Interpretation

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1 Predicting LOS of patients during their stay in the Intensive Care Unit in the MIMIC-III

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1.1 Objective

Accurately forecasting the Length of Stay (LOS) of patients in the Intensive Care Unit (ICU) is critical for resource allocation, clinical decision-making, and improving patient outcomes. This document outlines the development and optimization of a machine learning pipeline to predict ICU LOS using the MIMIC-III (Medical Information Mart for Intensive Care) dataset, a rich but challenging clinical database.

1.2 Challenges

- Skewed LOS distribution: Most patients stay 22 days, but a long tail of extended stays complicates modeling.
- Sparse, irregular time-series data: Clinical measurements (e.g., lab values, vitals) are recorded at varying frequencies.
- High-dimensional features: Thousands of potential predictors require careful selection to avoid overfitting

1.3 Why This Matters

- Clinical utility: Earlier, accurate LOS predictions can aid ICU bed management and discharge planning.
- Methodological insights: Demonstrates how to handle real-world clinical data constraints (missingness, skewness, high dimensionality).

2 Disease choice

We aimed to identify a disease that would provide: - Sufficient sample size: Enough ICU cases for robust statistical analysis - Clinical relevance: A condition with significant impact on ICU resource utilization - Temporal predictability: Clear patterns of clinical measurements within the critical first 24 hours of ICU admission

After querying the MIMIC-III database for conditions meeting these criteria, we selected Pneumonia (ICD-9 code 482.83) based on: - High prevalence in ICU populations - Well-defined clinical markers for monitoring - Consistent patterns of clinical deterioration that often require ICU admission

2.1 Loading relational MIMIC-III tables

We extracted and merged data from multiple MIMIC-III relational tables:

- PATIENTS table:
  - Demographic information (age, gender, ethnicity)
- ADMISSIONS table:
  - Hospital admission/discharge timestamps
  - Primary and secondary diagnoses
- ICUSTAYS table:
  - ICU admission/discharge timestamps
  - Length of stay calculation
- CHARTEVENTS table (first 24 hours):
  - Vital signs (heart rate, blood pressure, SpO)
  - Respiratory parameters (ventilator settings, FiO)
  - Neurological assessments (GCS scores)
- DIAGNOSES_ICD table:
  - Confirmation of primary pneumonia diagnosis
- D_ITEMS table:
  - Item description

[2]:
```
import pandas as pd
import matplotlib.pyplot as plt

data_path = "./data_sets/"

df_patients= pd.read_csv(data_path + 'PATIENTS.csv.gz')
df_admissions = pd.read_csv(data_path + 'ADMISSIONS.csv.gz')
df_icustays = pd.read_csv(data_path + 'ICUSTAYS.csv.gz')
df_diagnoses = pd.read_csv(data_path + 'DIAGNOSES_ICD.csv.gz', low_memory=False)
```

The integration of MIMIC-III's relational tables was carefully engineered to ensure data accuracy, temporal consistency, and clinical validity for our pneumonia cohort.

[3]:
```
# Filter for Pneumonia (ICD-9 = 48283)
df_diagnoses = df_diagnoses[df_diagnoses['ICD9_CODE'] ==␣
 ↪'48283'][['SUBJECT_ID', 'HADM_ID', 'ICD9_CODE']]

df_admissions_merged = pd.merge(
    df_diagnoses,
    df_admissions[['SUBJECT_ID', 'HADM_ID', 'ADMITTIME', 'ETHNICITY']],
    on=['SUBJECT_ID', 'HADM_ID'],
```

```
    how='left'
)

print('Number of hospital admissions: ', df_admissions_merged.shape[0])

df_icustays_merged = pd.merge(
    df_admissions_merged,
    df_icustays[['SUBJECT_ID', 'HADM_ID', 'ICUSTAY_ID', 'INTIME', 'LOS']],
    on=['SUBJECT_ID', 'HADM_ID'],
    how='left'
)

print('Number of icu stays: ', df_icustays_merged.shape[0])

df_icustays_patients_merged = pd.merge(
    df_icustays_merged,
    df_patients[['SUBJECT_ID', 'GENDER', 'DOB']],
    on='SUBJECT_ID',
    how='left'
)

df_icustays_patients_merged.head(3)
```

```
Number of hospital admissions:  264
Number of icu stays:  307
```

[3]:

	SUBJECT_ID	HADM_ID	ICD9_CODE	ADMITTIME	ETHNICITY
0	114	178393	48283	2146-08-29 01:18:00	UNKNOWN/NOT SPECIFIED
1	339	112625	48283	2187-04-20 23:10:00	BLACK/AFRICAN AMERICAN
2	285	165312	48283	2152-09-21 22:47:00	HISPANIC OR LATINO

	ICUSTAY_ID	INTIME	LOS	GENDER	DOB
0	258626	2146-08-29 17:59:00	1.8132	M	2098-05-09 00:00:00
1	221278	2187-04-20 23:10:50	31.7018	F	2120-07-17 00:00:00
2	238023	2152-09-21 22:48:50	28.6880	M	2107-05-16 00:00:00

There number icu stays which have chart events is of 140, this being enough to have a decent data frame.

[4]:
```
df_chart_events =  pd.read_csv(data_path + 'd_pneumonia.csv', low_memory=False)

# Merge df_merged with CHARTEVENTS (left join to preserve all ICU stays)
df_merged_with_chartevents = pd.merge(
    df_icustays_patients_merged,
    df_chart_events[['SUBJECT_ID', 'HADM_ID', 'ICUSTAY_ID', 'ITEMID',␣
 ↪'VALUENUM','CHARTTIME']].drop_duplicates(),
    on=['SUBJECT_ID', 'HADM_ID', 'ICUSTAY_ID'],
    how='left',
```

```
    indicator=True  # Adds a column '_merge' to show match status
)

has_chartevents = df_merged_with_chartevents['_merge'] == 'both'
no_chartevents = df_merged_with_chartevents['_merge'] == 'left_only'

icu_with_data = df_merged_with_chartevents[has_chartevents]['ICUSTAY_ID'].
 ↪unique()
icu_without_data = df_merged_with_chartevents[no_chartevents]['ICUSTAY_ID'].
 ↪unique()

print(f"ICU stays WITH CHARTEVENTS data: {len(icu_with_data)}")
print(f"ICU stays WITHOUT CHARTEVENTS data: {len(icu_without_data)}")

print(df_merged_with_chartevents.shape)

df_merged_with_chartevents.head(2)
```

```
ICU stays WITH CHARTEVENTS data: 145
ICU stays WITHOUT CHARTEVENTS data: 162
(986958, 14)
```

[4]:

	SUBJECT_ID	HADM_ID	ICD9_CODE	ADMITTIME	ETHNICITY	\
0	114	178393	48283	2146-08-29 01:18:00	UNKNOWN/NOT SPECIFIED	
1	114	178393	48283	2146-08-29 01:18:00	UNKNOWN/NOT SPECIFIED	

	ICUSTAY_ID	INTIME	LOS	GENDER	DOB	\
0	258626	2146-08-29 17:59:00	1.8132	M	2098-05-09 00:00:00	
1	258626	2146-08-29 17:59:00	1.8132	M	2098-05-09 00:00:00	

	ITEMID	VALUENUM	CHARTTIME	_merge
0	211.0	72.0	2146-08-30 10:00:00	both
1	581.0	102.0	2146-08-30 10:00:00	both

An inner join in the last merge could've saved this step, but now we need to remove the icu stays without chart events.

[5]:
```
df_final = df_merged_with_chartevents[df_merged_with_chartevents['_merge'] ==␣
 ↪'both'].copy()

# Optional: You can now drop the '_merge' column as it's no longer needed
df_final = df_final.drop(columns=['_merge'])

print(f"Shape of the original DataFrame: {df_merged_with_chartevents.shape}")
print(f"Shape of the final DataFrame (with data): {df_final.shape}")
df_final.head(3)
```

```
Shape of the original DataFrame: (986958, 14)
```

```
Shape of the final DataFrame (with data): (986796, 13)
```

[5]:

	SUBJECT_ID	HADM_ID	ICD9_CODE	ADMITTIME	ETHNICITY	\
0	114	178393	48283	2146-08-29 01:18:00	UNKNOWN/NOT SPECIFIED	
1	114	178393	48283	2146-08-29 01:18:00	UNKNOWN/NOT SPECIFIED	
2	114	178393	48283	2146-08-29 01:18:00	UNKNOWN/NOT SPECIFIED	

	ICUSTAY_ID	INTIME	LOS	GENDER	DOB	\
0	258626	2146-08-29 17:59:00	1.8132	M	2098-05-09 00:00:00	
1	258626	2146-08-29 17:59:00	1.8132	M	2098-05-09 00:00:00	
2	258626	2146-08-29 17:59:00	1.8132	M	2098-05-09 00:00:00	

	ITEMID	VALUENUM	CHARTTIME
0	211.0	72.0	2146-08-30 10:00:00
1	581.0	102.0	2146-08-30 10:00:00
2	618.0	20.0	2146-08-30 10:00:00

All of this steps were also done for bronchitis, but we were left with only 48 icu stays with chart events which is by far insuficient as a dataframe to train and validate a model.

3 Statistical analisys and visualization of patients with Pneumonia

3.1 Dataframe cleaning preparation for the analysis

- Since the time window of 24 hours was chosen for prediction, all chart events past that time will be discarded
- There are 4 very far outliers with LOS above 60 days and they will be discarded since they are not enough to prove helpful for the model training
- Based on the fact that 75% of the admissions have a LOS under 21 days and 87.2% have a LOS under 30 days, entries with more than that will also be discarded
- Not all ICU stays have all the item values present
  - The two possible approaces of dealing with that missing data are imputing 0 in their place or leaving them as null
  - Since XGBoost, the model planned to be trained, works well with missing values, these will be left as null
  - In order to mark their missing as a relevant feature, a count of the number of their appearances will be added for each item, 0 meaning a missing value

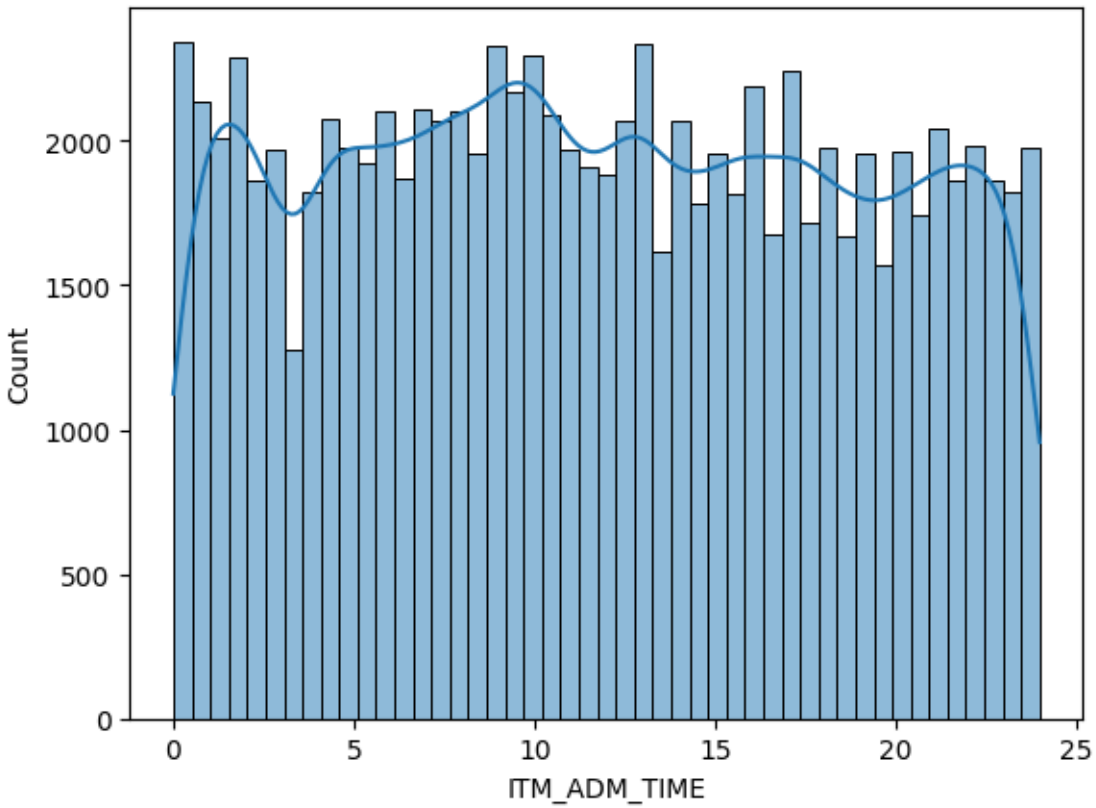
We need to take out all the events that happen outside of the first 24h windows of a patient's stay to be able to visualize a patient 24h in the ICU and its relation with items and also the simplify the dataframe.

[6]:
```
import seaborn as sns

df_final['INTIME'] = pd.to_datetime(df_final['INTIME'])
df_final['CHARTTIME'] = pd.to_datetime(df_final['CHARTTIME'])

df_final['ITM_ADM_TIME'] = (df_final['CHARTTIME'] - df_final['INTIME']).dt.
 ↪total_seconds() / 3600
```

```
df_final = df_final[(df_final['ITM_ADM_TIME'] <= 24) &␣
 ↪(df_final['ITM_ADM_TIME'] >= 0)]

print(df_final.shape)

sns.histplot(df_final['ITM_ADM_TIME'], kde=True)
```

```
(92430, 14)
```

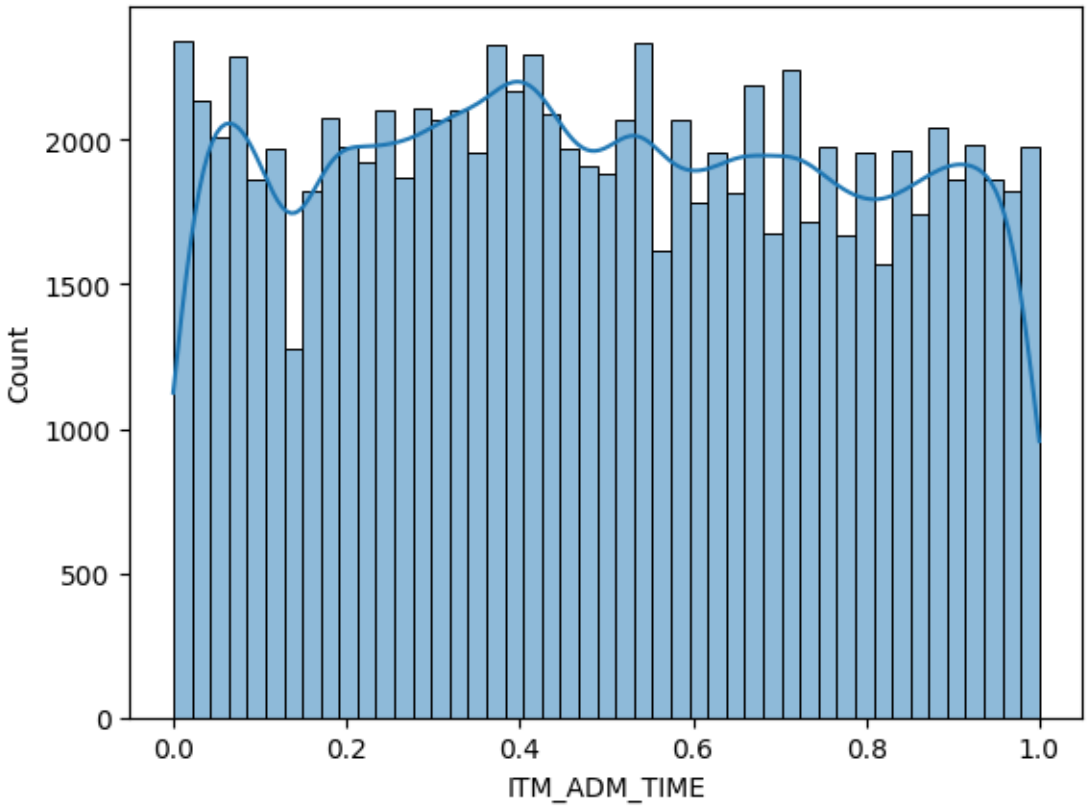
[6]: <Axes: xlabel='ITM_ADM_TIME', ylabel='Count'>



We normalize it to a time interval of (0, 1) to make any possible model easier to be trained and to be able to interpret results.

