ML Assignment 1 Report - Red and Blue

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First Half

Dataset Description

Kaggle Competition Link: Canadian Hospital Re-admittance Challenge | Kaggle

We were provided with a dataset containing records of patients who were admitted to hospitals in Canada. It presents us with demographic as well as diagnostic information for each record corresponding to a visit (encounter).

The aim of the challenge was to predict whether a patient would be *readmitted* within 30 days, after 30 days, or not at all.

Readmission of a patient generally indicates incorrect diagnosis or prescription, resulting in the risk of side effects and wastage of resources for both the hospital and the patient. Predicting readmission can prevent this.

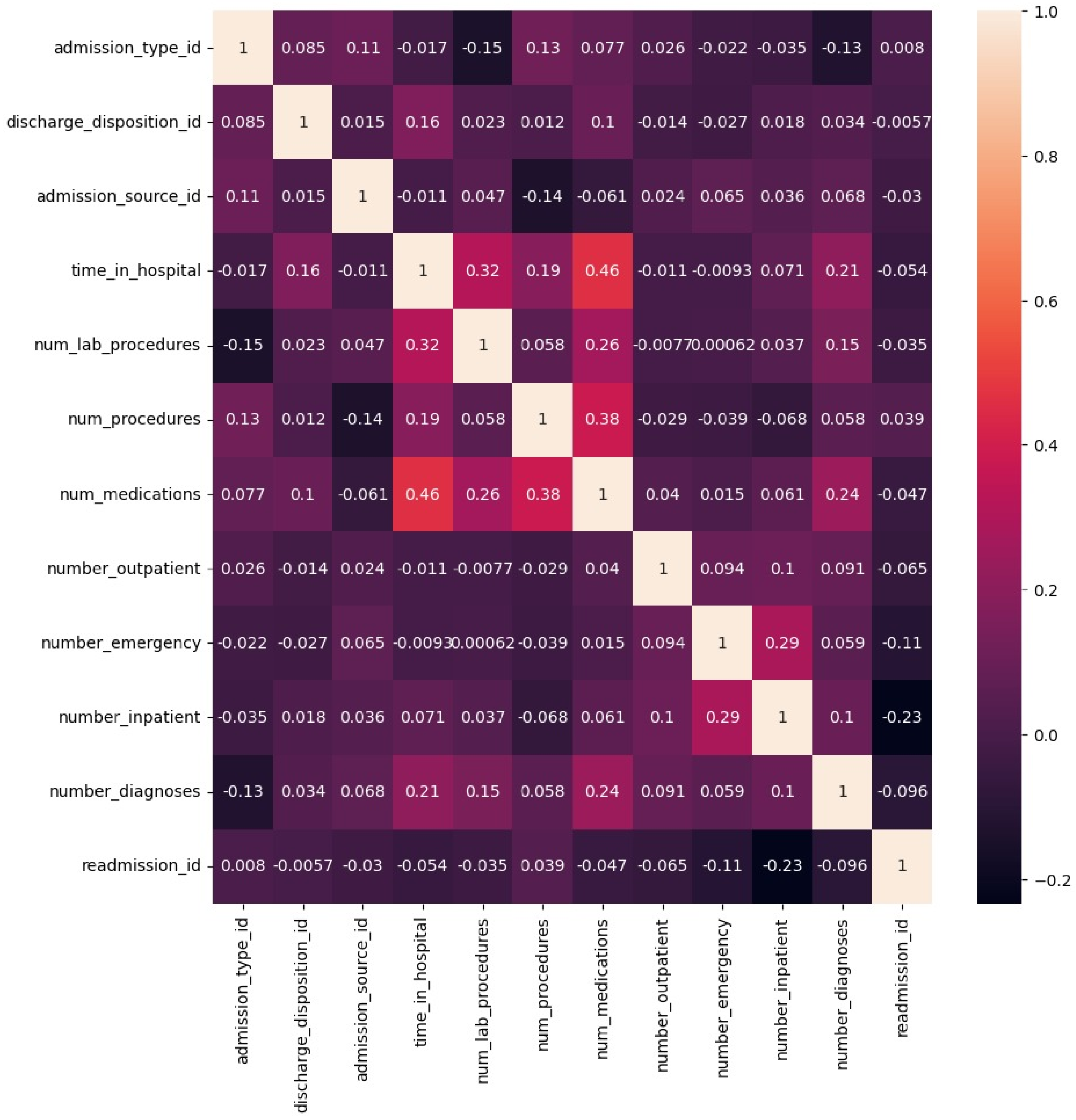
Description of Columns

Column Name	Description
enc_id	Unique identifier of an encounter
patient_id	Unique identifier of a patient
race	Race of the person
gender	Gender of the person
age	Age of the person grouped in 10-year intervals
weight	Weight in pounds
admission_type_id	Integer identifier corresponding to 9 distinct values
discharge_disposition_id	Integer identifier corresponding to 29 distinct values

Column Name	Description
admission_source_id	Integer identifier corresponding to 21 distinct values
time_in_hospital	Integer number of days between admission and discharge
payer_code	Integer identifier corresponding to 23 distinct values
medical_specialty	Integer identifier of a specialty of the admitting physician, corresponding to 84 distinct values
num_lab_procedures	Number of lab tests performed during the encounter
num_procedures	Number of procedures (other than lab tests) performed during the encounter
num_medications	Number of distinct generic names administered during the encounter
number_outpatient	Number of outpatient visits of the patient in the year preceding the encounter
number_emergency	Number of emergency visits of the patient in the year preceding the encounter
number_inpatient	Number of inpatient visits of the patient in the year preceding the encounter
diag_1	The primary diagnosis (coded as first three digits of ICD9)
diag_2	Secondary diagnosis (coded as first three digits of ICD9)
diag_3	Additional secondary diagnosis (coded as first three digits of ICD9)
number_diagnoses	Number of diagnoses entered to the system
max_glu_serum	Indicates the range of the result or if the test was not taken
A1Cresult	Indicates the range of the result or if the test was not taken
Columns corresponding to drug dosage	describe if there was any change in a given drug's dosage for this encounter. `["metformin", "repaglinide", "nateglinide", "chlorpropamide", "glimepiride", "acetohexamide", "glipizide", "glyburide", "tolbutamide", "pioglitazone", "rosiglitazone", "acarbose", "miglitol", "troglitazone", "tolazamide", "examide", "citoglipton", "insulin", "glyburide-metformin", "glipizide-metformin", "glimepiride-pioglitazone", "metformin-rosiglitazone", "metformin-pioglitazone"]`
change	Indicates if there was a change in diabetic medications (either dosage or generic name)
diabetesMed	Indicates if there was any diabetic medication prescribed
readmission_id	Days to inpatient readmission (label)

