 'P01042', 'P23
        142', 'P02790', 'Q9UHG2', 'P01834'])
        Top 10 least frequent UniProt IDs: dict_keys(['Q99829', 'Q99832', 'Q562R1', 'P01780', 'Q6UX71', '075326', 'P0
        6310', 'P19827', 'P36980', 'P02655'])
```

Summary stats

Out[]: visit id

The mean value of Normalized protein expression is 2712077; maximum value is 613851000, and minimum value is 84.6082. The variation is very large and there may be other factors impacting the NPX such as peptide kinds.

Visit month vs NPX

Because the large values and potential variability involved in the expression frequencies, we will use a logarithmic scale to NPX while looking the trend. The normalized protein expression is pretty stable across months, though the variance is very large.

```
In [ ]: # create a copy of the dataframe
        train_proteins_copy = train_proteins.copy()
        # calculate the logarithm of NPX
        train_proteins_copy["log_NPX"] = np.log(train_proteins_copy["NPX"])
        # set up the plot
        fig, ax = plt.subplots(figsize=(15, 5))
        sns.set_style('darkgrid')
        # create the boxplot and pointplot
        sns.boxplot(data=train_proteins_copy, x="visit_month", y="log_NPX", ax=ax)
        sns.pointplot(data=train_proteins_copy, x="visit_month", y="log_NPX", color="r", ci=None, linestyles=[":"], a
        # set the plot title and labels
        ax.set_title("NPX by Month", fontsize=15)
        ax.set_xlabel("Visit Month")
        ax.set_ylabel("NPX")
        plt.show()
        /var/folders/92/6467ymq56qn8qy3v68tsr84r0000gn/T/ipykernel_74699/3601816746.py:17: FutureWarning:
        The `ci` parameter is deprecated. Use `errorbar=None` for the same effect.
```