[7]:
```
df_final['ITM_ADM_TIME'] = df_final['ITM_ADM_TIME'] / 24.0

sns.histplot(df_final['ITM_ADM_TIME'], kde=True)
```

[7]: <Axes: xlabel='ITM_ADM_TIME', ylabel='Count'>



3.2 Patients overview

Three patients were chosen with little, medium and high LOS in order to visualize different trends.

A sorted CSV of the ICU stays has been generated using an sql query which is saved to the csv `norm_pneumonia.csv` to be able to chose said three examples.

[8]:
```
from statsmodels.nonparametric.smoothers_lowess import lowess

df = pd.read_csv("./data_sets/norm_pneumonia.csv")

df['ITM_ADM_TIME'] = df['NORMTIME']
df.drop(columns='NORMTIME')

# Define plotting function
def plot_icu_data(icu_id):
    filtered = df[df["ICUSTAY_ID"] == icu_id]
    value_min = 0
    value_max = 200
    filtered_limited = filtered[
        (filtered["VALUENUM"] >= value_min) & (filtered["VALUENUM"] <=␣
↪value_max)
```

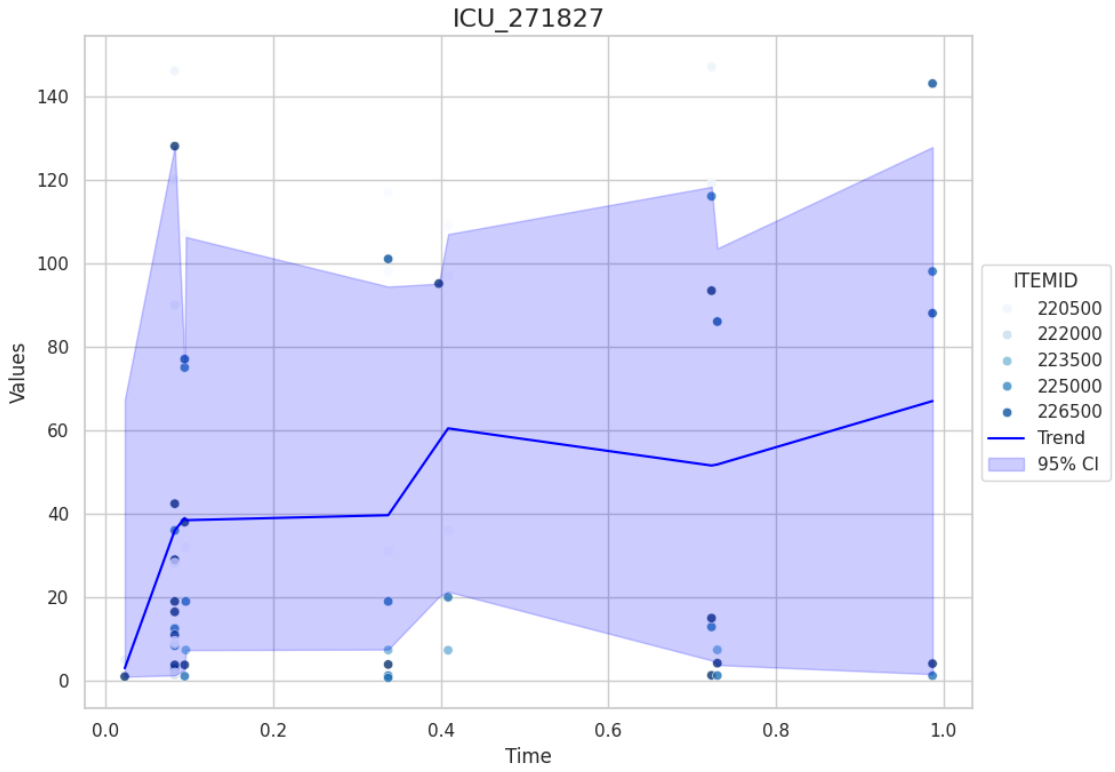
```
    ]

    # Prepare LOWESS smoothed values
    x = filtered_limited["ITM_ADM_TIME"]
    y = filtered_limited["VALUENUM"]
    lowess_smoothed = lowess(y, x, frac=0.3, return_sorted=True)
    lowess_x = lowess_smoothed[:, 0]
    lowess_y = lowess_smoothed[:, 1]

    # Bootstrap for confidence interval
    bootstraps = []
    for _ in range(100):
        sample = filtered_limited.sample(frac=1, replace=True)
        smoothed = lowess(sample["VALUENUM"], sample["ITM_ADM_TIME"], frac=0.3,␣
↪return_sorted=True)
        bootstraps.append(np.interp(lowess_x, smoothed[:, 0], smoothed[:, 1]))
    bootstraps = np.array(bootstraps)
    ci_lower = np.percentile(bootstraps, 2.5, axis=0)
    ci_upper = np.percentile(bootstraps, 97.5, axis=0)

    # Plot
    plt.figure(figsize=(10, 7))
    sns.set(style="whitegrid")

    sns.scatterplot(
        data=filtered_limited,
        x="ITM_ADM_TIME",
        y="VALUENUM",
        hue="ITEMID",
        palette="Blues",
        alpha=0.8
    )

    # Add LOWESS trend line
    plt.plot(lowess_x, lowess_y, color="blue", label="Trend")

    # Add ribbon (confidence interval)
    plt.fill_between(lowess_x, ci_lower, ci_upper, color="blue", alpha=0.2,␣
↪label="95% CI")

    # Adjust legend
    plt.legend(title="ITEMID", loc='center left', bbox_to_anchor=(1, 0.5))
    plt.title(f"ICU_{icu_id}", fontsize=16)
    plt.xlabel("Time")
    plt.ylabel("Values")
    plt.tight_layout()
    plt.show()
```

3.2.1 Small LOS

In this example we can see a slight increase of LOESS over time, but the trend is unstable do to sparse data and high variability.
Dense concentration of measurements in early stages suggest early implication of doctors that might suggest the shorter LOS.

[9]:
```
import numpy as np

plot_icu_data(icu_id=271827)
```

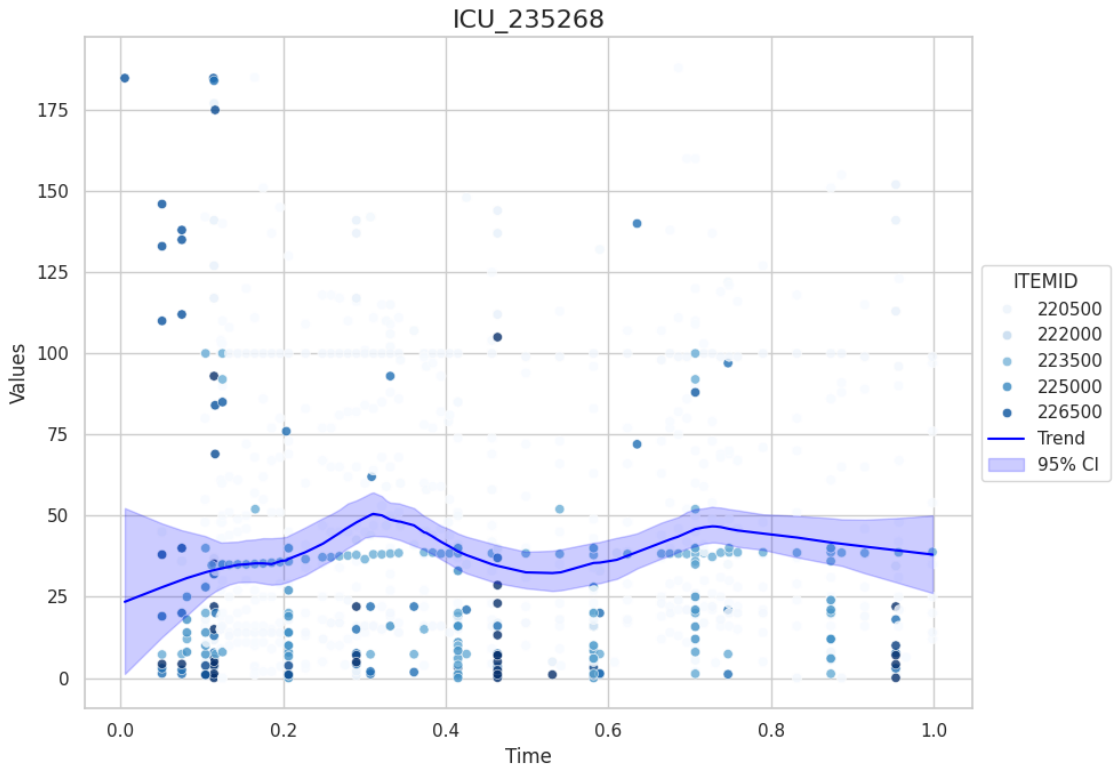
```
/home/cox/.local/lib/python3.10/site-
packages/statsmodels/nonparametric/smoothers_lowess.py:226: RuntimeWarning:
invalid value encountered in divide
  res, _ = _lowess(y, x, x, np.ones_like(x),
```



3.2.2 Medium LOS

Here, LOESS trend display a well formed curve and a consistent trajectory. Also, the evenly spread of items over the ICU stay suggest a stable and systematic mmonitoring over this time period.

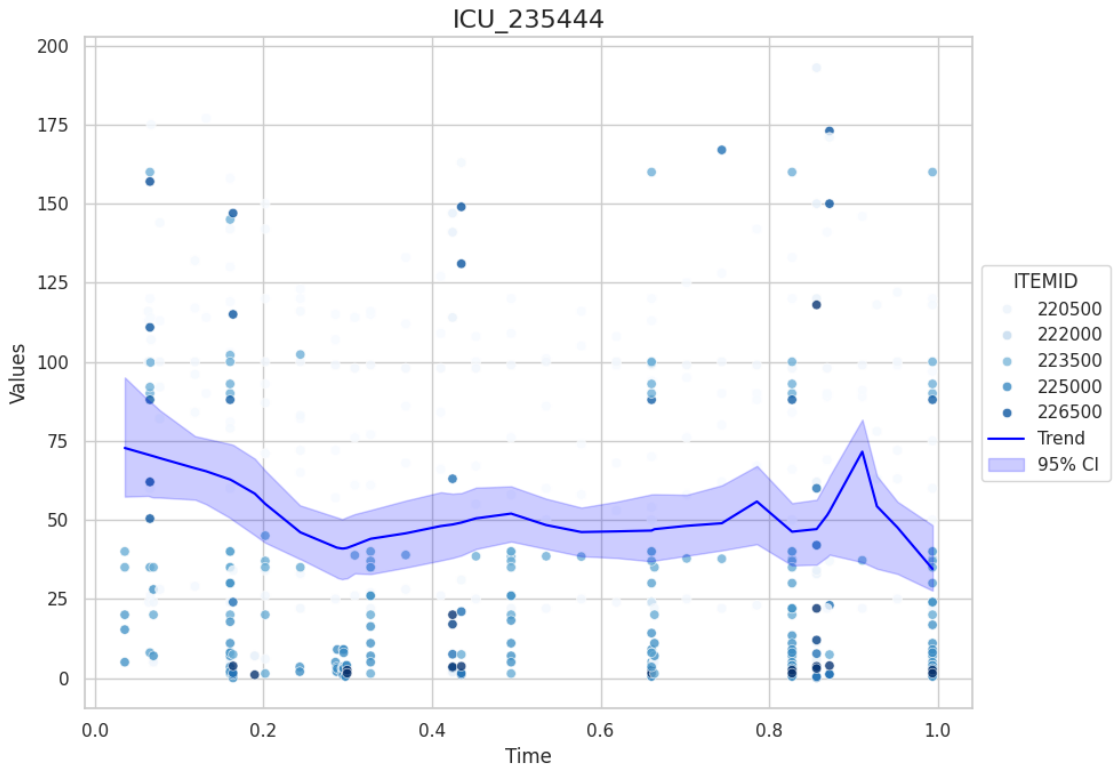
[10]:
```
plot_icu_data(icu_id=235268)
```



3.2.3 High LOS

This example ilustrates a slight downward slope, possibly due to treatment effects and the spike at 0.9 suggests a check-up.

[11]:
```
plot_icu_data(icu_id=235444)
```



4 Training and validation of a model to predict LOS

First of all our dataframe needs some processing for the model to be able to digest the data accordingly.

4.1 Data transformation

- The age of the patients is computed from the ICU admission time minus their birth date
  - Patients with ages greater than 89 years old are entered in the database to 300 in order to protect confidentiality
  - All the patients in this case will have their age moved to 91.4, the average of their group
- Categorical features of patients are encoded
  - Gender is label encoded, while ethnicity is encoded using one hot encoding for better model interpretation
- The distribution of the target variable, LOS, is right-skewed
  - In order to have that data better interpretable by a wider range of models, a *log transformation* will be applied on it ### Processing of DOB, INTIME and ADMITTIME To be able to make use of the dates, we transform them to pandas datetime format and create meaningful features out of them. These are the age, which is the difference between the time of admission in the ICU minus the date of birth, and the hospital time, which is the time of admission in the ICU minus the hospital admission time.

[12]:
```
df_final['DOB'] = pd.to_datetime(df_final['DOB'])
df_final['INTIME'] = pd.to_datetime(df_final['INTIME'])
df_final['ADMITTIME'] = pd.to_datetime(df_final['ADMITTIME'])

df_final['AGE'] = (
    (df_final['INTIME'].dt.year - df_final['DOB'].dt.year) +
    (df_final['INTIME'].dt.dayofyear - df_final['DOB'].dt.dayofyear) / 365.25
)
df_final['HOSP_TIME'] = (
    (df_final['INTIME'].dt.year - df_final['ADMITTIME'].dt.year) +
    (df_final['INTIME'].dt.dayofyear - df_final['ADMITTIME'].dt.dayofyear) /␣
 ↪365.25
)
# Can drop DOB, INTIME and ADMITE TIME
# df_merged.drop(columns=['DOB', 'ADMITTIME'], inplace=True)
```

In this dataset, patients older than 89 years old have been mapped to 300 years old out of privacy reasons. We need their actual age so it has meaning for the future model. This is done by assigning the average of this age group, 91.4, to all of them.

[13]:
```
df_final.loc[df_final['AGE'] > 89, 'AGE'] = 91.4
```

To make predictions on the LOS on patients at the 24 hour mark of their stay in ICU, the patients that stayed **more** than that, are not useful and will be discarded.

[14]:
```
df_final = df_final[df_final['LOS'] > 1]
df_final.head(3)
```

[14]:

	SUBJECT_ID	HADM_ID	ICD9_CODE	ADMITTIME	ETHNICITY
0	114	178393	48283	2146-08-29 01:18:00	UNKNOWN/NOT SPECIFIED
1	114	178393	48283	2146-08-29 01:18:00	UNKNOWN/NOT SPECIFIED
2	114	178393	48283	2146-08-29 01:18:00	UNKNOWN/NOT SPECIFIED

	ICUSTAY_ID	INTIME	LOS	GENDER	DOB	ITEMID	VALUENUM
0	258626	2146-08-29 17:59:00	1.8132	M	2098-05-09	211.0	72.0
1	258626	2146-08-29 17:59:00	1.8132	M	2098-05-09	581.0	102.0
2	258626	2146-08-29 17:59:00	1.8132	M	2098-05-09	618.0	20.0

	CHARTTIME	ITM_ADM_TIME	AGE	HOSP_TIME
0	2146-08-30 10:00:00	0.667361	48.306639	0.0
1	2146-08-30 10:00:00	0.667361	48.306639	0.0
2	2146-08-30 10:00:00	0.667361	48.306639	0.0

4.1.1 Ethnicity and gender processing

Categorical features of patients are to be encoded.