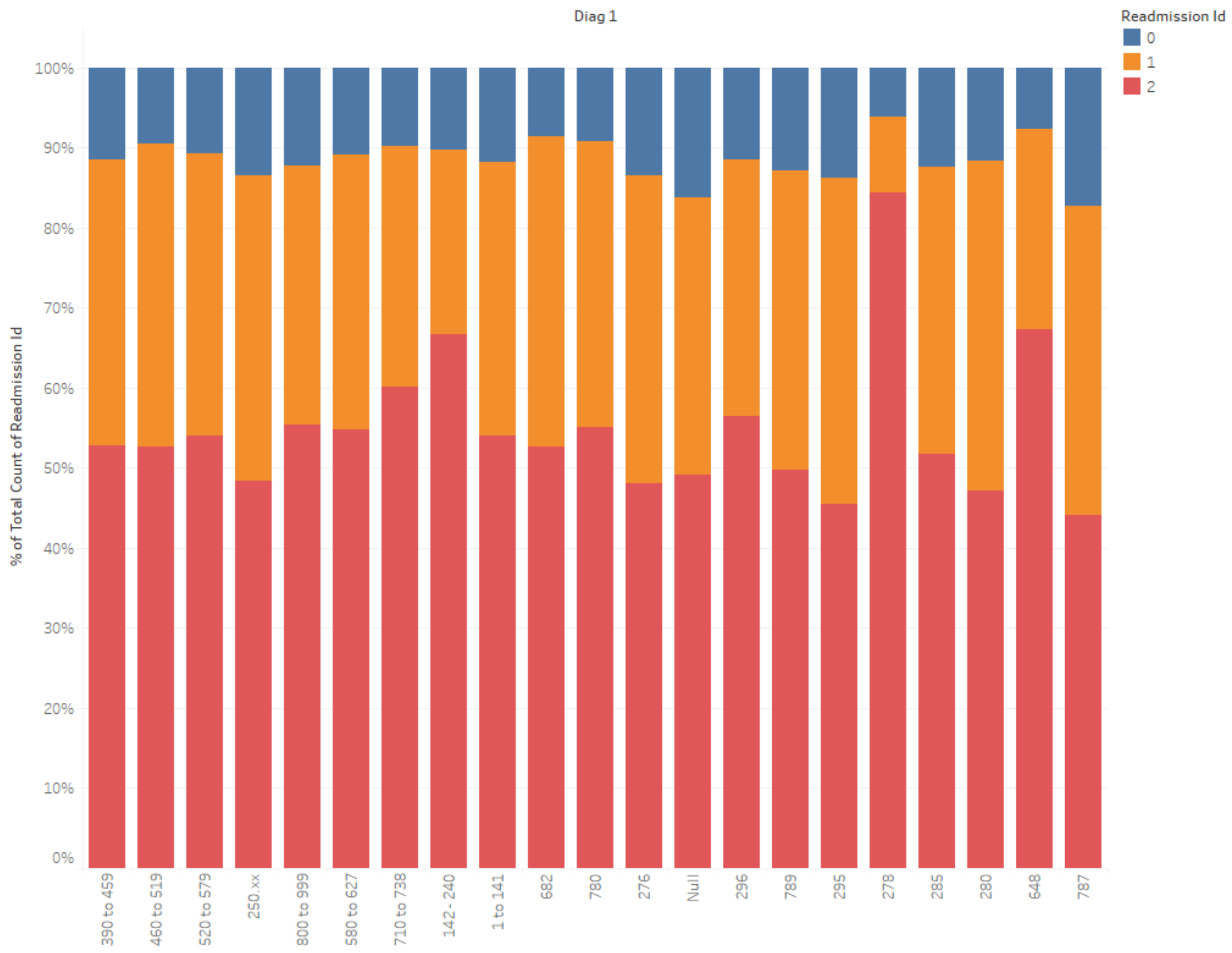
Exploratory Data Analysis

Correlation matrix for numerical columns, and `admission_type_id`, `admission_source_id`, `discharge_disposition_id`, and `readmission_id`.



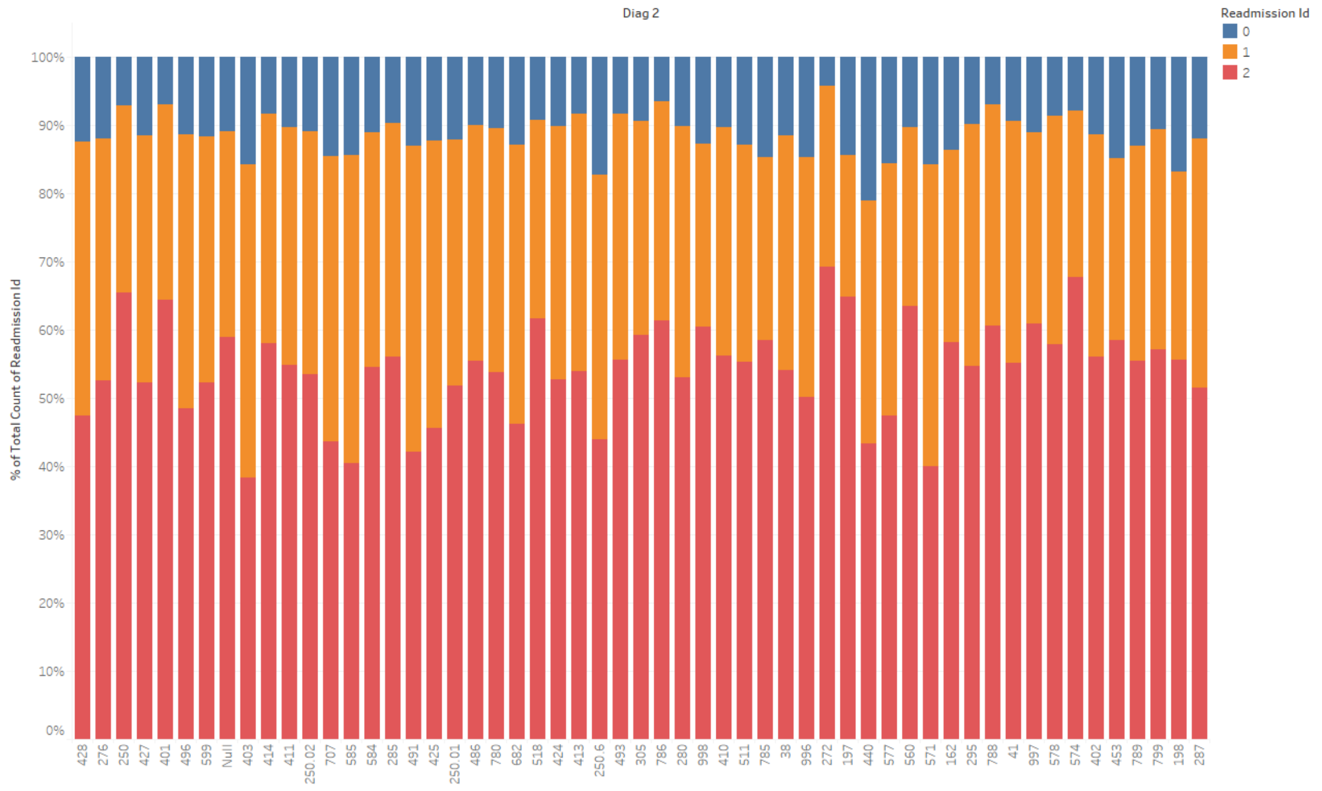
Plots to show how `readmission_id` is distributed across different grouped categories of `diag_1`, `diag_2`, `diag_3`.