Within this disease's sub data set there are different ethnicities, those that have less than 5 repre-

sentatives will be grouped together in an OTHER ethnicity.

[15]:
```
unique_ethnicities = df_final['ETHNICITY'].unique()
print(unique_ethnicities)

ethnicity_counts = df_final['ETHNICITY'].value_counts()
print(ethnicity_counts)

rare_ethnicities = ['HISPANIC/LATINO - PUERTO RICAN', 'WHITE - RUSSIAN',
                    'HISPANIC/LATINO - DOMINICAN', 'ASIAN - CHINESE',
                    'UNABLE TO OBTAIN', 'PATIENT DECLINED TO ANSWER']

df_final['ETHNICITY'] = df_final['ETHNICITY'].replace(rare_ethnicities, 'OTHER')

ethnicity_counts = df_final['ETHNICITY'].value_counts()
print(ethnicity_counts)
```

```
['UNKNOWN/NOT SPECIFIED' 'BLACK/AFRICAN AMERICAN' 'HISPANIC OR LATINO'
 'ASIAN' 'WHITE' 'OTHER' 'WHITE - RUSSIAN'
 'HISPANIC/LATINO - PUERTO RICAN' 'ASIAN - CHINESE' 'UNABLE TO OBTAIN'
 'PATIENT DECLINED TO ANSWER']
ETHNICITY
WHITE                              77730
BLACK/AFRICAN AMERICAN              5450
UNKNOWN/NOT SPECIFIED               2309
HISPANIC OR LATINO                  1810
ASIAN                               1268
OTHER                                883
WHITE - RUSSIAN                      813
UNABLE TO OBTAIN                     753
PATIENT DECLINED TO ANSWER           400
ASIAN - CHINESE                      376
HISPANIC/LATINO - PUERTO RICAN       215
Name: count, dtype: int64
ETHNICITY
WHITE                      77730
BLACK/AFRICAN AMERICAN      5450
OTHER                       3440
UNKNOWN/NOT SPECIFIED       2309
HISPANIC OR LATINO          1810
ASIAN                       1268
Name: count, dtype: int64
```

The gender is encoded using a Label Encoder since in this data set it has 2 values.

But in the case of ethnicities, using a Label Encoder to encode these values would create an ordinal relationship between them, which will make them lose their meaning. Instead, the etnicities are one hot encoded, with the first column being dropped to prevent multicollinearity.

[16]:
```
from sklearn.preprocessing import LabelEncoder

gender_encoder = LabelEncoder()

df_final['GENDER'] = gender_encoder.fit_transform(df_final['GENDER'])

print("Gender Classes:", gender_encoder.classes_)

df_final = pd.get_dummies(
    df_final,
    columns=['ETHNICITY'],
    prefix='ETH',
    drop_first=True
    )


df_final.head(3)
```

```
Gender Classes: ['F' 'M']
```

[16]:

	SUBJECT_ID	HADM_ID	ICD9_CODE	ADMITTIME	ICUSTAY_ID	\
0	114	178393	48283	2146-08-29 01:18:00	258626	
1	114	178393	48283	2146-08-29 01:18:00	258626	
2	114	178393	48283	2146-08-29 01:18:00	258626	

	INTIME	LOS	GENDER	DOB	ITEMID	VALUENUM	\
0	2146-08-29 17:59:00	1.8132	1	2098-05-09	211.0	72.0	
1	2146-08-29 17:59:00	1.8132	1	2098-05-09	581.0	102.0	
2	2146-08-29 17:59:00	1.8132	1	2098-05-09	618.0	20.0	

	CHARTTIME	ITM_ADM_TIME	AGE	HOSP_TIME	\
0	2146-08-30 10:00:00	0.667361	48.306639	0.0	
1	2146-08-30 10:00:00	0.667361	48.306639	0.0	
2	2146-08-30 10:00:00	0.667361	48.306639	0.0	

	ETH_BLACK/AFRICAN AMERICAN	ETH_HISPANIC OR LATINO	ETH_OTHER	\
0	False	False	False	
1	False	False	False	
2	False	False	False	

	ETH_UNKNOWN/NOT SPECIFIED	ETH_WHITE
0	True	False
1	True	False
2	True	False

[52]:
```
df_icustays_patients_merged.describe().T
```

[52]:

	count	mean	min	\
SUBJECT_ID	307.0	33228.550489	114.0	
HADM_ID	307.0	150245.521173	100395.0	
ICUSTAY_ID	307.0	252298.661238	200387.0	
INTIME	307	2150-10-01 05:11:23.130293248	2100-12-10 12:50:48	
LOS	307.0	15.420087	0.0705	
DOB	307	2080-01-13 13:12:42.214983680	1805-12-07 00:00:00	
AGE	307.0	65.235295	19.350445	

	25%	50%	\
SUBJECT_ID	11215.0	25474.0	
HADM_ID	125328.0	152895.0	
ICUSTAY_ID	230449.5	253214.0	
INTIME	2125-01-24 21:55:23.500000256	2150-04-22 17:40:51.000000512	
LOS	4.42235	11.9535	
DOB	2056-08-04 00:00:00	2088-08-09 00:00:00	
AGE	57.278234	67.956194	

	75%	max	std
SUBJECT_ID	49267.5	99715.0	28758.748753
HADM_ID	174117.5	199845.0	27775.541971
ICUSTAY_ID	275776.0	299728.0	28329.125649
INTIME	2174-08-08 07:02:47.000000512	2207-12-13 20:57:20	NaN
LOS	21.613	84.0409	13.732065
DOB	2110-02-18 00:00:00	2173-02-23 00:00:00	NaN
AGE	76.819302	91.4	15.791862

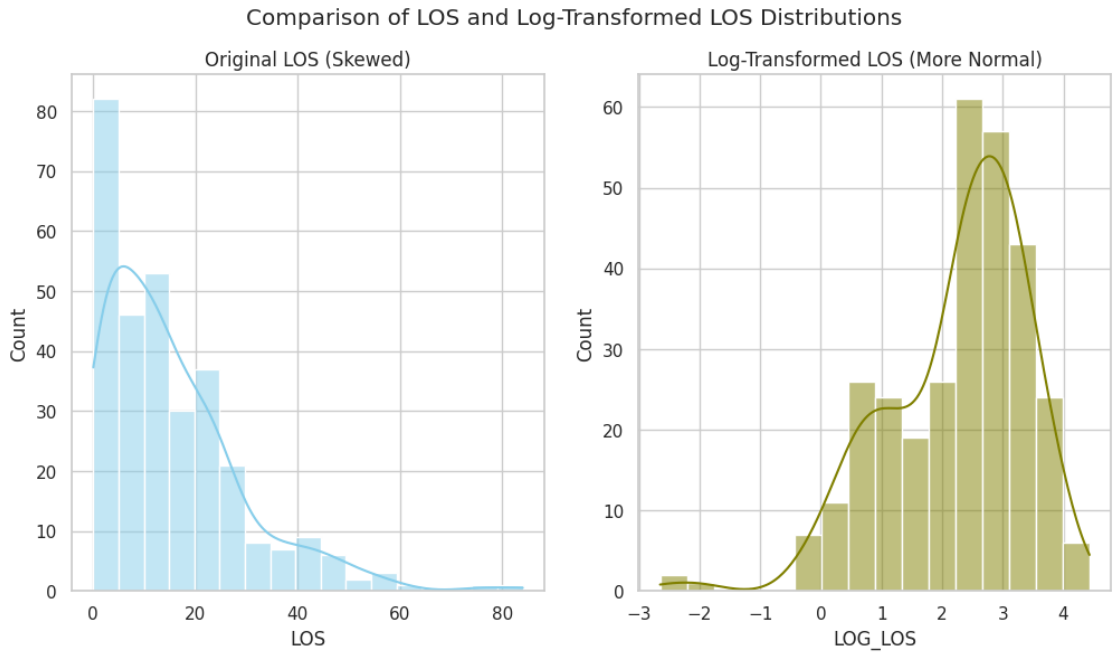
- Based on the fact that 75% of the admissions have a LOS under 21 days and 87.2% have a LOS under 30 days, entries with more than that will also be discarded
- Not all ICU stays have all the item values present
  - The two possible approaces of dealing with that missing data are imputing 0 in their place or leaving them as null
  - Since XGBoost, the model planned to be trained, works well with missing values, these will be left as null
  - In order to mark their missing as a relevant feature, a count of the number of their appearances will be added for each item, 0 meaning a missing value

[17]:
```
print('Initial size: ', df_final.shape[0])
df_final = df_final[df_final['LOS'] <= 30]
print('Current size: ', df_final.shape[0])
```

```
Initial size:  92007
Current size:  87861
```

Without removal of the outliers, the LOS distribution was right skewed, which would've suggested using the log of the LOS. But after the elimination, log becomes left skewed.

[18]:
```
import matplotlib.pyplot as plt

df_final_log = df_icustays_patients_merged.copy()


df_final_log['LOG_LOS'] = np.log(df_final_log['LOS'])

fig, axes = plt.subplots(1, 2, figsize=(12, 6))
fig.suptitle('Comparison of LOS and Log-Transformed LOS Distributions')

sns.histplot(df_final_log['LOS'], kde=True, ax=axes[0], color='skyblue')
axes[0].set_title('Original LOS (Skewed)')

sns.histplot(df_final_log['LOG_LOS'], kde=True, ax=axes[1], color='olive')
axes[1].set_title('Log-Transformed LOS (More Normal)')

# plt.tight_layout()
plt.show()
```

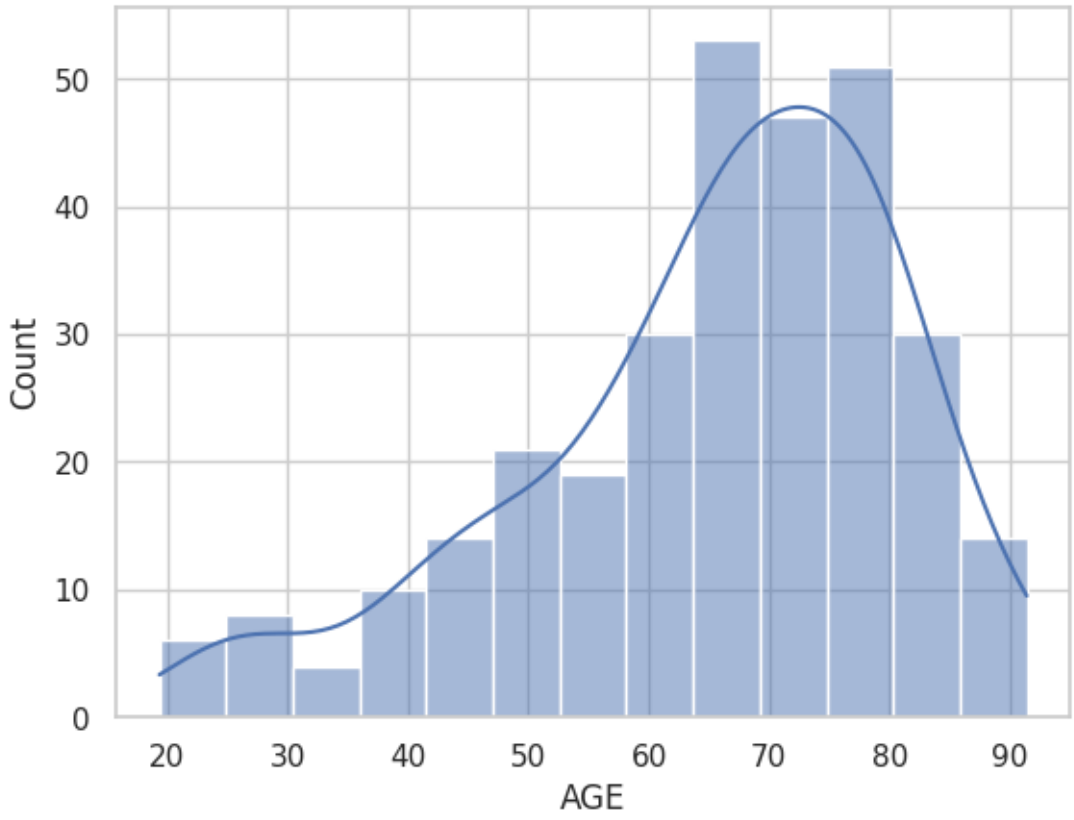


Age distribution looks good.

[19]:
```
df_icustays_patients_merged['DOB'] = pd.
 ↪to_datetime(df_icustays_patients_merged['DOB'])
df_icustays_patients_merged['INTIME'] = pd.
 ↪to_datetime(df_icustays_patients_merged['INTIME'])
```

```
df_icustays_patients_merged['AGE'] = (
    (df_icustays_patients_merged['INTIME'].dt.year -␣
 ↪df_icustays_patients_merged['DOB'].dt.year) +
    (df_icustays_patients_merged['INTIME'].dt.dayofyear -␣
 ↪df_icustays_patients_merged['DOB'].dt.dayofyear) / 365.25
)

df_icustays_patients_merged.loc[df_icustays_patients_merged['AGE'] > 89, 'AGE']␣
 ↪= 91.4  # Handle MIMIC-III's >89 group

sns.histplot(df_icustays_patients_merged['AGE'], kde=True)
```

[19]: <Axes: xlabel='AGE', ylabel='Count'>



4.2 Feature Engineering

- The time-stamps of each chart event will be normalized as starting from the addmission time
- Given the time-stamped nature of the item entries, the item values for each ICU stay will be aggregated into the following 5 features per item:
  - average
  - standard deviation

  - trend
  - range
  - count
- Since not all ICU stays have the same items in their respective events, only the items with more than 78% appearance will be selected as features
  - This criteria means selecting the first 32 items, multiplied by the number of 5 metrics for each, giving 160 features
  - This sorting is performed by an SQL query, that saves the results into `items_appearance_pneumonia.csv` ### Items aggregation We need to introduce the items into our dataframe, we do that by calculating a set of aggregate features for the top 32 most frequent items in our disease.