Percentage of Readmission IDs in Various Groupings of diag_1



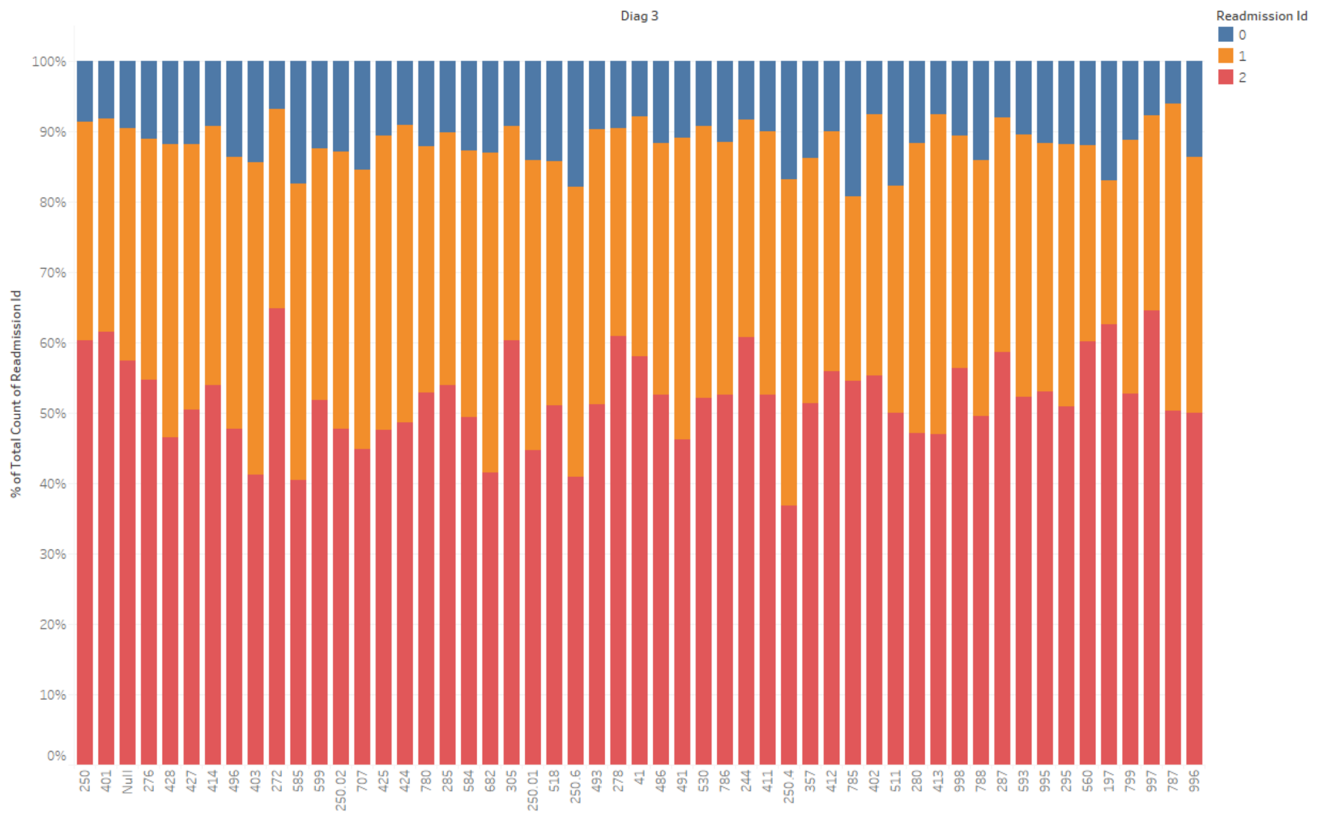
% of Total Count of Readmission Id for each Diag 1. Color shows details about Readmission Id. The view is filtered on Exclusions (Diag 1,Readmission Id), which keeps 63 members. Percents are based on each column of the table.

Percentage of Readmission IDs in Various Groupings of diag_2



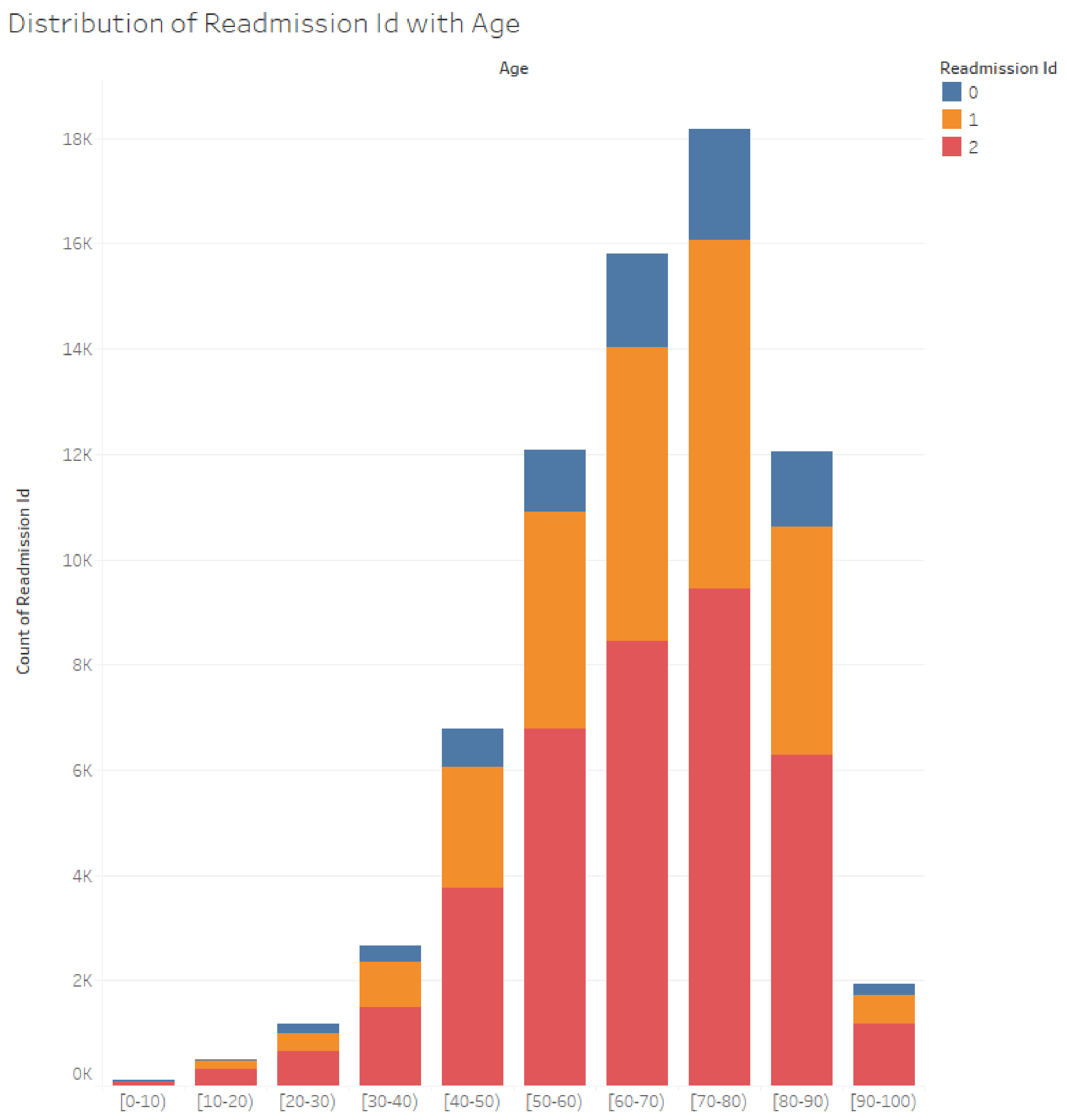
% of Total Count of Readmission Id for each Diag 2. Color shows details about Readmission Id. The data is filtered on Exclusions (Diag 1,Readmission Id), which keeps 63 members. The view is filtered on Exclusions (Diag 2,Readmission Id), which keeps 195 members. Percents are based on each column of the table.

Percentage of Readmission IDs in Various Groupings of diag_3

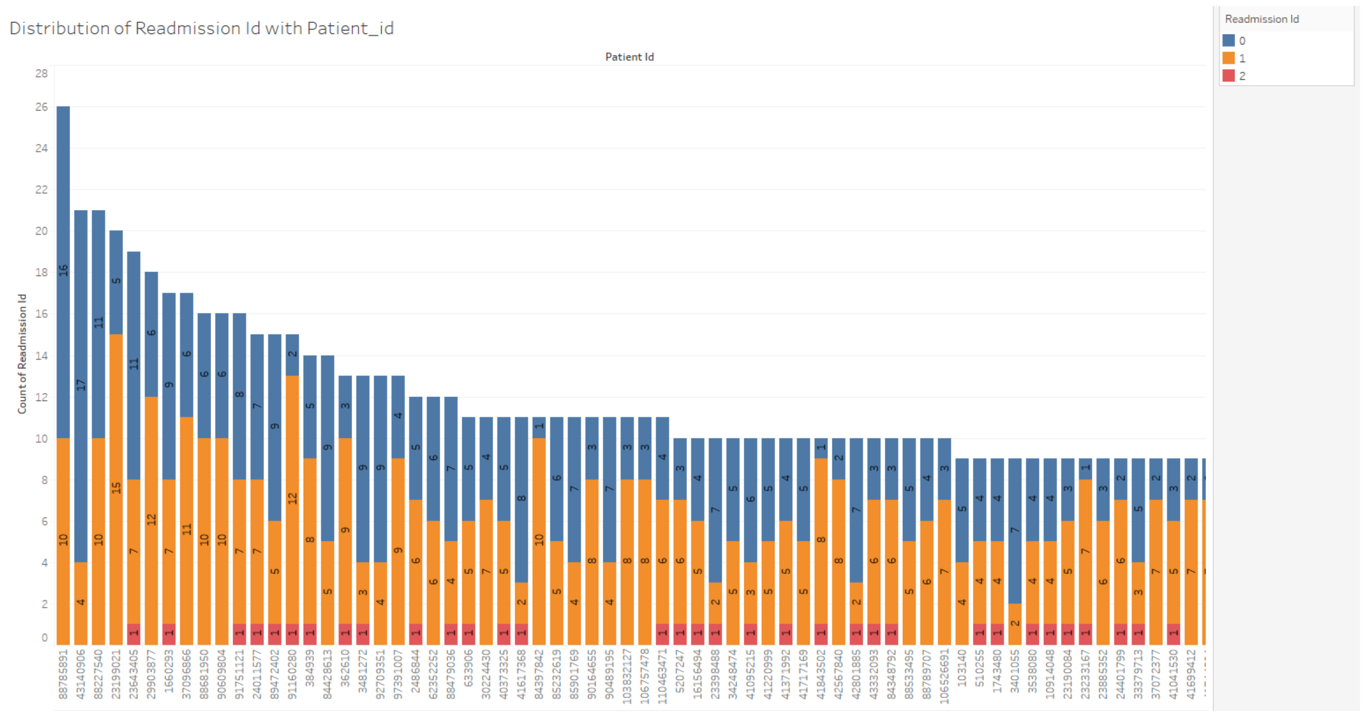


% of Total Count of Readmission Id for each Diag 3. Color shows details about Readmission Id. The data is filtered on Exclusions (Diag 1,Readmission Id) and Exclusions (Diag 2,Readmission Id). The Exclusions (Diag 1,Readmission Id) filter keeps 63 members. The Exclusions (Diag 2,Readmission Id) filter keeps 195 members. The view is filtered on Exclusions (Diag 3,Readmission Id) and Diag 3. The Exclusions (Diag 3,Readmission Id) filter keeps 331 members. The Diag 3 filter excludes 536. Percents are based on each column of the table.

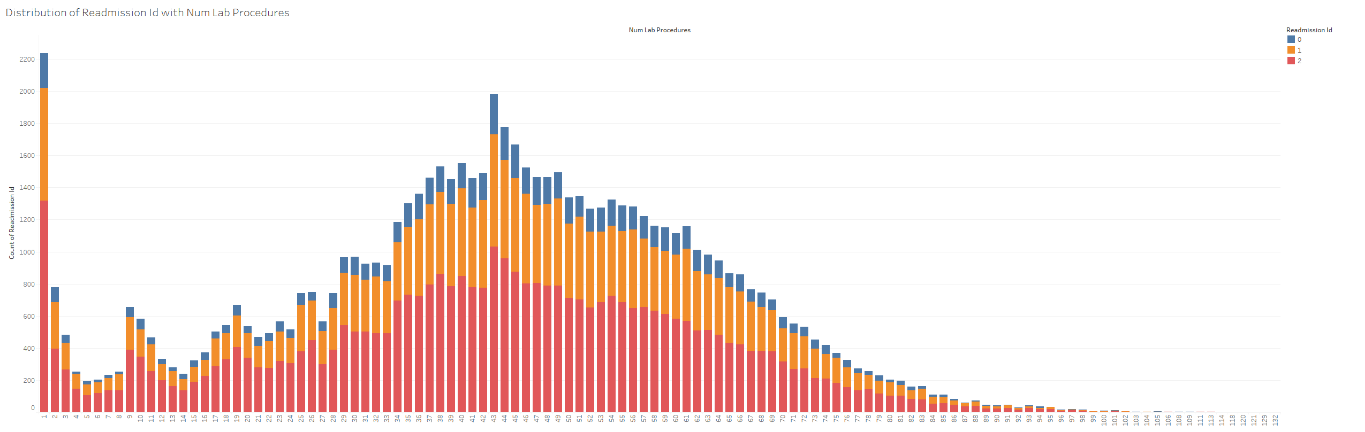
Distribution of `readmission_id` across age