[20]:
```
static_features = df_final.drop_duplicates(subset=['SUBJECT_ID', 'HADM_ID',␣
↪'ICUSTAY_ID'])[
    ['SUBJECT_ID', 'HADM_ID', 'ICUSTAY_ID','HOSP_TIME', 'AGE', 'GENDER',
     'ETH_BLACK/AFRICAN AMERICAN', 'ETH_HISPANIC OR LATINO',
     'ETH_OTHER', 'ETH_UNKNOWN/NOT SPECIFIED', 'ETH_WHITE','LOS']
]

static_features.head()
```

[20]:

	SUBJECT_ID	HADM_ID	ICUSTAY_ID	HOSP_TIME	AGE	GENDER	\
0	114	178393	258626	0.000000	48.306639	1	
13145	285	165312	238023	0.000000	45.353183	1	
21486	605	115545	248569	0.000000	91.400000	0	
46380	3482	192399	202786	0.002738	55.577687	1	
48072	2090	138877	256557	0.000000	76.605065	1	

	ETH_BLACK/AFRICAN AMERICAN	ETH_HISPANIC OR LATINO	ETH_OTHER	\
0	False	False	False	
13145	False	True	False	
21486	False	False	False	
46380	False	False	False	
48072	False	False	False	

	ETH_UNKNOWN/NOT SPECIFIED	ETH_WHITE	LOS
0	True	False	1.8132
13145	False	False	28.6880
21486	False	False	16.8598
46380	False	True	4.9694
48072	False	True	10.0869

[21]:
```
import pandas as pd
import numpy as np

# The 'features_df' (for mapping names) is now a separate, optional argument.
```

```
def create_feature_matrix(df_events, df_static, item_ids, features_df=None,␣
↪agg_list=None):
    """
    Creates a feature matrix by combining static data with aggregated␣
↪time-series features.
    This version correctly accepts a list of ITEMIDs and robustly flattens␣
↪MultiIndex columns.

    Args:
        df_events (pd.DataFrame): Time-series data with 'SUBJECT_ID', 'ITEMID',␣
↪'VALUENUM', 'CHARTTIME'.
        df_static (pd.DataFrame): Static patient data with 'SUBJECT_ID'.
        item_ids (list): A Python list of ITEMIDs to use for feature generation.
        features_df (pd.DataFrame, optional): For mapping ITEMID to readable␣
↪names.
                                                Must have 'ITEMID' and␣
↪'item_name' columns. Defaults to None.
        agg_list (list, optional): Aggregations to compute. Defaults to␣
↪['mean', 'std', 'count', 'range', 'trend'].

    Returns:
        pd.DataFrame: Combined static + aggregated features, with NaN filled as␣
↪0.
    """
    if agg_list is None:
        agg_list = ['mean', 'std', 'count', 'range', 'trend']

    # 1. Filter relevant ITEMIDs from the provided list
    df_filtered = df_events[df_events['ITEMID'].isin(item_ids)].copy()
    df_filtered['CHARTTIME'] = pd.to_datetime(df_filtered['CHARTTIME'])

    # 2. Define aggregation calculations
    def calculate_aggregated_features(group):
        vals = group['VALUENUM']
        count = vals.count()
        features = {}
        for agg in agg_list:
            features[agg] = 0
        if count == 0:
            return pd.Series(features)
        if 'count' in agg_list: features['count'] = count
        if 'mean' in agg_list: features['mean'] = vals.mean()
        if 'std' in agg_list: features['std'] = vals.std() if count > 1 else 0
        if 'range' in agg_list: features['range'] = vals.max() - vals.min() if␣
↪count > 1 else 0
        if 'trend' in agg_list and count > 1:
```

```
            group = group.sort_values('CHARTTIME')
            time_in_hours = (group['CHARTTIME'] - group['CHARTTIME'].iloc[0]).
↪dt.total_seconds() / 3600.0
            valid_indices = time_in_hours.notna() & vals.notna()
            if valid_indices.sum() > 1:
                slope = np.polyfit(time_in_hours[valid_indices],␣
↪vals[valid_indices], 1)[0]
                features['trend'] = slope if np.isfinite(slope) else 0
        return pd.Series(features)

    # 3. Compute aggregations
    item_stats = (
        df_filtered.groupby(['SUBJECT_ID', 'ITEMID'])
        .apply(calculate_aggregated_features)
        .unstack(fill_value=0)
    )

    # 4. Flatten MultiIndex columns
    if isinstance(item_stats.columns, pd.MultiIndex):
        if features_df is not None:
            # Ensure data types match for mapping
            features_df['ITEMID'] = features_df['ITEMID'].astype(int)
            itemid_to_label = dict(zip(features_df['ITEMID'],␣
↪features_df['item_name']))
            item_stats.columns = [
                f"{agg}_{itemid_to_label.get(int(itemid), f'ITEM_{itemid}')}"
                for agg, itemid in item_stats.columns
            ]
        else: # If no features_df is provided, use default names
            item_stats.columns = [
                f"{agg}_ITEM_{itemid}" for agg, itemid in item_stats.columns
            ]

    item_stats = item_stats.reset_index()

    # 5. Merge with static data
    model_data = pd.merge(
        df_static,
        item_stats,
        on='SUBJECT_ID',
        how='left'
    ).fillna(0)

    return model_data
```

The top features have been achieved by quering the dataset and exporting it to `items_appearance_pneumonia` .

[22]:
```
top_features_df = pd.read_csv(data_path + 'items_appearance_pneumonia.csv')

top_features_df.head()
```

[22]:

	rank	ITEMID	item_name	VALUEUOM	stay_count
0	1	220645.0	Sodium (serum)	mEq/L	135
1	2	220615.0	Creatinine	mg/dL	135
2	3	220602.0	Chloride (serum)	mEq/L	135
3	4	225624.0	BUN	mg/dL	135
4	5	227443.0	HCO3 (serum)	mEq/L	135

[23]:
```
top32_features = top_features_df[top_features_df['rank'] <= 32]['ITEMID'].
↪to_list()

print('The number of items is: ', len(top32_features))
```

```
The number of items is:  32
```

For each of these items the mean, standard deviation, count, trend and range are calculated and inserted as features in the dataframe.

[24]:
```
model_data_full = create_feature_matrix(
    df_final,
    static_features,
    top32_features, # The list of ITEMIDs
    features_df=top_features_df # The dataframe for naming
)
print(model_data_full.shape)
model_data_full.head(1)
```

```
(126, 172)

/tmp/ipykernel_1368/3013210344.py:53: DeprecationWarning: DataFrameGroupBy.apply
operated on the grouping columns. This behavior is deprecated, and in a future
version of pandas the grouping columns will be excluded from the operation.
Either pass `include_groups=False` to exclude the groupings or explicitly select
the grouping columns after groupby to silence this warning.
  .apply(calculate_aggregated_features)
```

[24]:

	SUBJECT_ID	HADM_ID	ICUSTAY_ID	HOSP_TIME	AGE	GENDER	\
0	114	178393	258626	0.0	48.306639	1	

	ETH_BLACK/AFRICAN AMERICAN	ETH_HISPANIC OR LATINO	ETH_OTHER	\
0	False	False	False	

	ETH_UNKNOWN/NOT SPECIFIED	…	trend_Calcium non-ionized	\
0	True	…	0.0	

	trend_Phosphorous	trend_TCO2 (calc) Arterial	trend_SpO2 Desat Limit	\

```
0                0.0                          0.0                       0.0

   trend_Anion gap  trend_Potassium (serum)  trend_HCO3 (serum)  \
0              0.0                      0.0                 0.0

   trend_Platelet Count  trend_Prothrombin time  trend_INR
0                   0.0                     0.0        0.0

[1 rows x 172 columns]
```

Also, for a better prediction we add the SOFA score, which is widely used in real life.

[25]:
```
# Define SOFA-related ITEMIDs
sofa_itemids = {
    'RESPIRATION': [220224, 223835],  # PaO , FiO
    'COAGULATION': [828],           # Platelets
    'LIVER': [225690],                 # Bilirubin
    'CARDIOVASCULAR': [220052],       # MAP
    'CNS': [198],                     # GCS
    'RENAL': [220615]           # Creatinine
}

# 1. Flatten the list of ITEMIDs
all_sofa_ids = [item for sublist in sofa_itemids.values() for item in sublist]

# 2. Apply the filter directly
df_sofa_components = df_chart_events[df_chart_events['ITEMID'].
 ↪isin(all_sofa_ids)]

print(f"Found {len(df_sofa_components)} SOFA-related measurements.")
df_sofa_components.head(1)
```

```
Found 67420 SOFA-related measurements.
```

[25]:
```
   ROW_ID  SUBJECT_ID  HADM_ID  ICUSTAY_ID  ITEMID           CHARTTIME  \
0  170754        1709   127294      207018  220052  2118-01-04 12:15:00

             STORETIME     CGID  VALUE  VALUENUM VALUEUOM  WARNING  ERROR  \
0  2118-01-04 14:22:00  19783.0  124.0     124.0     mmHg      0.0    0.0

  RESULTSTATUS STOPPED
0          NaN     NaN
```

[26]:
```
# Extract PaO  and FiO  (assuming FiO  is in %, e.g., 50% = 0.5)
df_pao2 = df_sofa_components[df_sofa_components['ITEMID'] == 220224]
df_fio2 = df_sofa_components[df_sofa_components['ITEMID'] == 223835]
df_pao2
```

```
# Merge and calculate PaO/FiO ratio
df_respiration = pd.merge(
    df_pao2[['SUBJECT_ID', 'HADM_ID', 'ICUSTAY_ID', 'CHARTTIME', 'VALUENUM']],
    df_fio2[['SUBJECT_ID', 'HADM_ID', 'ICUSTAY_ID', 'CHARTTIME', 'VALUENUM']],
    on=['SUBJECT_ID', 'HADM_ID', 'ICUSTAY_ID', 'CHARTTIME'],
    suffixes=('_PAO2', '_FIO2')
)

df_respiration['PAO2_FIO2_RATIO'] = df_respiration['VALUENUM_PAO2'] /␣
 ↪(df_respiration['VALUENUM_FIO2'] / 100)

# Assign SOFA Respiration Subscore (0-4)
df_respiration['SOFA_RESPIRATION'] = pd.cut(
    df_respiration['PAO2_FIO2_RATIO'],
    bins=[0, 100, 200, 300, 400, float('inf')],
    labels=[4, 3, 2, 1, 0],
    right=False
)

df_respiration.head(2)
```

[26]:
```
   SUBJECT_ID  HADM_ID  ICUSTAY_ID           CHARTTIME  VALUENUM_PAO2  \
0        3482   192399      202786 2152-11-18 20:00:00          106.0
1       12110   105928      212945 2172-03-02 09:00:00          154.0

   VALUENUM_FIO2  PAO2_FIO2_RATIO SOFA_RESPIRATION
0           30.0       353.333333                1
1           50.0       308.000000                1
```

[27]:
```
df_platelets = df_sofa_components[df_sofa_components['ITEMID'] == 828].copy()

df_platelets['SOFA_COAGULATION'] = pd.cut(
    df_platelets['VALUENUM'],
    bins=[0, 20, 50, 100, 150, float('inf')],
    labels=[4, 3, 2, 1, 0],
    right=False
)
df_platelets.head(3)
```

[27]:
```
          ROW_ID  SUBJECT_ID  HADM_ID  ICUSTAY_ID  ITEMID  \
941838  35644178         285   165312      238023     828
942333  35661979         285   165312      238023     828
942532  35667689         285   165312      238023     828

                  CHARTTIME           STORETIME     CGID  VALUE  VALUENUM  \
941838  2152-09-26 01:03:00  2152-09-26 02:08:00  15331.0  181.0     181.0
```

```
942333  2152-10-12 01:42:00  2152-10-12 02:39:00  15331.0  260.0     260.0
942532  2152-10-18 02:29:00  2152-10-18 03:48:00  15331.0  333.0     333.0

       VALUEUOM  WARNING  ERROR RESULTSTATUS   STOPPED SOFA_COAGULATION
941838      NaN      NaN    NaN        Final  NotStopd                0
942333      NaN      NaN    NaN        Final  NotStopd                0
942532      NaN      NaN    NaN        Final  NotStopd                0
```

[28]:
```
df_bilirubin = df_sofa_components[df_sofa_components['ITEMID'] == 225690].copy()

df_bilirubin['SOFA_LIVER'] = pd.cut(
    df_bilirubin['VALUENUM'],
    bins=[0, 1.2, 2.0, 6.0, 12.0, float('inf')],
    labels=[0, 1, 2, 3, 4],
    right=False
)

df_bilirubin.head(3)
```

[28]:
```
     ROW_ID  SUBJECT_ID  HADM_ID  ICUSTAY_ID  ITEMID            CHARTTIME  \
33   170787        1709   127294      207018  225690  2118-01-04 12:45:00
269  171808        1709   127294      207018  225690  2118-01-06 04:50:00
333  171233        1709   127294      207018  225690  2118-01-05 03:08:00

                STORETIME     CGID  VALUE  VALUENUM VALUEUOM  WARNING  ERROR  \
33   2118-01-04 14:39:00  20889.0    1.9       1.9    mg/dL      1.0    0.0
269  2118-01-06 05:27:00  20889.0    2.5       2.5    mg/dL      1.0    0.0
333  2118-01-05 04:03:00  20889.0    2.3       2.3    mg/dL      1.0    0.0

    RESULTSTATUS STOPPED SOFA_LIVER
33           NaN     NaN          1
269          NaN     NaN          2
333          NaN     NaN          2
```

[29]:
```
df_vasopressors = df_sofa_components[df_sofa_components['ITEMID'] == 220052].
  ↪copy()

# Assign SOFA Cardiovascular Subscore
df_vasopressors['SOFA_CARDIOVASCULAR'] = pd.cut(
    df_vasopressors['VALUENUM'],
    bins=[0, 70, float('inf')],
    labels=[1, 0],  # 1 if MAP < 70, else 0
    right=False
)

df_vasopressors['SOFA_CARDIOVASCULAR'].value_counts()
```

[29]:
```
SOFA_CARDIOVASCULAR
0    25909
1     7634
Name: count, dtype: int64
```

[30]:
```
df_gcs = df_sofa_components[df_sofa_components['ITEMID'] == 198].copy()

df_gcs['SOFA_CNS'] = pd.cut(
    df_gcs['VALUENUM'],
    bins=[0, 6, 9, 12, 14, 16],
    labels=[4, 3, 2, 1, 0],
    right=False
)
df_gcs.head(2)
```

[30]:

	ROW_ID	SUBJECT_ID	HADM_ID	ICUSTAY_ID	ITEMID	CHARTTIME	STORETIME	CGID	VALUE	VALUENUM	VALUEUOM	WARNING	ERROR	RESULTSTATUS	STOPPED	SOFA_CNS
940886	35647251	285	165312	238023	198	2152-09-28 03:00:00	2152-09-28 05:36:00	14997.0	9.0	9.0	points	NaN	NaN	NaN	NotStopd	2
940923	35654790	285	165312	238023	198	2152-10-04 07:00:00	2152-10-04 06:45:00	17048.0	11.0	11.0	points	NaN	NaN	NaN	NotStopd	2

We aggregate all the SOFA scores into one.

[31]:
```
df_creatinine = df_sofa_components[df_sofa_components['ITEMID'] == 220615].
↪copy()

df_creatinine['SOFA_RENAL'] = pd.cut(
    df_creatinine['VALUENUM'],
    bins=[0, 1.2, 2.0, 3.5, 5.0, float('inf')],
    labels=[0, 1, 2, 3, 4],
    right=False
)

df_creatinine.head()
```

[31]:

	ROW_ID	SUBJECT_ID	HADM_ID	ICUSTAY_ID	ITEMID	CHARTTIME
23	170777	1709	127294	207018	220615	2118-01-04 12:45:00
114	170225	1709	127294	207018	220615	2118-01-03 05:23:00
259	171798	1709	127294	207018	220615	2118-01-06 04:50:00
323	171223	1709	127294	207018	220615	2118-01-05 03:08:00
553	173781	1709	127294	207018	220615	2118-01-10 22:59:00

```
                STORETIME     CGID  VALUE  VALUENUM VALUEUOM  WARNING  ERROR  \
23    2118-01-04 14:39:00  20889.0    7.1       7.1    mg/dL      1.0    0.0
114   2118-01-03 07:01:00  20889.0    6.6       6.6    mg/dL      1.0    0.0
259   2118-01-06 05:27:00  20889.0    4.8       4.8    mg/dL      1.0    0.0
323   2118-01-05 04:03:00  20889.0    6.0       6.0    mg/dL      1.0    0.0
553   2118-01-10 23:55:00  20889.0    6.7       6.7    mg/dL      1.0    0.0

    RESULTSTATUS STOPPED SOFA_RENAL
23           NaN     NaN          4
114          NaN     NaN          4
259          NaN     NaN          3
323          NaN     NaN          4
553          NaN     NaN          4
```

[32]:
```
# Merge all subscores
df_sofa_scores = pd.concat([
    df_respiration[['SUBJECT_ID', 'HADM_ID', 'ICUSTAY_ID', 'SOFA_RESPIRATION']],
    df_platelets[['SUBJECT_ID', 'HADM_ID', 'ICUSTAY_ID', 'SOFA_COAGULATION']],
    df_bilirubin[['SUBJECT_ID', 'HADM_ID', 'ICUSTAY_ID', 'SOFA_LIVER']],
    df_vasopressors[['SUBJECT_ID', 'HADM_ID', 'ICUSTAY_ID',␣
 ↪'SOFA_CARDIOVASCULAR']],
    df_gcs[['SUBJECT_ID', 'HADM_ID', 'ICUSTAY_ID', 'SOFA_CNS']],
    df_creatinine[['SUBJECT_ID', 'HADM_ID', 'ICUSTAY_ID', 'SOFA_RENAL']]
])
df_sofa_scores = df_sofa_scores.fillna(0)
df_sofa_scores.head(2)
```