Distribution of `readmission_id` across patient_id

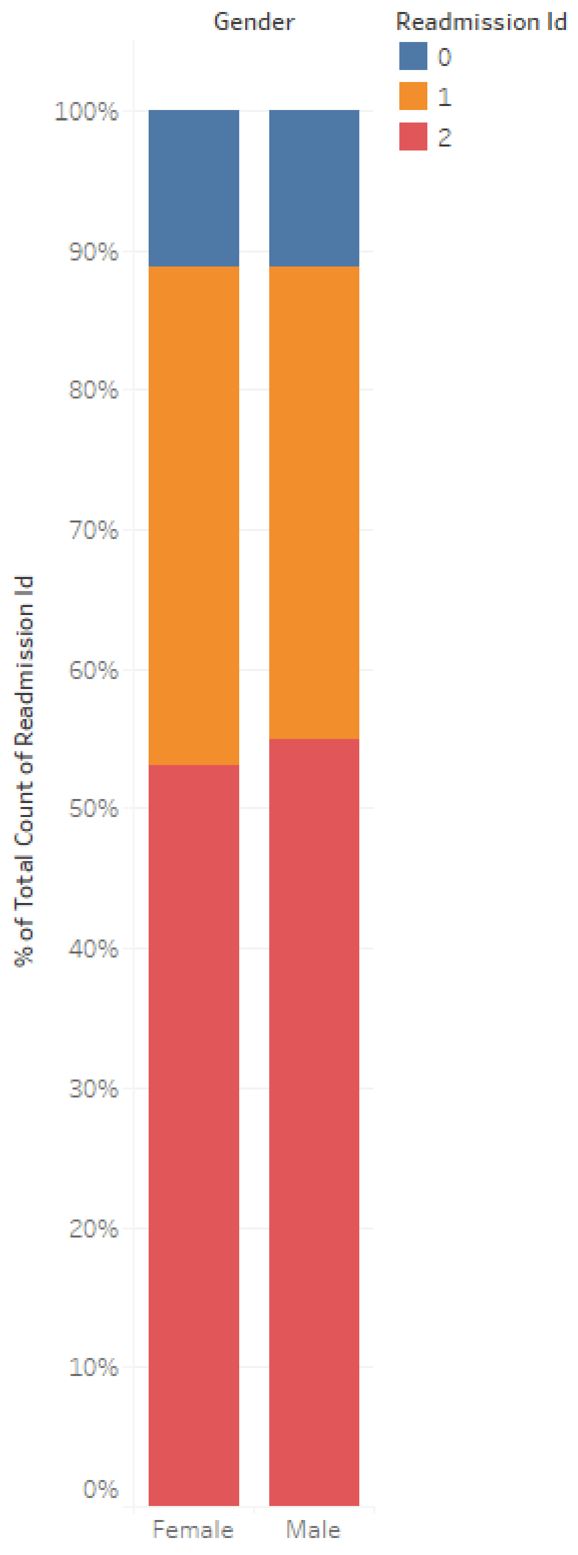


Distribution of `readmission_id` with `num_lab_procedures`



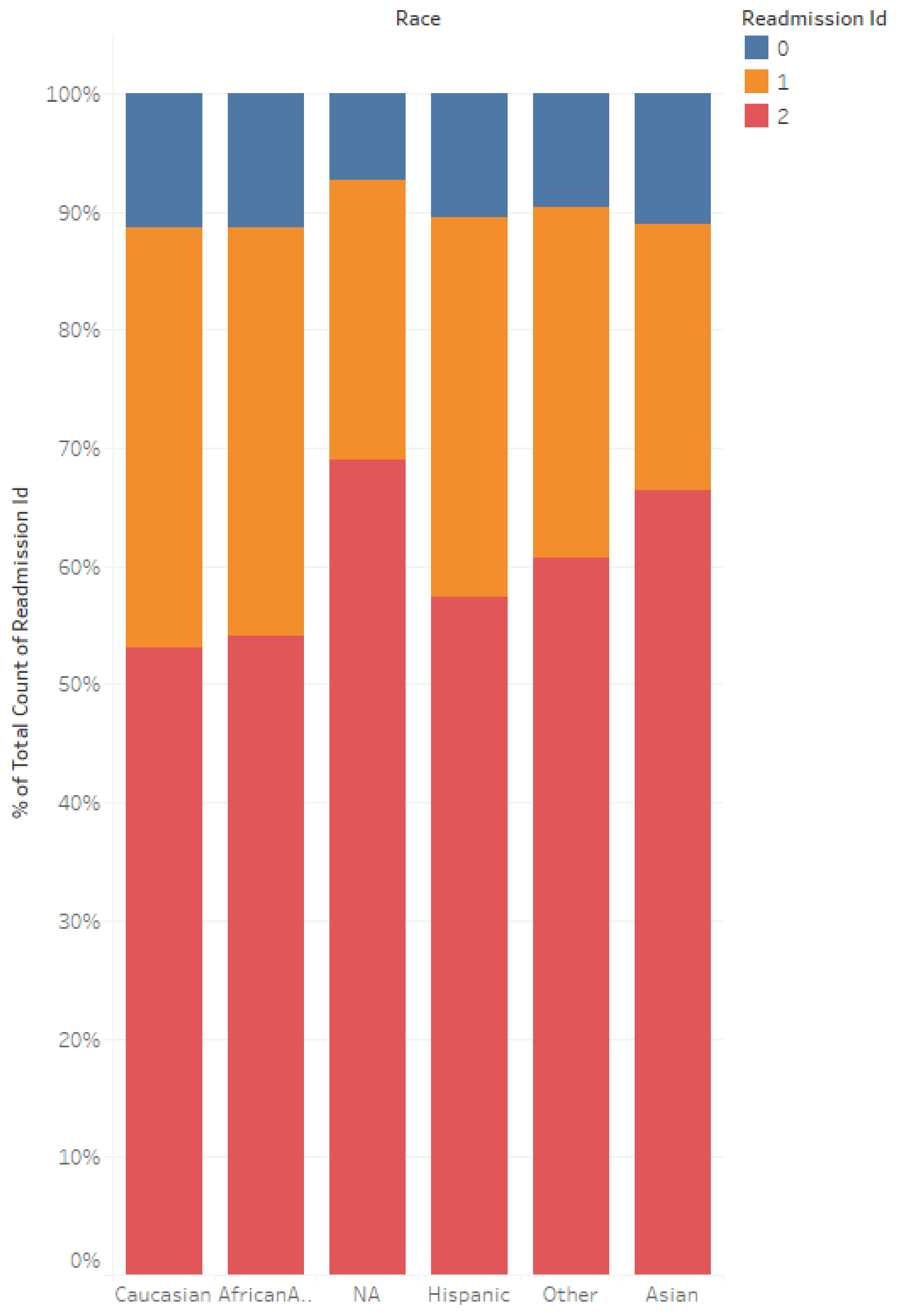
Distribution of `readmission_id` across genders

Gender



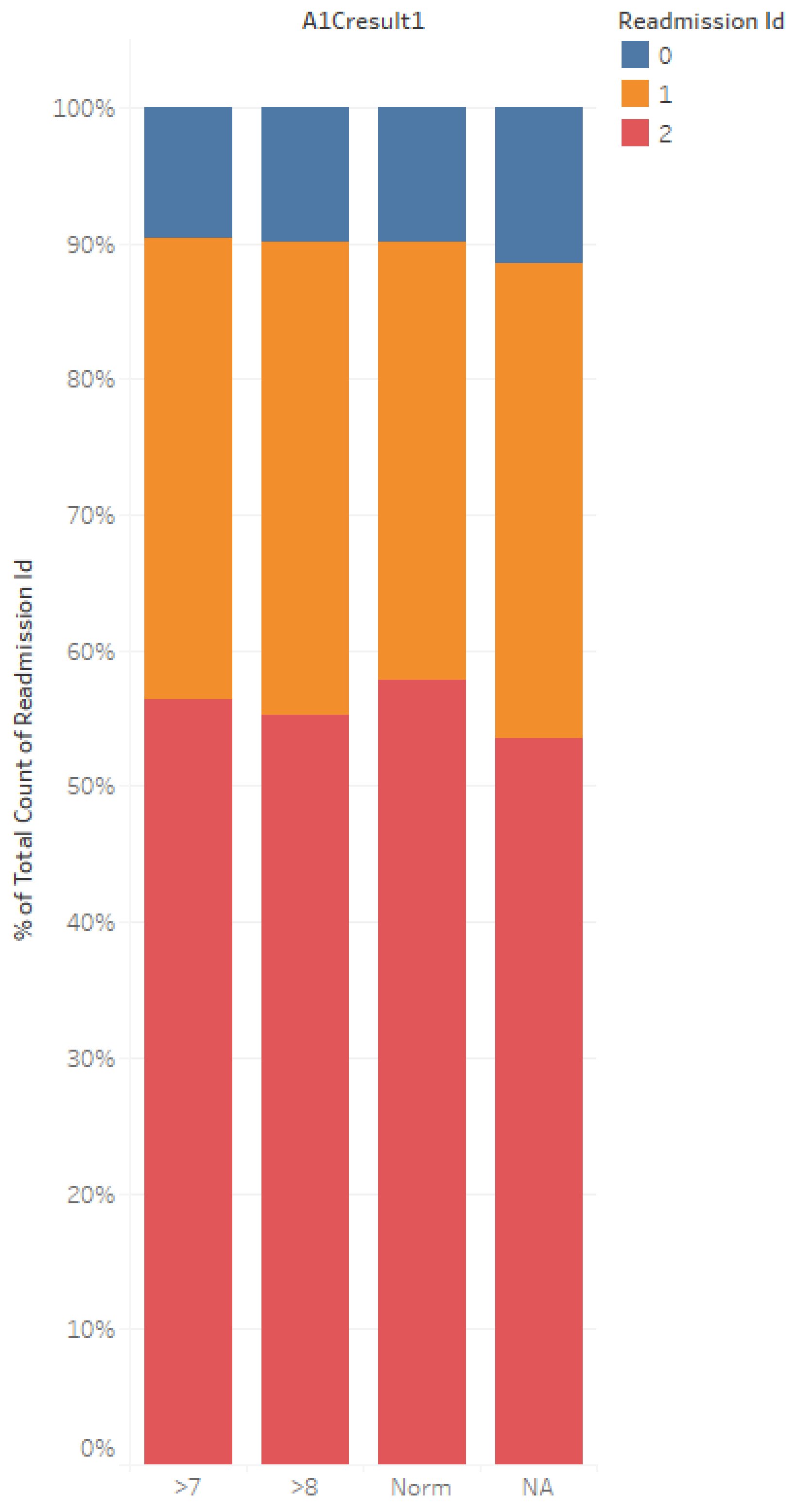
Distribution of `readmission_id` across races

Race

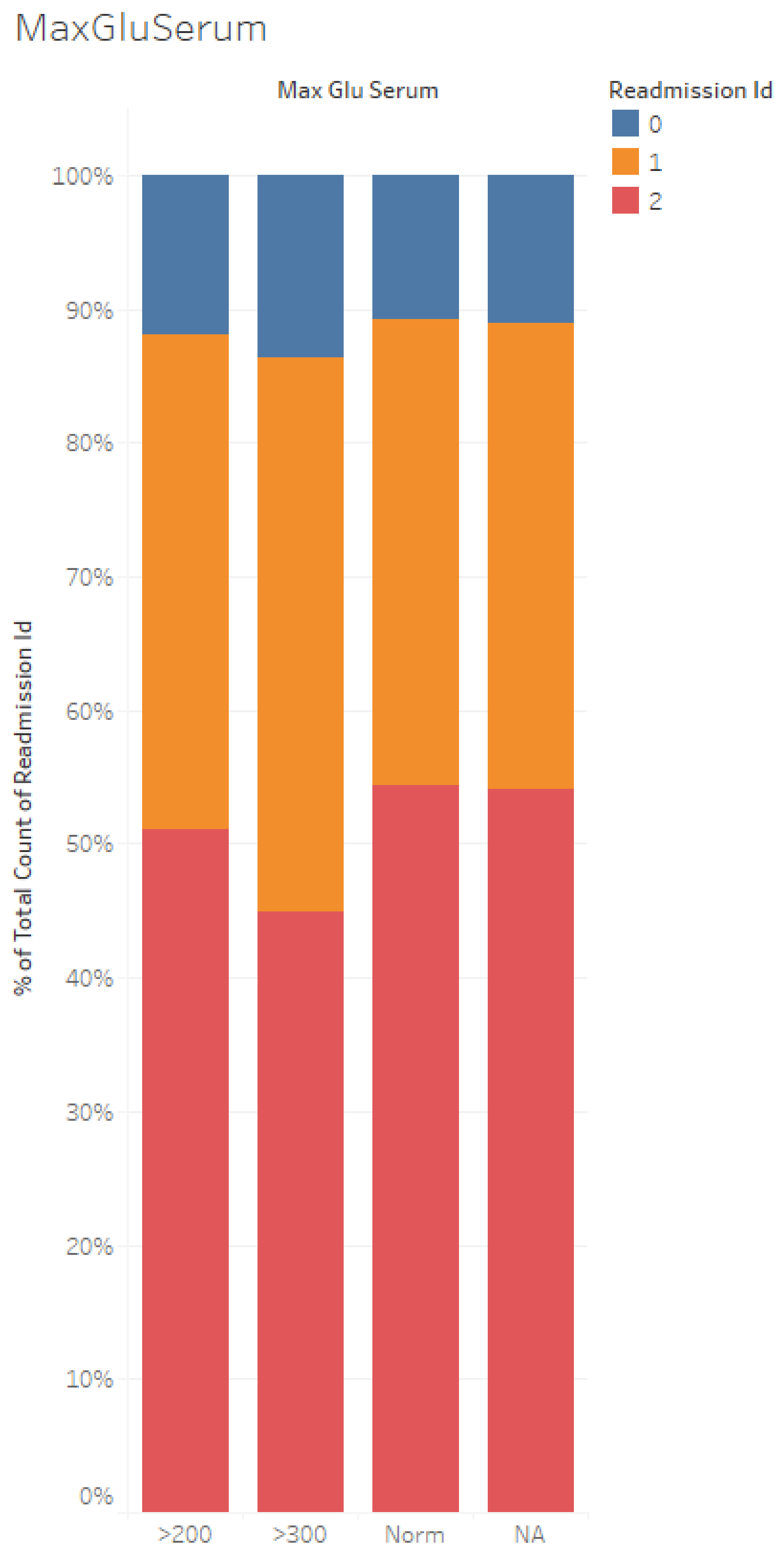


Distribution of `readmission_id` across A1Cresults

A1Cresult



Distribution of `readmission_id` across `max_glu_serum` ranges



- Tools used for plotting were Tableau and Seaborn.

Data Processing

Dropping Columns

Column Dropped	Reason
payer_code	39.55% null values, does not affect readmission of a patient
weight	96.84% null values
max_glu_serum	94.77% null values
A1Cresult	83.32% null values
patient_id	Replaced with a new column to reflect the frequency of patient_id in data
Columns corresponding to drug dosage	Dropped after introducing 4 new columns to reflect the count of *Up*, *Down*, *No*, and *Steady* for each encounter_id
diag_1, diag_2, diag_3	Dropped after experimenting with various sub-groupings of these columns and dropping the rest. No significant improvement was observed in validation score.

Dropping null rows

We initially considered dropping rows corresponding to null values in *race*, *diag_1*, *diag_2*, and *diag_3* as they had *2.27%*, *0.02%*, *0.34%*, and *1.38%* null values respectively. We observed that this did not improve our validation score, when compared with imputing values.

Imputing

For all categorical columns, null values were imputed with a new category, denoted by *"0"*.
For all numerical columns, none of them were observed to have null values.
Prior to this, we experimented by imputing with mode, the validation accuracy decreased slightly, prompting us to rethink our strategy.

Outlier Detection

We tried outlier detection on the numerical columns, ['time_in_hospital', 'num_lab_procedures', 'num_procedures', 'num_medications', 'number_diagnoses']

It was observed that removing these outliers improved the validation score but did not generalize well to unseen data when submitted to Kaggle. We believe this is due to the fact that number of rows in the validation set decreased, leading to a higher validation score.

The definition for upper and lower whiskers is as follows:

```
Q1 = df_copy[attr].quantile(0.25)   # 1st quartile
Q3 = df_copy[attr].quantile(0.75)   # 3rd quartile
IQR = Q3 - Q1                       # Inter-quartile range
lower_whisker = Q1 - 1.5 * IQR
upper_whisker = Q3 + 1.5 * IQR
```

Grouping Columns

Diagnosis Columns (diag_1, diag_2, diag_3)

Grouping Function

```python
def change_diagnosis(value):
    if value >= 1 and value <= 139:
        return "D1"
    elif value <= 239:
        return "D2"
    elif value <= 279:
        return "D3"
    elif value <= 289:
        return "D4"
    elif value <= 319:
        return "D5"
    elif value <= 389:
        return "D6"
    elif value <= 459:
        return "D7"
    elif value <= 519:
        return "D8"
    elif value <= 579:
        return "D9"
    elif value <= 629:
        return "D9"
    elif value <= 679:
        return "D10"
    elif value <= 709:
        return "D11"
    elif value <= 739:
        return "D12"
    elif value <= 759:
        return "D13"
    elif value <= 779:
        return "D14"
    elif value <= 799:
        return "D15"
    elif value <= 999:
        return "D16"
    elif value == 1000:
        return "D17"
    else:
        return "D0"
```

This grouping strategy followed the standard ICD9 Codes. These categorical values were later one-hot encoded. However, it was later noticed that this grouping did not increase the validation score on Kaggle, we decided to drop the 3 columns. This provided a significant boost in terms of training time.

Age variable

In order to deal with the categorical variable `age` which has values like `[0-10)`, `[10-20)` and so on, we tried the following approaches:

- We tried label encoding the variable. Label encoding captures the inherent order of the age categories. The label encoding would assign consecutive numerical values, such as `0` for `[0-10)`, 1 for [10-20), 2 for [20-30), and so on. This maintains the natural order, allowing the algorithm to understand and leverage the ordinal nature of the data.

```
label_encoder = LabelEncoder()
df["age"] = label_encoder.fit_transform(df["age"])
```

- We also tried an average-based approach to convert the column to a numerical variable:

```
def change_age(value):
    if(value == '[0-10)'):
        return 5
    elif(value == '[10-20)'):
        return 15
    elif(value == '[20-30)'):
        return 25
    elif(value == '[30-40)'):
        return 35
    elif(value == '[40-50)'):
        return 45
    elif(value == '[50-60)'):
        return 55
    elif(value == '[60-70)'):
        return 65
    elif(value == '[70-80)'):
        return 75
    elif(value == '[80-90)'):
        return 85
    elif(value == '[90-100)'):
        return 95
```

However we noticed that both these approaches led to a very similar validation score as well as accuracy on Kaggle. Hence, we continued with the Label Encoding approach.