[32]:
```
   SUBJECT_ID  HADM_ID  ICUSTAY_ID SOFA_RESPIRATION SOFA_COAGULATION  \
0        3482   192399      202786                1                0
1       12110   105928      212945                1                0

  SOFA_LIVER SOFA_CARDIOVASCULAR SOFA_CNS SOFA_RENAL
0          0                   0        0          0
1          0                   0        0          0
```

[33]:
```
# 1. First ensure each component has only one score per ICU stay by taking the␣
 ↪worst (max) score
sofa_components = ['SOFA_RESPIRATION', 'SOFA_COAGULATION', 'SOFA_LIVER',
                   'SOFA_CARDIOVASCULAR', 'SOFA_CNS', 'SOFA_RENAL']

df_sofa_scores_aggregated = df_sofa_scores.groupby(
    ['SUBJECT_ID', 'HADM_ID', 'ICUSTAY_ID']
)[sofa_components].max().reset_index()

# 2. Verify uniqueness
print(f"Before aggregation: {len(df_sofa_scores)} records")
```

```
print(f"After aggregation: {len(df_sofa_scores_aggregated)} unique ICU stays")
print("Duplicate check:", df_sofa_scores_aggregated.
  ↪duplicated(subset=['SUBJECT_ID', 'HADM_ID', 'ICUSTAY_ID']).any())

# 3. Now merge with main data
df_model_full_with_sofa = pd.merge(
    left=model_data_full,
    right=df_sofa_scores_aggregated,
    how='left',
    on=['SUBJECT_ID', 'HADM_ID', 'ICUSTAY_ID'],
    validate='one_to_one'  # This will now pass
)

# 4. Calculate total SOFA (handle missing components as 0)
df_model_full_with_sofa['total_sofa'] =␣
  ↪df_model_full_with_sofa[sofa_components].fillna(0).sum(axis=1)
```

```
Before aggregation: 37829 records
After aggregation: 146 unique ICU stays
Duplicate check: False
```

[34]:
```
df_model_full_with_sofa = df_model_full_with_sofa.drop(columns=sofa_components)
df_model_full_with_sofa.head()
```

[34]:

	SUBJECT_ID	HADM_ID	ICUSTAY_ID	HOSP_TIME	AGE	GENDER	\
0	114	178393	258626	0.000000	48.306639	1	
1	285	165312	238023	0.000000	45.353183	1	
2	605	115545	248569	0.000000	91.400000	0	
3	3482	192399	202786	0.002738	55.577687	1	
4	2090	138877	256557	0.000000	76.605065	1	

	ETH_BLACK/AFRICAN AMERICAN	ETH_HISPANIC OR LATINO	ETH_OTHER	\
0	False	False	False	
1	False	True	False	
2	False	False	False	
3	False	False	False	
4	False	False	False	

	ETH_UNKNOWN/NOT SPECIFIED	…	trend_Phosphorous	\
0	True	…	0.000000	
1	False	…	0.000000	
2	False	…	0.089292	
3	False	…	0.000000	
4	False	…	-0.021077	

	trend_TCO2 (calc) Arterial	trend_SpO2 Desat Limit	trend_Anion gap	\
0	0.000000	0.000000e+00	0.000000	

```
1                    0.000000           0.000000e+00         0.000000
2                   -0.073447          -7.002831e-16         0.137920
3                    0.243856          -5.129622e-02         0.000000
4                   -0.016348           1.739162e-15         0.075682

   trend_Potassium (serum)  trend_HCO3 (serum)  trend_Platelet Count  \
0                 0.000000            0.000000              0.000000
1                 0.000000            0.000000              0.000000
2                -0.124548            0.433000              0.082418
3                 0.000000            0.000000              0.000000
4                -0.031053           -0.258931             -1.545801

   trend_Prothrombin time  trend_INR  total_sofa
0                0.000000   0.000000           0
1                0.000000   0.000000           0
2                0.000000   0.000000           3
3                0.000000   0.000000           0
4                0.055427   0.013857           4

[5 rows x 173 columns]
```

- 160 features, plus the encoded categorical ones, for each entry being too many for such a small number of entries (about 140), careful feature selection is necessary
- The filtering of the features will be performed in three steps (proven useful by iterative experiments):
  1. Filtering out the features with a *variance lower* than 1%
  2. Building a *correlation matrix* on the remaining features and determine the pairs with correlation higher than 0.9
     - Out of these pairs, only one of them is worth keeping, so the other one is dropped
  3. Training a dummy XGBoost model in order to extract the permutation importance of the features
     - Drop the features with a contribution to the RMS less than 1%

4.2.1 Dropping features with less than 1% variance

Said features that do not change are not usefull in our training.

[35]:
```
from sklearn.feature_selection import VarianceThreshold
# only works on numerical features
selector = VarianceThreshold(threshold=0.01)  # drop features with <1% variance

model_data_full = df_model_full_with_sofa.copy()

non_numerical_feature_cols = ['SUBJECT_ID','HADM_ID','ICUSTAY_ID','LOS']

feature_cols = [col for col in model_data_full.columns if col not in␣
 ↪non_numerical_feature_cols]
```

```
features_df = model_data_full[feature_cols]
selector.fit(features_df)

kept_cols = features_df.columns[selector.get_support()]

print(f"Original number of features: {len(feature_cols)}")
print(f"Number of features kept: {len(kept_cols)}")

final_cols_to_keep = non_numerical_feature_cols + kept_cols.tolist()
df_selected = model_data_full[final_cols_to_keep]

print("\nShape of the new DataFrame:", df_selected.shape)
print("\nFirst 5 rows of the new DataFrame with selected features:")
df_selected.head(3)
```

```
Original number of features: 169
Number of features kept: 154

Shape of the new DataFrame: (126, 158)

First 5 rows of the new DataFrame with selected features:
```

[35]:

	SUBJECT_ID	HADM_ID	ICUSTAY_ID	LOS	AGE	GENDER	\
0	114	178393	258626	1.8132	48.306639	1	
1	285	165312	238023	28.6880	45.353183	1	
2	605	115545	248569	16.8598	91.400000	0	

	ETH_BLACK/AFRICAN AMERICAN	ETH_HISPANIC OR LATINO	ETH_OTHER	\
0	False	False	False	
1	False	True	False	
2	False	False	False	

	ETH_UNKNOWN/NOT SPECIFIED	…	trend_Resp Alarm - High	\
0	True	…	0.000000e+00	
1	False	…	0.000000e+00	
2	False	…	-4.747817e-16	

	trend_Arterial Base Excess	trend_BUN	trend_TCO2 (calc) Arterial	\
0	0.000000	0.000000	0.000000	
1	0.000000	0.000000	0.000000	
2	-0.118072	1.967882	-0.073447	

	trend_SpO2 Desat Limit	trend_Anion gap	trend_HCO3 (serum)	\
0	0.000000e+00	0.00000	0.000	
1	0.000000e+00	0.00000	0.000	
2	-7.002831e-16	0.13792	0.433	

```
   trend_Platelet Count  trend_Prothrombin time  total_sofa
0              0.000000                     0.0           0
1              0.000000                     0.0           0
2              0.082418                     0.0           3

[3 rows x 158 columns]
```

[36]:
```
dropped_cols_mask = ~selector.get_support()
dropped_cols = features_df.columns[dropped_cols_mask]
# Dropped columns
print(len(dropped_cols))
dropped_cols
```

```
15
```

[36]:
```
Index(['HOSP_TIME', 'std_PH (Arterial)', 'range_PH (Arterial)',
       'trend_Hemoglobin', 'trend_O2 saturation pulseoxymetry',
       'trend_Creatinine', 'trend_Magnesium',
       'trend_O2 Saturation Pulseoxymetry Alarm - High',
       'trend_O2 Saturation Pulseoxymetry Alarm - Low', 'trend_PH (Arterial)',
       'trend_Resp Alarm - Low', 'trend_Calcium non-ionized',
       'trend_Phosphorous', 'trend_Potassium (serum)', 'trend_INR'],
      dtype='object')
```

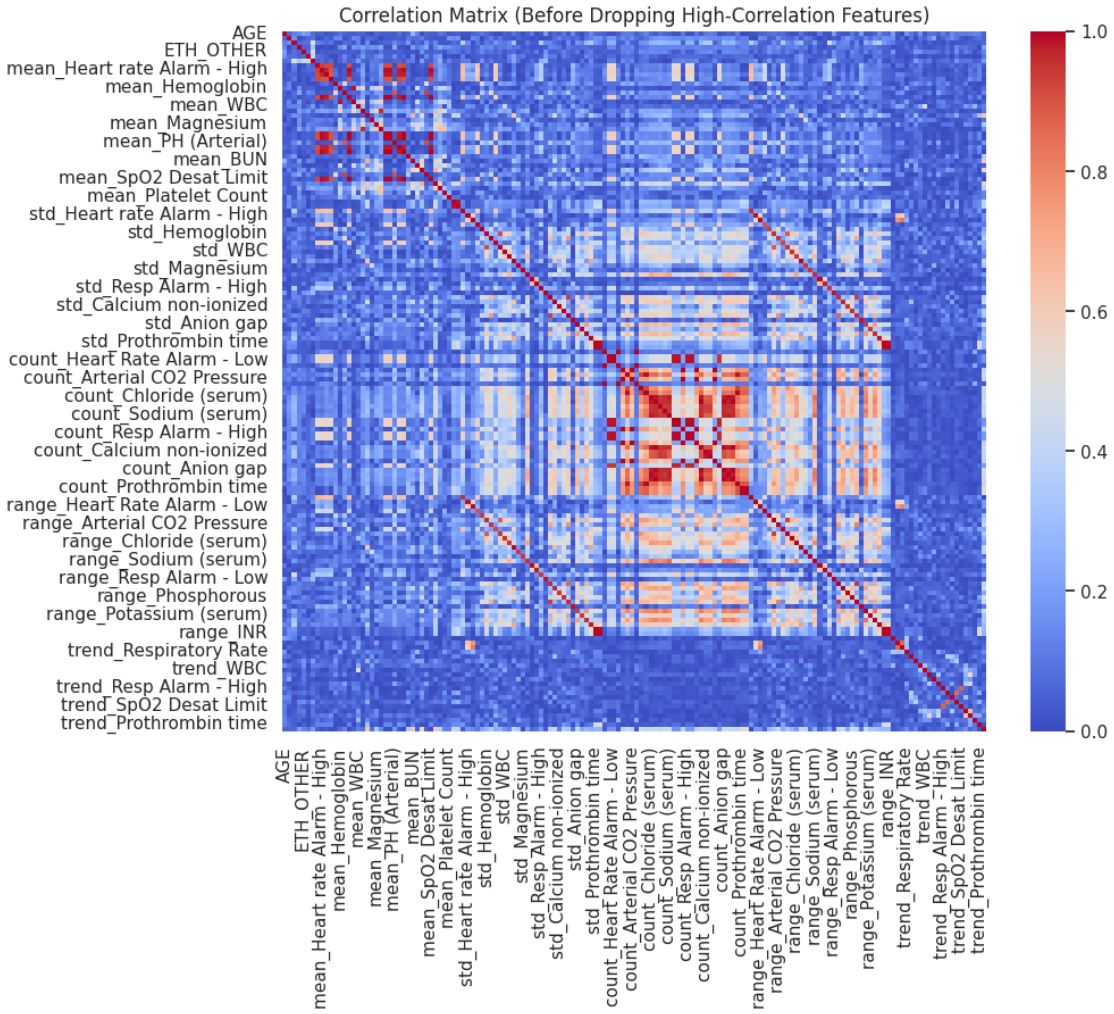
Droppin features with very low variance results in dropping **15 features**.

4.2.2 Dropping highly correlated features

By dropping highly correlated features, we keep item value importance and greatly decrease multicollinearity.

[37]:
```
X = df_selected.drop(columns=non_numerical_feature_cols)

corr_matrix = X.corr().abs()

print("Generating heatmap for features before correlation-based removal...")

plt.figure(figsize=(10, 8))
sns.heatmap(corr_matrix, cmap='coolwarm', annot=False)
plt.title('Correlation Matrix (Before Dropping High-Correlation Features)')
plt.show()
```

```
Generating heatmap for features before correlation-based removal…
```



[38]:
```
df_selected.columns
```

[38]:
```
Index(['SUBJECT_ID', 'HADM_ID', 'ICUSTAY_ID', 'LOS', 'AGE', 'GENDER',
       'ETH_BLACK/AFRICAN AMERICAN', 'ETH_HISPANIC OR LATINO', 'ETH_OTHER',
       'ETH_UNKNOWN/NOT SPECIFIED',
       …
       'trend_Resp Alarm - High', 'trend_Arterial Base Excess', 'trend_BUN',
       'trend_TCO2 (calc) Arterial', 'trend_SpO2 Desat Limit',
       'trend_Anion gap', 'trend_HCO3 (serum)', 'trend_Platelet Count',
       'trend_Prothrombin time', 'total_sofa'],
      dtype='object', length=158)
```

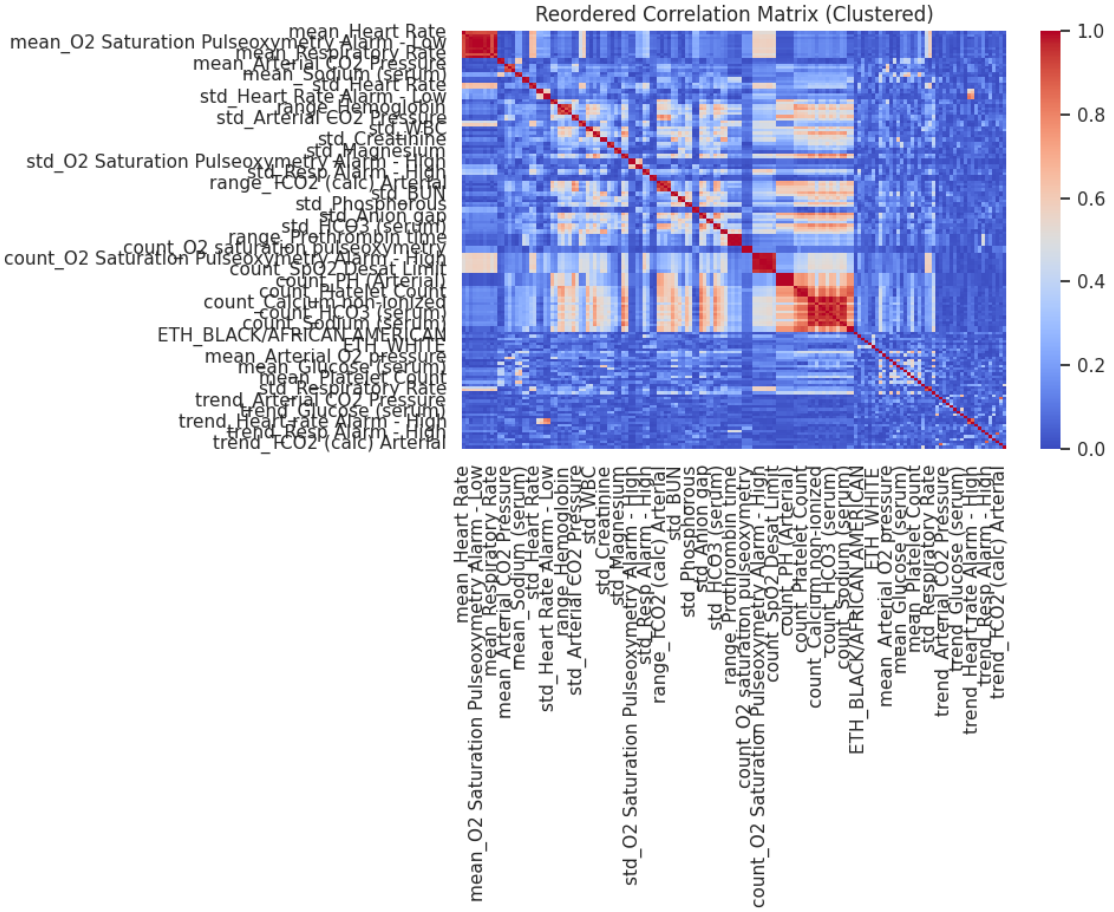
We tried to debug the correlation matrix because we thought it would eliminate way too many features. But, it turns out clusters are bigger than 2, so for example in a cluster of 10, we eliminate 9 features resulting in only 1 remaining.