Feature Engineering

Counting Changes in Drug Dosage

The different drugs have 4 possible values: `Up`, `Down`, `Steady`, and `No`.

We decided to introduce 4 new columns, each of which counts the number of Up's, Down's, Steady's and No's for each row across all rows. We then drop all the columns that corresponds to drugs. This was done in order to capture the *change* in these columns, since they were very sparse to begin with (most values were `No`).

```
drugs_cols = ["metformin", "repaglinide", "nateglinide", "chlorpropamide", "glimepiride",
"acetohexamide", "glipizide", "glyburide", "tolbutamide", "pioglitazone", "rosiglitazone",
"acarbose", "miglitol", "troglitazone", "tolazamide", "examide", "citoglipton", "insulin",
"glyburide-metformin", "glipizide-metformin", "glimepiride-pioglitazone", "metformin-
rosiglitazone", "metformin-pioglitazone"]

def count_up(row):
    return sum([1 for col in drugs_cols if row[col] in ['Up']])

def count_down(row):
    return sum([1 for col in drugs_cols if row[col] in ['Down']])

def count_steady(row):
    return sum([1 for col in drugs_cols if row[col] in ['Steady']])

def count_no(row):
    return sum([1 for col in drugs_cols if row[col] in ['No']])

# Apply the function row-wise
df['count_up'] = df.apply(count_up, axis=1)
df['count_down'] = df.apply(count_down, axis=1)
df['count_steady'] = df.apply(count_steady, axis=1)
df['count_no'] = df.apply(count_no, axis=1)
df.drop(drugs_cols, axis=1, inplace=True)
```

Grouping Numerical values for inpatient / outpatient / emergency

For the number_outpatient, number_emergency and number_inpatient, we tried adding the three values and assigning a new column called num_visits.

```
df['num_visits'] = df["number_outpatient"] + df["number_inpatient"] + df["number_emergency"]
df.drop(["number_outpatient", "number_inpatient", "number_emergency"],axis=1, inplace = True)
```

However we noticed that this approach led to a very similar validation score to when the three columns existed individually. Hence, we stuck with the 3 original columns.

Frequency for patient_id

- **Train Data:** We introduced a new column called `f_patient_id` which counts the number of visits for a given patient_id and assigns that number to all rows that corresponds to that patient_id.

```
df['f_patient_id'] = df['patient_id'].copy(deep=True)
cnt_dict = df['patient_id'].value_counts()
for i in df['patient_id']:
    idx = df[df['f_patient_id'] == i].index
    df.loc[idx, 'f_patient_id'] = cnt_dict[i]
df.drop(['patient_id'], axis=1, inplace=True)
```

- **Test Data:** For the test data, in `f_patient_id`, we added the number of visits for that patient_id, from the train and test data and assign it to that column,

```
cnt_dict_1 = test_df['patient_id'].value_counts()
test_df['f_patient_id'] = test_df['patient_id'].copy(deep=True)
for i in test_df['patient_id']:
    idx = test_df[test_df['f_patient_id'] == i].index
    if cnt_dict.get(i) != None and cnt_dict[i] != 0:
        test_df.loc[idx, 'f_patient_id'] = cnt_dict_1[i] + cnt_dict[i]
    else:
        test_df.loc[idx, 'f_patient_id'] = cnt_dict_1[i]
```

Model Selection and Training

Logistic Regression, KNN Classifier, and Decision Tree Classifier

In our initial attempt to train a model, we made use of *logistic regression, KNN classifier, and Decision Tree Classifier*. We observed that logistic regression and KNN classifier returned poor results and the decision tree classifier returned considerably better results. After tweaking the hyper parameters for a while, the team decided to switch to an ensemble method, *Random Forest Classifier*.

Random Forest Classifier

Based on the observations from previous assumptions, we tried using random forest classifier to classify the given data. The results obtained were a significant improvement over decision trees after tuning the hyper parameters, but the accuracy score still seemed below par (about *0.57*). Our next approach was to try various boosting techniques to see if they generalize better.

XGBoost Classifier, CatBoost Classifier

Both models gave significantly better results on the validation set as well as on Kaggle, which were further improved by hyper parameter tuning. The reason they were not chosen as the final model was only due to LGBM Classifier giving slightly better results.

LGBMClassifier - Final Model Used

We finally decided to make use of LGBM classifier from our set of boosting methods. This model with tuned hyper parameters gave the best results on Kaggle, as well as an validation score on par with XGBoost and CatBoost.

2-Model and 3-Model Approaches

Having tried various single model setups , we tried 2 different strategies involving multiple models to improve the prediction accuracy.

The first was creating a 2-model setup. The first model was created to predict whether the `readmission_id` was zero or not. The reason for this choice was that the percentage of records where readmission id was zero is around 10% which is very less. Once a record is classified to have a non-zero `readmission_id`, it is sent to another model which was trained to choose between `readmission_id` 1 or 2. This model was trained only on data which has `readmission_id` 1 or 2. The 2 model setup was an interesting strategy for the problem but the 1 / 2 classifier struggled to classify records correctly, reducing the accuracy of the whole setup. This was the reason why this strategy was dropped.

The 3-model setup trains 3 different models to predict whether a data point has a particular `readmission_id` or not. This way the 3 models predict a particular class with a certain probability. Once the models predict the class with a probability, the `readmission_id` is considered to be the class with maximum probability. This is also a good setup but this idea failed due to the poor accuracy of the classifier for `readmission_id` 1. The class 1 classifier could not find the necessary features to predict class 1 correctly leading to records with `readmission_id` as class 1 to be classified as class 2. This decreased the accuracy of the overall setup *(0.708 on Kaggle)*. Hence we decided to drop both the strategies.

Hyper parameter Tuning

Grid Search and Cross Validation

In an attempt to discover the best hyperparameters for some of the above models, we used the `RandomCV` and `GridSearchCV` cross validation methods. The returned hyper parameter values did improve the validation score slightly, but after carefully considering the tradeoff in training time, we decided to use only select hyper parameter values.

RandomCV

```
from sklearn.model_selection import RandomizedSearchCV
# Create the random grid
random_grid = {'n_estimators': [int(x) for x in np.linspace(start = 200, stop = 2000, num =
10)],
                'max_features': ['log2', 'sqrt', 'none'],
                'max_depth': [int(x) for x in range(1, 13)],
                'min_samples_split': [x for x in range(2, 100, 5)],
                'min_samples_leaf': [x for x in range(3, 15)],
                'bootstrap': [True, False],
                'criterion': ['gini', 'entropy', 'log_loss'],
                'oob_score': [True, False],
                'class_weight': ['balanced', 'balanced_subsample']}

# Use the random grid to search for best hyperparameters
# First create the base model to tune
rf = RandomForestClassifier()
# Random search of parameters, using 3 fold cross validation,
# search across 100 different combinations, and use all available cores
rf_random = RandomizedSearchCV(estimator = rf, param_distributions = random_grid, n_iter = 100,
cv = 3, verbose=2, random_state=0, n_jobs = -1, scoring='accuracy')
# Fit the random search model
rf_random.fit(X_train, Y_train)
print(rf_random.best_params_)
```

GridSearchCV

```
from sklearn.model_selection import GridSearchCV
# Create the parameter grid based on the results of random search
param_grid = {
    'bootstrap': [True],
    'max_depth': [80, 90, 100, 110],
    'max_features': [2, 3],
    'min_samples_leaf': [3, 4, 5],
    'min_samples_split': [8, 10, 12],
    'n_estimators': [100, 200, 300, 1000]
}
# Create a based model
rf = RandomForestClassifier()
# Instantiate the grid search model
grid_search = GridSearchCV(estimator = rf, param_grid = param_grid, cv=3, n_jobs=-1, verbose =
2)

# # Fit the grid search to the data
# grid_search.fit(X_train, Y_train)
print(grid_search.best_params_)
best_grid = grid_search.best_estimator_
```

Validation

In addition to using Grid Search cross validation as described above, we used `accuracy_score` and `f1_score` metrics to gauge the performance of our model.
We also made use of `confusion_matrix` to understand which classes were being wrongly classified, and made strides to improve predictions based on these insights.
Lastly, for some of the models described earlier, we also made use of the `predict_proba` method to interpret the predicted probabilities of each class, for each test point.