[39]:
```
import networkx as nx

upper = corr_matrix.where(np.triu(np.ones(corr_matrix.shape), k=1).astype(bool))

# Step 3: Extract highly correlated feature pairs (threshold > 0.9)
high_corr_pairs = upper.stack()[upper.stack() > 0.9]

print(f"Number of high-correlation feature pairs (corr > 0.9):␣
 ↪{len(high_corr_pairs)}")

df_reduced = df_selected.drop(columns=['HADM_ID', 'ICUSTAY_ID', 'LOS',␣
 ↪'SUBJECT_ID'])

# Step 4: Build graph and find connected components (clusters)
G = nx.Graph()
G.add_edges_from(high_corr_pairs.index.tolist())

clusters = list(nx.connected_components(G))

print(f"Number of correlated feature clusters: {len(clusters)}")

# Step 5: Debug cluster sizes
for i, group in enumerate(clusters):
    print(f"Cluster {i+1}: size = {len(group)} → dropping {len(group) - 1}")

# Step 6: Compute features to drop (keep first in each group)
to_drop_groups = [list(group)[1:] for group in clusters if len(group) > 1]
to_drop = [item for sublist in to_drop_groups for item in sublist]

print(f"Total number of features to drop: {len(to_drop)}")
print("Features being dropped:", to_drop)

# Step 7: Drop the features
df_reduced = df_reduced.drop(columns=to_drop)

# Step 8: Reorder features for visual inspection
ordered_features = [feat for group in clusters for feat in sorted(group)]
remaining_features = [f for f in df_reduced.columns if f not in␣
 ↪ordered_features]
ordered_features += sorted(remaining_features)

reordered_corr = corr_matrix.loc[ordered_features, ordered_features]

# Step 9: Plot the reordered correlation matrix
plt.figure(figsize=(10, 8))
sns.heatmap(reordered_corr, cmap='coolwarm', annot=False)
plt.title("Reordered Correlation Matrix (Clustered)")
```

```
plt.tight_layout()
plt.show()
```

```
Number of high-correlation feature pairs (corr > 0.9): 171
Number of correlated feature clusters: 38
Cluster 1: size = 10 → dropping 9
Cluster 2: size = 2 → dropping 1
Cluster 3: size = 3 → dropping 2
Cluster 4: size = 2 → dropping 1
Cluster 5: size = 2 → dropping 1
Cluster 6: size = 2 → dropping 1
Cluster 7: size = 2 → dropping 1
Cluster 8: size = 2 → dropping 1
Cluster 9: size = 2 → dropping 1
Cluster 10: size = 4 → dropping 3
Cluster 11: size = 2 → dropping 1
Cluster 12: size = 2 → dropping 1
Cluster 13: size = 2 → dropping 1
Cluster 14: size = 2 → dropping 1
Cluster 15: size = 2 → dropping 1
Cluster 16: size = 2 → dropping 1
Cluster 17: size = 2 → dropping 1
Cluster 18: size = 2 → dropping 1
Cluster 19: size = 2 → dropping 1
Cluster 20: size = 2 → dropping 1
Cluster 21: size = 2 → dropping 1
Cluster 22: size = 2 → dropping 1
Cluster 23: size = 4 → dropping 3
Cluster 24: size = 2 → dropping 1
Cluster 25: size = 2 → dropping 1
Cluster 26: size = 2 → dropping 1
Cluster 27: size = 2 → dropping 1
Cluster 28: size = 2 → dropping 1
Cluster 29: size = 2 → dropping 1
Cluster 30: size = 2 → dropping 1
Cluster 31: size = 2 → dropping 1
Cluster 32: size = 4 → dropping 3
Cluster 33: size = 3 → dropping 2
Cluster 34: size = 7 → dropping 6
Cluster 35: size = 5 → dropping 4
Cluster 36: size = 4 → dropping 3
Cluster 37: size = 11 → dropping 10
Cluster 38: size = 2 → dropping 1
Total number of features to drop: 73
Features being dropped: ['mean_Resp Alarm - Low', 'mean_SpO2 Desat Limit',
'mean_O2 Saturation Pulseoxymetry Alarm - High', 'mean_O2 Saturation
Pulseoxymetry Alarm - Low', 'mean_O2 saturation pulseoxymetry', 'mean_Heart
```

Rate', 'mean_Heart rate Alarm - High', 'mean_Respiratory Rate', 'mean_Heart Rate Alarm - Low', 'mean_Hematocrit (serum)', 'mean_Arterial CO2 Pressure', 'mean_PH (Arterial)', 'mean_Sodium (serum)', 'mean_Prothrombin time', 'std_Heart Rate', 'std_Heart rate Alarm - High', 'range_Heart Rate Alarm - Low', 'std_Arterial O2 pressure', 'std_Hematocrit (serum)', 'std_Hemoglobin', 'range_Hematocrit (serum)', 'range_Arterial CO2 Pressure', 'range_O2 saturation pulseoxymetry', 'std_WBC', 'range_Chloride (serum)', 'range_Creatinine', 'std_Glucose (serum)', 'range_Magnesium', 'range_Sodium (serum)', 'std_O2 Saturation Pulseoxymetry Alarm - High', 'range_O2 Saturation Pulseoxymetry Alarm - Low', 'range_Resp Alarm - High', 'std_Resp Alarm - Low', 'std_TCO2 (calc) Arterial', 'range_Arterial Base Excess', 'range_TCO2 (calc) Arterial', 'range_BUN', 'std_Calcium non-ionized', 'std_Phosphorous', 'range_SpO2 Desat Limit', 'range_Anion gap', 'std_Potassium (serum)', 'std_HCO3 (serum)', 'range_Platelet Count', 'std_INR', 'range_Prothrombin time', 'std_Prothrombin time', 'count_Heart Rate', 'count_O2 saturation pulseoxymetry', 'count_O2 Saturation Pulseoxymetry Alarm - High', 'count_Resp Alarm - Low', 'count_Heart Rate Alarm - Low', 'count_Resp Alarm - High', 'count_O2 Saturation Pulseoxymetry Alarm - Low', 'count_SpO2 Desat Limit', 'count_Arterial CO2 Pressure', 'count_Arterial O2 pressure', 'count_PH (Arterial)', 'count_TCO2 (calc) Arterial', 'count_Hematocrit (serum)', 'count_Platelet Count', 'count_Hemoglobin', 'count_Anion gap', 'count_Creatinine', 'count_Phosphorous', 'count_Sodium (serum)', 'count_Chloride (serum)', 'count_Magnesium', 'count_BUN', 'count_Potassium (serum)', 'count_Glucose (serum)', 'count_HCO3 (serum)', 'count_INR']



Elimination by correlation, resulting **73 features** eliminated.

[40]:
```
df_final_selected_elimcorr = df_selected.drop(columns=to_drop)
df_final_selected_noelimcorr = df_selected

print(f"\nFinal number of features: {df_final_selected_elimcorr.shape[1] -␣
↪len(non_numerical_feature_cols)}")
print("Shape of the final DataFrame:", df_final_selected_elimcorr.shape)
print("\nFirst 5 rows of the final DataFrame:")
df_final_selected_elimcorr.head(1)
```

```
Final number of features: 81
Shape of the final DataFrame: (126, 85)

First 5 rows of the final DataFrame:
```

[40]:

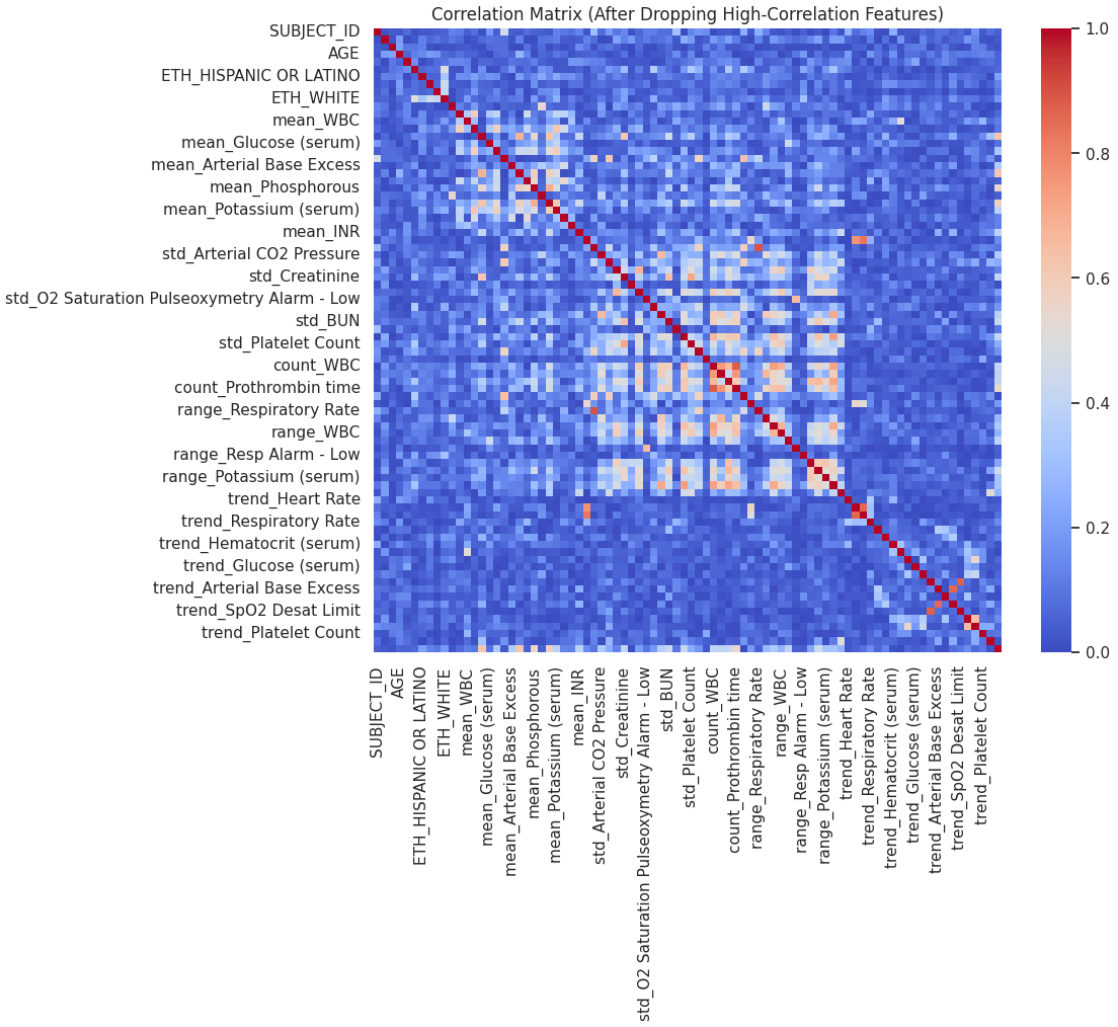
	SUBJECT_ID	HADM_ID	ICUSTAY_ID	LOS	AGE	GENDER	\
0	114	178393	258626	1.8132	48.306639	1	

```
   ETH_BLACK/AFRICAN AMERICAN  ETH_HISPANIC OR LATINO  ETH_OTHER  \
0                       False                   False      False

   ETH_UNKNOWN/NOT SPECIFIED  …  trend_Resp Alarm - High  \
0                       True  …                      0.0

   trend_Arterial Base Excess  trend_BUN  trend_TCO2 (calc) Arterial  \
0                         0.0        0.0                         0.0

   trend_SpO2 Desat Limit  trend_Anion gap  trend_HCO3 (serum)  \
0                     0.0              0.0                 0.0

   trend_Platelet Count  trend_Prothrombin time  total_sofa
0                   0.0                     0.0           0

[1 rows x 85 columns]
```

Steps of eliminating the highly correlated features: - Isolate Features (X): We start with df_variance_selected, the DataFrame that has already been filtered for low variance. We create X which contains only the feature columns from this set. - Correlation Matrix: We compute the correlation matrix for X and take the absolute value, as we're interested in the strength of the correlation, not its direction (positive or negative). - Upper Triangle: The line np.triu(…) creates a mask for the upper triangle of the matrix (everything above the main diagonal). We do this because a correlation matrix is symmetrical (corr(A,B) is the same as corr(B,A)), and we only need to check each pair of features once to avoid redundancy. - Find Columns to Drop: We iterate through the columns of our upper-triangle view. If any value in a column is greater than our threshold (0.9), we add that column's name to our to_drop list. This effectively keeps one feature from each highly correlated pair and flags the other for removal. - Create Final DataFrame: We drop the columns in the to_drop list from df_variance_selected to produce our final, cleaned dataset df_final_selected.

[41]:
```
final_features = df_final_selected_elimcorr.drop(columns='LOS')

# Calculate the new correlation matrix
final_corr_matrix = final_features.corr().abs()

print("\nGenerating heatmap for the final set of features...")

plt.figure(figsize=(10, 8))
sns.heatmap(final_corr_matrix, cmap='coolwarm', annot=False, vmin=0, vmax=1)
plt.title('Correlation Matrix (After Dropping High-Correlation Features)')
plt.show()
```

```
Generating heatmap for the final set of features…
```



4.2.3 Permutation importance

This filter will discard features that contribute less than 1% to the RMSE.

[42]:
```
import pandas as pd
import numpy as np
from sklearn.model_selection import GroupKFold
from sklearn.metrics import mean_squared_error
from sklearn.inspection import permutation_importance
from xgboost import XGBRegressor

def filter_low_importance_features(df, target_column, group_column=None,␣
↪threshold=0.01, n_splits=5, n_repeats=5):
    """
    Filter features based on permutation importance across multiple GroupKFold␣
↪splits.
```

```
    Parameters:
    - df: DataFrame containing features and target
    - target_column: Name of the target column
    - group_column: Name of the column used for grouping (optional)
    - threshold: Minimum relative importance to keep a feature (default: 0.01)
    - n_splits: Number of splits for GroupKFold (default: 5)
    - n_repeats: Number of repeats for permutation importance (default: 5)

    Returns:
    - DataFrame with selected features and target column
    """
    # Prepare data
    y = df[target_column]
    X = df.drop(columns=[target_column, 'HADM_ID', 'SUBJECT_ID', 'ICUSTAY_ID',␣
↪'LOS'])
    groups = df[group_column] if group_column else np.arange(len(df))

    # Initialize model and cross-validator
    model = XGBRegressor(n_estimators=1000, early_stopping_rounds=10,␣
↪eval_metric='rmse', verbosity=0)
    gkf = GroupKFold(n_splits=n_splits)

    # Store importances from all folds
    fold_importances = []

    for train_idx, val_idx in gkf.split(X, y, groups):
        X_train, X_val = X.iloc[train_idx], X.iloc[val_idx]
        y_train, y_val = y.iloc[train_idx], y.iloc[val_idx]

        # Fit model with early stopping
        model.fit(X_train, y_train, eval_set=[(X_val, y_val)], verbose=False)

        # Calculate permutation importance
        result = permutation_importance(
            model, X_val, y_val,
            n_repeats=n_repeats,
            scoring='neg_root_mean_squared_error',
            random_state=42
        )
        fold_importances.append(result.importances_mean)

    # Average importances across all folds
    avg_importances = np.mean(fold_importances, axis=0)
    relative_importances = avg_importances / np.sum(avg_importances)

    # Select features meeting importance threshold
```

```
    important_features = X.columns[relative_importances >= threshold]
    print(f"Retaining {len(important_features)} features out of {X.shape[1]}␣
 ↪with importance  {threshold:.1%}")

    # Return selected features plus target column
    return df[important_features.tolist() + [target_column]]

# Example usage:
df_final_selected = filter_low_importance_features(
    df_final_selected_elimcorr,
    target_column='LOS',
    group_column='SUBJECT_ID',
    threshold=0.01
)
```

```
Retaining 20 features out of 81 with importance  1.0%
```

[43]:
```
df_final_selected.head(3)
```

[43]:

	AGE	ETH_UNKNOWN/NOT SPECIFIED	mean_Arterial O2 pressure	\
0	48.306639	True	0.0	
1	45.353183	False	0.0	
2	91.400000	False	183.0	

	mean_Glucose (serum)	mean_Magnesium	mean_Arterial Base Excess	mean_BUN	\
0	0.0	0.000000	0.0	0.000000	
1	0.0	0.000000	0.0	0.000000	
2	127.5	2.333333	-4.5	54.333333	

	mean_Calcium non-ionized	mean_Phosphorous	mean_TCO2 (calc) Arterial	…	\
0	0.0	0.000000	0.00	…	
1	0.0	0.000000	0.00	…	
2	6.6	1.933333	21.25	…	

	mean_Platelet Count	std_Arterial Base Excess	\
0	0.0	0.000000	
1	0.0	0.000000	
2	179.5	3.109126	

	count_Heart rate Alarm - High	range_Potassium (serum)	range_HCO3 (serum)	\
0	0.0	0.0	0.0	
1	0.0	0.0	0.0	
2	3.0	3.4	7.0	

	trend_Respiratory Rate	trend_Arterial CO2 Pressure	\
0	0.000000	0.000000	
1	0.000000	0.000000	

```
2                0.084494                      0.176256

   trend_SpO2 Desat Limit  total_sofa      LOS
0            0.000000e+00           0   1.8132
1            0.000000e+00           0  28.6880
2           -7.002831e-16           3  16.8598

[3 rows x 21 columns]
```

Permutance importance results in dropping **73 features**.

4.3 Model choice, training and validation

4.3.1 1. Data Preparation

- The test holdout will be 20% out of the total number of entries
  - Although this leaves the model with less training data, a larger test dataset is essential for comprehensive model evaluation
- The model will be trained using 5-fold cross-validation
- It starts by preparing the data. It separates the features (like age and gender) from the target variable (LOS). It also creates a new "interaction" feature by multiplying a patient's age and gender, which can sometimes help the model find more complex patterns. The data is then split into a training set for teaching the model and a test set for evaluating its performance.

[44]:
```
import pandas as pd
import numpy as np
from xgboost import XGBRegressor
from sklearn.model_selection import train_test_split, GridSearchCV, KFold,␣
 ↪cross_val_score
from sklearn.metrics import mean_absolute_error, r2_score, mean_squared_error,␣
 ↪median_absolute_error
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler
import shap
import matplotlib.pyplot as plt
df_perm_selected = df_final_selected.copy()
# 1. Enhanced Data Preparation
def prepare_data(df):
    X = df.drop(columns=['LOS', 'SUBJECT_ID', 'HADM_ID', 'ICUSTAY_ID'],␣
 ↪errors='ignore')
    y = df['LOS']

    # Add interaction terms for top features (example)
    if 'AGE' in X.columns and 'GENDER' in X.columns:
        X['AGE_GENDER_INTERACTION'] = X['AGE'] * X['GENDER']
```

```
    return X, y

X, y = prepare_data(df_perm_selected)
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.2, random_state=42, stratify=pd.qcut(y, q=5)
)
```

4.3.2 2. Model selection

4.3.3 Choosing the appropriate algorithm

- XGBoost (Extreme Gradinent Boosting) is a great fit for this pipeline, having the following advantages:
  - Good handling of tabular data
  - Good performance on moderate-sized data
  - Robustness for missing values and mixed data types (encoded categorical and numerical values)
  - Explainable feature importance for interpretability
  - Very good handling of non-linear relationships
  - Includes regulation for preventing overfitting
- Alternatives considered:
  - Random forests
    - Are simpler but offer less accurate results
    - Filtering of feature importance is already done during the preprocessing part of the pipeline
  - Neural Networks
    - Need much larger ammounts of instances and data, would need to consider a different diagnostic ### Defining the evaluation strategy
- The key metrics that will be tracked to evaluate the performance of the model are:
  - RMSE (Root Mean Squared Error)
    - Penalizes large errors, especially useful in such critical medical cases
    - RMSE chosen instead of MSE for better interpretability by converting the result back to the original units (days)
  - MAE (Mean Absolute Error)
    - Easily interpretable as the average days mispredicted
  - R^2
    - Explains the variance captured by the model
    - Results from 0 increasing to one indicate increasing performance, while results lower than 0 indincate performance worse than predicting the average
- These metrics can be extracted from the five-fold cross-validation training, but more reliably on the test data holdout

4.3.4 3. Model Training and Tuning

4.3.5 Training the model on the training set

- As previously stated, the model will be trained using 5-fold cross-validation
  - This solves the problem of biased results of a single train-test split

  - The cross-validation approach aims to reduce overfitting and variance in the chosen perfomance metrics
  - The data utilization is maximized, every ICU stay being used four times for training and one time for testing
- Grouping ICU stays by patient ids is essential, since one patient can have multiple ICU stays
  - This grouping can prevent data leakage, not allowing ICU stays of patients to be split across training, validation and test data
  - This approach better represents real-world performance ### Hyperparameter tuning
- Grid search is chosen for automating the hyperparameter tuning of the model
  - It works by systematically testing the combinations of predefined hyperparameters in order to find the best performing model
  - Seamlessly integrates the five-fold cross-validation
  - Automatically balances the bias-variance tradeoff
  - Provides explainable results, making the best combination of hyperparameters available for inspection
- The code uses a powerful machine learning algorithm called XGBoost. It sets up a pipeline that first standardizes the data (scaling all features to have a similar range) and then trains the XGBoost model.

- To find the best version of the model, it uses GridSearchCV to automatically test many different combinations of settings (hyperparameters), like the model's depth and learning rate. This process uses cross-validation to ensure the chosen settings are robust and perform well on unseen data.

[45]:
```
# 2. Enhanced Model Training with Pipeline
pipeline = Pipeline([
    ('scaler', StandardScaler()),
    ('xgb', XGBRegressor(random_state=42, early_stopping_rounds=30))
])

params = {
    'xgb__max_depth': [3, 5, 7],
    'xgb__learning_rate': [0.01, 0.05, 0.1],
    'xgb__n_estimators': [100, 200, 300],
    'xgb__subsample': [0.8, 1.0],
    'xgb__colsample_bytree': [0.8, 1.0],
    'xgb__reg_alpha': [0, 0.1, 1],
    'xgb__reg_lambda': [0, 0.1, 1]
}

scaler = StandardScaler()
X_test_scaled = scaler.fit(X_train).transform(X_test)

cv_splitter = KFold(n_splits=5, shuffle=True, random_state=42)

print("Running enhanced GridSearchCV...")
model = GridSearchCV(
    estimator=pipeline,
```

```
    param_grid=params,
    cv=cv_splitter,
    scoring='neg_root_mean_squared_error',
    n_jobs=-1,
    verbose=1
)
model.fit(X_train, y_train, xgb__eval_set=[(X_test_scaled, y_test)],␣
 ↪xgb__verbose=False)
print("GridSearchCV complete.")

from sklearn.base import clone
```

```
Running enhanced GridSearchCV…
Fitting 5 folds for each of 972 candidates, totalling 4860 fits
GridSearchCV complete.
```

4.3.6 4. Model Evaluation

- Once the best model is found and trained, the code thoroughly evaluates its performance. It calculates several key metrics:
- RMSE (Root Mean Squared Error): The typical error in the model's LOS predictions.
- MAE (Mean Absolute Error): The average absolute difference between predicted and actual LOS.
- R^2 (R-squared): How much of the variation in LOS the model can explain.

[53]:
```
# 3. Comprehensive Evaluation
def evaluate_model(model, X, y):
    estimator_for_cv = clone(model.best_estimator_)

    # Disable the early stopping parameter for this specific cross-validation␣
 ↪run
    # The pipeline step is 'xgb', so we use 'xgb__early_stopping_rounds'
    estimator_for_cv.set_params(xgb__early_stopping_rounds=None)


    cv_scores = cross_val_score(estimator_for_cv, X, y,
                                cv=cv_splitter,␣
 ↪scoring='neg_root_mean_squared_error')
    print(f"Cross-validated RMSE: {-cv_scores.mean():.4f} ± {cv_scores.std():.
 ↪4f}")

    predictions = model.predict(X_test)

    metrics = {
        'MAE': mean_absolute_error(y_test, predictions),
        'RMSE': np.sqrt(mean_squared_error(y_test, predictions)),
```

```
        'R2': r2_score(y_test, predictions)
    }

    print("\n--- Final Model Performance ---")
    for name, value in metrics.items():
        print(f"{name}: {value:.4f}")

    # Prediction error plot - not presenting relevant information
    # plt.figure(figsize=(8, 6))
    # plt.scatter(y_test, predictions, alpha=0.3)
    # plt.plot([y.min(), y.max()], [y.min(), y.max()], 'k--')
    # plt.xlabel('True Values')
    # plt.ylabel('Predictions')
    # plt.title('Prediction Error Plot')
    # plt.show()

    return metrics

metrics = evaluate_model(model, X_train, y_train)
```

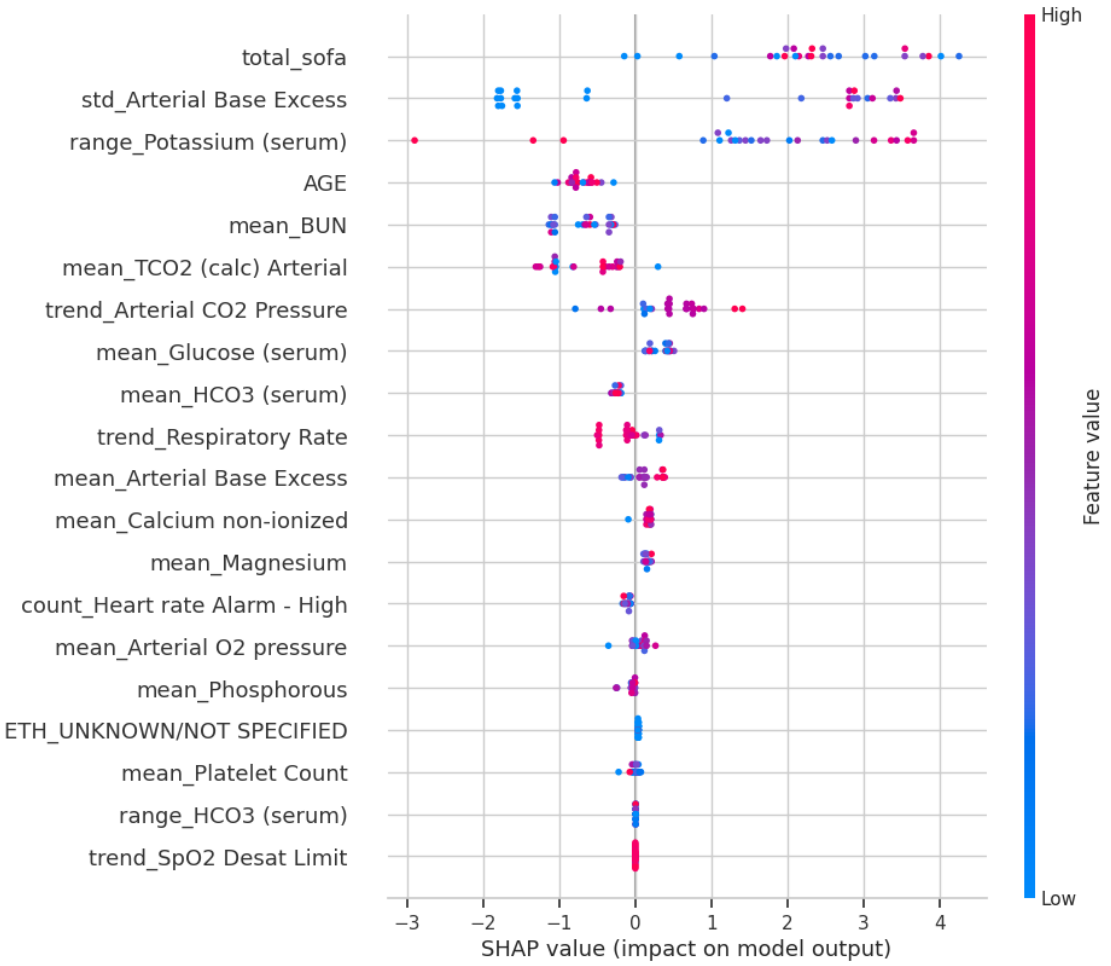
```
Cross-validated RMSE: 7.4830 ± 1.9958

--- Final Model Performance ---
MAE: 5.4606
RMSE: 6.9130
R2: 0.2117
```

4.3.7 5. Model Interpretation with SHAP

- SHAP, LIME
- feature importance
- SHAP (Shape additive explanations) is a very useful tool for explaining how machine learning models make predictions
  - It assigns a feature importance value for a specific predicion, showing how much a feature contributed to the model's output
  - A baseline (expected value) is computed to represent the average prediction of the model over the dataset, SHAP using it to explain how features push the prediction above or below this baseline
  - Positive values indicate a fature increasing the LOS predicion, while negative values indicate decreasing it
  - SHAP can also be used for global interpretability, generatin a bar plot for feature values across all patients
- LIME (Local Interpretable Model-agnostic Explanations) is used to explain only individual predictions
  - approximating the model behaviour with another simpler, interpretabe model (like linear regression or decision rules)
  - It explains individual predictions by creating small variations of the input, querying the model, and fitting the simple interpretable model to approximate the model's behavior

locally.
  - It highlights key features for a specific case using the surrogate model's coefficients.
- Finally, the code uses the SHAP (SHapley Additive Explanations) library to understand why the model makes its predictions. This is a crucial step for model interpretability. It generates a "beeswarm" plot that shows not only which features are most important for predicting LOS but also how the value of each feature (e.g., high vs. low age) impacts the prediction.

[47]:
```
# 4. Enhanced SHAP Analysis
def shap_analysis(model, X, sample_size=500):
    # Use best estimator from GridSearchCV
    best_model = model.best_estimator_.named_steps['xgb']

    # Sample data for faster computation
    if len(X) > sample_size:
        X_sample = X.sample(sample_size, random_state=42)
    else:
        X_sample = X

    # Compute SHAP values
    explainer = shap.Explainer(best_model)
    shap_values = explainer(X_sample)

    shap.plots.beeswarm(shap_values, max_display=20)

    return shap_values

shap_values = shap_analysis(model, X_test)
```



The top features in the XGBoost model for predicting hospital stays are total_sofa (organ failure severity), std_Creatinine (kidney instability), and mean_BUN (kidney/metabolic health). Respiratory issues (count_Resp Alarm - High, trend_Arterial O2 pressure) and heart rate variability (range_Heart Rate) also matter. Key lab values include platelets, bicarbonate, magnesium, and WBCs. The model uses both trends and extreme values to predict longer stays.

a. Single Patient Analysis Firstly, the code randomly selects one specific patient from the test set. It then shows the model's predicted Length of Stay (LOS) for this individual versus their actual, true LOS, providing a clear example of the model's performance on a single case.