Final Results

Model	Result on Kaggle	Approach
KNN Classifier	0.528	-
Random Forest Classifier	0.564	One-Hot Encoding after grouping diags
Random Forest Classifier	0.566	One-Hot Encoding after grouping diags, admission_source_id, admission_type_id, discharge_disposition_id
Random Forest Classifier	0.574	Hyper Parameter Tuning
Random Forest Classifier	0.576	Dropping select drug dosage columns where majority of values belong to one category
Random Forest Classifier	0.578	Added outlier detection
XGB Classifier	0.584	Dropped all diags, no groupings for ids

XGB Classifier	0.598	Keep enc_id, patient_id
LGBM Classifier	0.604	Switched to LGBM classifier
LGBM Classifier	0.609	Hyper Parameter Tuning
LGBM Classifier	0.608	Hyper Parameter Tuning
LGBM Classifier	0.637	Use frequency of patient_id as a column
LGBM Classifier	0.643	Hyper Parameter Tuning
LGBM Classifier	0.648	test_patient_id_freq = train_patient_freq
LGBM Classifier	0.721	test_patient_id_freq = train_patient_freq + test_patient_freq. Count Up, Down, No, and Steady separately in drug dosage columns
LGBM Classifier	0.725	Hyper Parameter Tuning

Best Accuracy with 3-model approach: 0.708 on Kaggle.
Best Accuracy (Overall) = *0.725 on Kaggle*

Second Half

In this section of the assignment, we employed both the SVM model and Artificial Neural Networks in an attempt to enhance the accuracy of predicting the Readmission ID. Employing the established preprocessing methods, we noted that while the accuracy of the SVM model and the Neural Network model approached that of the ensemble models, the LGBM classifier consistently demonstrated superior accuracy in predicting the patient's readmission ID.

Artificial Neural Networks

Details For Preprocessing and Feature Engineering

Initially, we went ahead with the same preprocessing and feature engineering done for the first half of the project, but soon realized that it was cumbersome to improve the accuracy (on Kaggle) beyond 56%.

We felt that due to the nature of hidden layers, it might be best to reduce our processing to a minimal level, and let the network itself learn the relationships between different features.

With that in mind, we started with a clean train.csv file (the one provided as part of the assignment) and:

- Engineered a new column to store the frequencies of patient ids (similar to the first half).
- Categorical columns were one-hot encoded.
- Missing values in numerical columns were imputed using the `mean` strategy.
- patient_id and enc_id were dropped.

Subsequently, an Artificial Neural Network was constructed to forecast the readmission ID. Given the nature of the problem as a Multi-class classification one, our strategy involved crafting a Neural Network equipped with a cross-entropy loss function, alongside ReLU and Softmax Activation functions implemented within the hidden layers. A model comprising 4 hidden layers was selected for this objective. This choice ensures an adequate quantity of hidden layers to enhance the model's performance while remaining sufficiently compact to facilitate swift weight updates via back-propagation.

Note: To implement the Neural Network itself, we made use of the TensorFlow and Keras frameworks due to their simple and intuitive interfaces. A sequential (`tf.keras.Sequential`) model was built using `tf.keras.layers.Dense` and `tf.keras.layers.Dropout` as layers.

Through multiple iterations of experiments and training, the following hyperparameters were decided upon:

Hyperparameters For The Neural Network

```
# Building the neural network for multi-class classification
model = tf.keras.Sequential([
    tf.keras.layers.Dense(128, activation='relu', input_shape=(X_train.shape[1],)),
    tf.keras.layers.Dropout(0.2),
    tf.keras.layers.Dense(64, activation='relu'),
    tf.keras.layers.Dense(3, activation='softmax')
])

model.compile(optimizer='adam', loss='categorical_crossentropy', metrics=['accuracy'])
```

Hidden Layer 1 - Dense

- Number of input features - 128
- Number of output features - 64
- Activation Function - ReLU

Dropout Layer

- Dropout: 0.2

Hidden Layer 2

- Number of input features - 64
- Number of output features - 3
- Activation Function - ReLU

Output Layer

- Number of input features - 3
- Number of output features - 3
- Activation Function - Softmax

Loss Function and Optimizer

- Loss Function - Categorical Cross-Entropy
- Optimizer - Adam
- Metric - Accuracy

Each layer within the model incorporates batch normalization, a technique applied to ensure that successive layers receive appropriately scaled data, thereby enhancing the ease of processing.

Training Details

- Number of Epochs - 10

Epoch	Loss	Accuracy	Val Loss	Val Accuracy
1	0.7940	0.6566	0.7364	0.6939
2	0.7251	0.7013	0.7190	0.7104
3	0.7053	0.7134	0.7101	0.7122
4	0.6940	0.7191	0.7043	0.7143
5	0.6840	0.7217	0.7052	0.7143
6	0.6769	0.7248	0.7007	0.7157
7	0.6735	0.7245	0.7126	0.7155
8	0.6661	0.7272	0.7131	0.7033
9	0.6600	0.7295	0.7171	0.7099
10	0.6546	0.7316	0.7147	0.7157

Switching To PyTorch: Based on the above implementation using TensorFlow, a copy of it was also written in Pytorch, the details of which are similar to what has been described above.

Best Scores on Kaggle

- TensorFlow implementation - 0.722
- PyTorch implementation - 0.722

Support Vector Machine

Details For Preprocessing and Feature Engineering

Initially, we went ahead with the same preprocessing and feature engineering done for the first half of the project, but soon realized that it was cumbersome to improve the accuracy (on Kaggle) beyond 60%.

With that in mind, we started with a clean train.csv file (the one provided as part of the assignment) and:

- Engineered a new column to store the frequencies of patient ids (similar to the first half).
- Categorical columns were one-hot encoded.
- Missing values in numerical columns were imputed using the `mean` strategy.
- patient_id and enc_id were dropped.

Subsequently, we trained multiple SVM models using different kernels, such as `poly` and `rbf` to forecast the readmission ID.

Through multiple iterations of experiments and training, the following hyperparameters were decided upon:

Hyperparameters For Different

```
# SVM with Polynomial Kernel
svm_poly = SVC(kernel='poly', degree=3, random_state=42)
svm_poly.fit(X_train, y_train)
y_pred_poly = svm_poly.predict(X_val)
accuracy_poly = accuracy_score(y_val, y_pred_poly)
print(f'Polynomial Kernel Accuracy: {accuracy_poly}')
```

```
# SVM with RBF Kernel
svm_rbf = SVC(kernel='rbf', random_state=42)
svm_rbf.fit(X_train, y_train)
y_pred_rbf = svm_rbf.predict(X_val)
accuracy_rbf = accuracy_score(y_val, y_pred_rbf)
print(f'RBF Kernel Accuracy: {accuracy_rbf}')
```

Metric For Evaluations

- Metric - Accuracy

Training Details

Kernel	Accuracy
poly (degree=3)	0.7142
rbf	0.7127

Best Scores on Kaggle

- Using `poly` kernel with degree 3: `0.721`
- Using `rbf` kernel: `0.72`