[48]:
```
import lime
import lime.lime_tabular
from sklearn.pipeline import Pipeline
import matplotlib.pyplot as plt
import numpy as np

# 1. Prepare the explainer with feature names
```

```
best_model = model.best_estimator_.named_steps['xgb']
explainer_shap = shap.Explainer(best_model, feature_names=X.columns.tolist())

feature_names = X.columns.tolist()

np.random.seed(42)
sample_idx = np.random.choice(X_test.index)
instance = X_test.loc[[sample_idx]]
true_value = y_test.loc[sample_idx]

# Scale the instance using the same scaler
instance_scaled = scaler.transform(instance)

# Make prediction
prediction = best_model.predict(instance_scaled)[0]

print(f"\n=== Analyzing Prediction for Instance #{sample_idx} ===")
print(f"True LOS: {true_value:.2f} days")
print(f"Predicted LOS: {prediction:.2f} days")
print(f"Difference: {abs(prediction-true_value):.2f} days\n")
```

```
=== Analyzing Prediction for Instance #62 ===
True LOS: 9.30 days
Predicted LOS: 6.59 days
Difference: 2.71 days
```

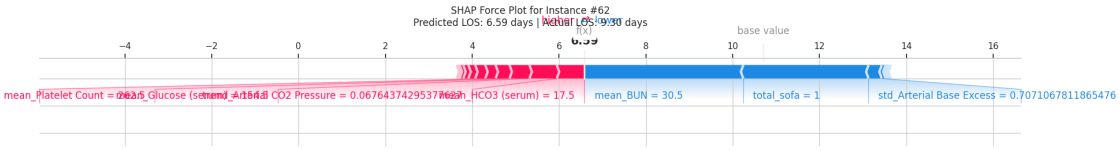
b. Deep Dive with SHAP Using the SHAP library, the code generates detailed explanations for this one prediction:

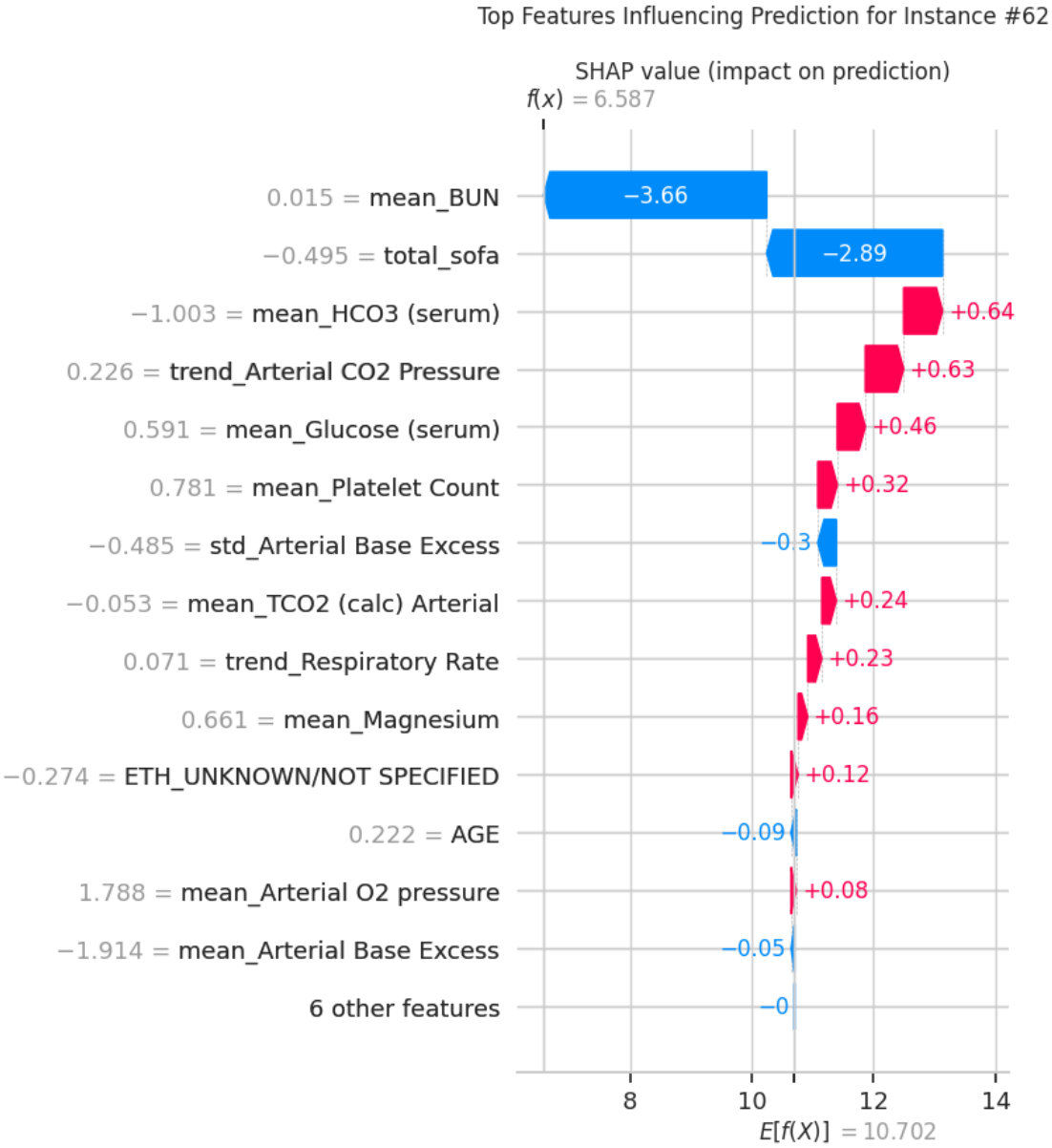
- Force Plot: This visual shows the "push and pull" of each feature. Features in red pushed the prediction higher (increasing the predicted LOS), while features in blue pushed it lower.
- Waterfall Plot: This provides a step-by-step breakdown of how each feature's value moved the prediction from the baseline average to its final output. Detailed List: It prints a ranked list of every feature and its exact impact (the SHAP value) on this one prediction.

[49]:
```
# 2. Generate SHAP values for our instance
shap_values = explainer_shap(instance_scaled)

# 3. Custom force plot with better formatting
plt.figure(figsize=(12, 4))
force_plot = shap.plots.force(
    explainer_shap.expected_value,
    shap_values.values[0],
    instance.values[0],
    feature_names=feature_names,
```

```
    matplotlib=True,
    show=False
)
plt.title(f"SHAP Force Plot for Instance #{sample_idx}\nPredicted LOS:␣
 ↪{prediction:.2f} days | Actual LOS: {true_value:.2f} days",
          pad=20)
plt.tight_layout()
plt.show()

# 4. Enhanced waterfall plot
plt.figure(figsize=(4, 2))
shap.plots.waterfall(
    shap_values[0],
    max_display=15,
    show=False
)
plt.title(f"Top Features Influencing Prediction for Instance #{sample_idx}",␣
 ↪pad=20)
plt.xlabel("SHAP value (impact on prediction)")
plt.tight_layout()
plt.show()

# 5. Print detailed feature impacts
# print("\n=== Detailed Feature Impacts ===")
# print(f"{'Feature':<40} | {'Value':<15} | {'SHAP Effect':<15}")
# print("-" * 75)
# for i in np.argsort(-np.abs(shap_values.values[0])):
#     print(f"{feature_names[i]:<40} | {instance.values[0][i]:<15.3f} |␣
 ↪{shap_values.values[0][i]:<15.3f}")
```

<Figure size 1200x400 with 0 Axes>





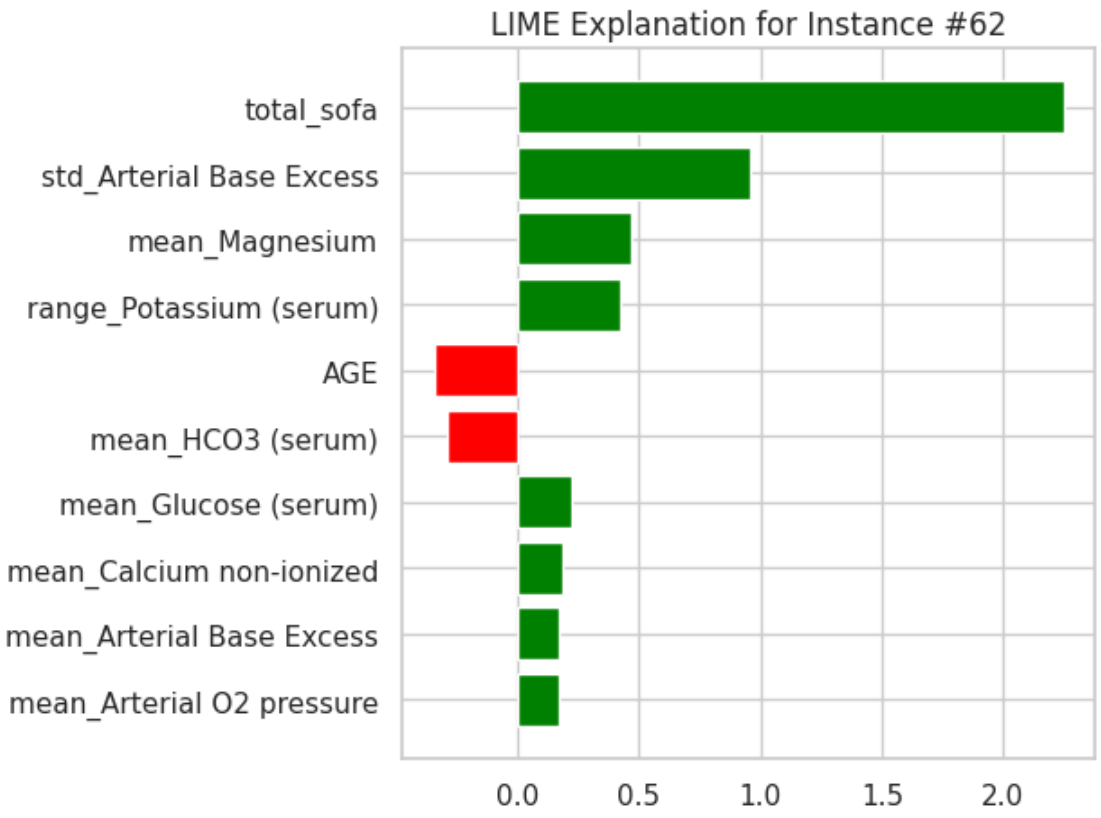
The SHAP force plot shows that the model predicted a hospital stay of 10.81 days for patient #62, while the actual stay was 9.30 days—a slight overestimation. The prediction was influenced most by higher magnesium and arterial CO2 pressure, which increased the forecasted stay, while lower total SOFA and serum HCO3 levels reduced it. BUN had a minor positive effect. The base prediction started around 10.81 days, with SOFA, HCO3, CO2 pressure, and magnesium being the most impactful factors.

c. An Alternative View with LIME Next, the code uses a different explanation library, LIME (Local Interpretable Model-agnostic Explanations), to get a second opinion on the same prediction. LIME works by creating a simpler, temporary model that mimics the behavior of the complex XGBoost model just for this one patient. It then generates a plot showing which features

this simpler model found most important.

[50]:
```
# 4. LIME Explanation
print("\nLIME Explanation:")

# Create LIME explainer (using pre-scaled data)
explainer_lime = lime.lime_tabular.LimeTabularExplainer(
    training_data=scaler.transform(X_train),
    feature_names=feature_names,
    mode='regression',
    discretize_continuous=False
)

# Explain the instance
exp = explainer_lime.explain_instance(
    instance_scaled[0],
    best_model.predict,
    num_features=10
)

# Plot LIME explanation
fig = exp.as_pyplot_figure()
plt.title(f"LIME Explanation for Instance #{sample_idx}")
plt.tight_layout()
plt.show()
```

```
LIME Explanation:
```



The LIME explanation shows which features most influenced the model's prediction for this specific patient (Instance #62). The total SOFA score (measuring organ dysfunction) had the strongest positive impact, suggesting worse organ failure led to a longer predicted hospital stay. Bicarbonate levels and creatinine fluctuations (kidney function) also pushed the prediction higher, while improving oxygen levels reduced the predicted stay.

This breakdown helps clinicians understand why the model predicted a certain length of stay, highlighting critical factors like organ failure and lab trends. If the SOFA score is high, for example, it signals the patient may need closer monitoring.

5 Appendix - Model Optimization Steps

5.1 Further features and hyperparameters tuning

- After completing the initial pipeline, the evaluated performance is poor, indicating the need for further tuning
- The initial pipeline and its performance will be described, followed by noting its measured performance
- Every following tuning of the pipeline will be mentioned, evaluated and labeled as meaningful or not based on the improvement it adds

5.1.1 The initial pipeline

- Features:
  - Patients-related: age, gender, time in the hospital before admission in ICU, ethnicity
  - Events: time-stamped values of items are aggregated into: average, standard deviation, trend, range (max-min), count
    - Data not present replaced with 0
  - Target (ICU stay): log transformed
- Feature selection:
  - first items with most appearances: 32
    - 168 features
  - filter by variance: <1%
    - 153 features left
  - fileter by correlation: >0.9
    - 79 features left
  - filter by contribution to RMSE (permutation imporance): <1%
    - 9 features left
- Cosen model: XGBoost
- Hyperparameters:
  - Grid search:
    - max depth: 3, 5, 7, 10
    - learning rate: .01, .1
    - nr of estimators: 100, 200
    - reg_alpha: .1
- Evaluation on test data:
  - MAE: 9.69 days
  - RMSE: 13.47 days
  - R^2: -0.29

5.1.2 Pipeline modification

- Removing cross-validation and and grid search, default XGBoost parameters
  - Evaluation:
    - MAE: 10.08 days
    - RMSE: 13.73 days
    - R^2: -0.34
  - Verdict: Cross-validation and grid search are helpful
- Removing only grid search
  - Evaluation:
    - MAE: 10.63 days
    - RMSE: 13.09 days
    - R^2: -0.5
  - Verdict: Grid search is helpful
- Removing filtering by contribution to RMSE (permutation importance)
  - Evaluation:
    - MAE: 9.45
    - RMSE: 12.79
    - R^2: -0.16

    - Verdict: Tuning of the treshold for this filter may prove useful
- Eliminate filtering by correlation and permutation importance
    - Evaluation:
        * MAE: 8.6
        * RMSE: 11.74
        * R^2: 0.02
    - Verdict: Correlation proves to be a problem, needs tuning or removal

5.1.3 Pipeline modification after dropping pattients with LOS > 30 days

- Given that 75% of patients stay in the ICU for less than 22 days, removing patients with LOS greater than 30 days seems like a good trade-off
- New results after limiting entries and discarding all feature filters
    - Evaluation:
        * MAE: 5.94
        * RMSE: 6.9
        * R^2: -0.17
    - Verdict: Based on the R^2, promissing gains can be added with filters
- Adding only filtering by variance
    - Evaluation:
        * MAE: 5.90
        * RMSE: 7.04
        * R^2: -0.19
    - Verdict: Same results
- Adding filtering by correlation
    - Evaluation:
        * MAE: 6.28
        * RMSE: 7.21
        * R^2: -0.24
    - Verdict: Filtering by correlation gives worse results
- Adding all filters
    - Remaining with only 7 relevant features
    - Evaluation:
        * MAE: 5.93
        * RMSE: 6.95
        * R^2: -0.16
    - Verdict: **Best version so far**
- Leaving only variance and permutation importance feature filters
    - Remaining with 14 relevant features
    - Evaluation:
        * MAE: 6.05
        * RMSE: 7.07
        * R^2: -0.19
    - Verdict: Filtering by correlation helps XGBoost in permutation importance filtering
- Adding all filters and *imputing missing values with 0*
    - Remaining with only 7 relevant features
    - Evaluation:
        * MAE: 6.20

    - RMSE: 6.90
    - R^2: -0.14
  - Verdict: Worse results, XGBoost works well with missing values

5.1.4 Final Pipeline with Optimized Hyperparameters

- Feature selection:
  - Applied all filters (variance, correlation, permutation importance)
- Final features: 20 most relevant features

-Model: XGBoost with optimized hyperparameters

- Early stopping rounds enabled during training
- Best parameters from grid search
- Evaluation:
  - Cross-validated RMSE: 7.4830 ± 1.9958
- Final test performance:
  - MAE: 5.4606 days
  - RMSE: 6.9130 days
  - R^2: 0.2117
- Verdict:
- Best performing version achieved
  - Significant improvement over initial pipeline (R^2 from -0.29 to +0.21)
  - Cross-validation shows reasonable stability (±2 days RMSE variation)
  - Early stopping helped prevent overfitting while maintaining performance
  - Minimal feature set (20 features) provides good interpretability

This final version represents the optimal balance between performance and complexity, with all optimization steps contributing to the improved results. The positive R^2 value indicates the model now explains some variance in the data, unlike the initial pipeline which performed worse than a simple mean predictor.