MIMIC ML/DL

Learning objectives

- Make us of MIMIC-IV for mortality prediction on patients diagnosed with sepsis.
- Make use of scikit-learn built-in binary classification models for mortality prediction.
- Build, train, and evaluate a neural network (PyTorch) for mortality prediction.

Set up and pre-requisites

- First thing we need to do is make sure latest google-colab is installed and import required Python modules.
- Main libraries required are PyTorch, scikit-learn, NumPy, pandas, and matplotlib.

```
!pip install -U pip google-colab --quiet
import errno
import os
import matplotlib.pyplot as plt
 mport numpy as np
 mport pandas as pd
# PyTorch dependencies
 mport torch
 Google Colab dependencies
from google.colab import drive
from google.colab import files
 scikit-learn models and metrics
from sklearn.base import BaseEstimator, ClassifierMixin
from sklearn.ensemble import RandomForestClassifier
from sklearn.linear_model import LogisticRegression
from sklearn.metrics import roc_auc_score, f1_score, precision_score, recall_score, accuracy_score, roc_curve
from sklearn.model_selection import train_test_split
from sklearn.naive_bayes import GaussianNB
from sklearn.neighbors import KNeighborsClassifier
from sklearn.preprocessing import StandardScaler
from sklearn.svm import LinearSVC
from sklearn.tree import DecisionTreeClassifier
from sklearn.utils.validation import check_X_y, check_is_fitted
 rom torch.utils.data import DataLoader, Dataset
```

Set up and pre-requisites

- Jupyter notebook assumes MIMIC-IV dataset (https://physionet.org/content/mimiciv/2.2/) has been previously downloaded from PhysioNet, unzipped, and uploaded to Google Drive.
- Thus, we need to mount Google Colab to Google Drive.
- String constants for multiple column names found in MIMIC-IV are also defined.

drive.mount('/content/drive')

```
ICU KEY - 'icu'
HOSP KEY = "hosp"
LONG TITLE_KEY = 'long_title'
ICD CODE KEY - 'icd code'
ICD VERSION KEY = 'icd version'
SEQ_NUM_KEY = 'seq_num
SUBJECT ID KEY - 'subject id'
DISCHTIME KEY = 'dischtime'
DEATHTIME KEY - 'deathtime'
ADMIT_PROVIDER_ID_KEY = 'admit_provider_id'
DISCHARGE_LOCATION_KEY = 'discharge location'
EDREGTIME_KEY = 'edregtime
ANCHORE_YEAR_GROUP_KEY = 'anchor_year_group'
ANCHOR YEAR KEY = 'anchor year'
ANCHOR AGE KEY - 'anchor age'
RACE KEY = 'race'
DOD KEY = 'dod'
LAST CAREUNIT KEY = 'last careunit'
INTIME KEY - 'intime'
OUTTIME_KEY = 'outtime'
LOS KEY - 'los'
STAY ID KEY = 'stay id'
LABEL KEY - 'label'
VALUE KEY - 'value'
VALUENUM KEY = 'valuenum'
VALUEUOM KEY - 'valueuom'
FLAG KEY - "flag"
REF RANGE LOWER_KEY = 'ref_range_lower'
REF_RANGE_UPPER_KEY = 'ref_range_upper'
PRIORITY KEY - 'priority'
SPECIMEN ID KEY = 'specimen id'
ORDER PROVIDER ID KEY - 'order provider id'
CATEGORY KEY - 'category'
FLUID KEY = 'fluid'
LABEVENT ID KEY - 'labevent id'
CHARTTIME KEY - 'charttime'
ADMIT AGE_KEY = 'admit_age'
FIRST CAREUNIT KEY - 'first careunit'
ADMISSION TYPE KEY - 'admission type'
HOSPITAL_EXPIRE_FLAG_KEY = 'hospital_expire_flag'
INSURANCE KEY - 'insurance'
ADMISSION LOCATION KEY - 'admission location'
MARITAL STATUS KEY = 'marital status'
```

- Helper method shown on the right is used to read MIMIC-IV csv data files into a pandas data frame.
- MIMIC-IV files are split into hosp and icu directories. Thus, we need to check if target csv file exists in either directory.

```
def pandas_read_csv(mimic_csv_file_name: str, low_memory=False, chunksize=None) -> pd.DataFrame:
    """
    Read CSV file from MIMIC-IV dataset into a pandas DataFrame.
    """
    # change path of mimic data directory (in mounted Google Drive)
    mimic_root_dir_path = '/content/drive/MyDrive/mimiciv/2.2'

# mimic-iv is split into 'hosp' and 'icu' directories
    hosp_dir_path = os.path.join(mimic_root_dir_path, ICU_KEY)
    icu_dir_path = os.path.join(mimic_root_dir_path, HOSP_KEY)

# check if desired file name exists in either 'hosp' or 'icu' directory,
    # else raise FileNotFoundError
    if os.path.exists(os.path.join(hosp_dir_path, mimic_csv_file_name)):
        file_path = os.path.join(hosp_dir_path, mimic_csv_file_name)
        return pd.read_csv(file_path, low_memory=low_memory, chunksize=chunksize)
    elif os.path.exists(os.path.join(icu_dir_path, mimic_csv_file_name)):
        file_path = os.path.join(icu_dir_path, mimic_csv_file_name)
        return pd.read_csv(file_path, low_memory=low_memory, chunksize=chunksize)
    else:
        raise FileNotFoundError(errno.ENOENT, os.strerror(errno.ENOENT), mimic_csv_file_name)
```

- Helper method (first half) shown on the right is used to read, filter, merge, and return raw MIMIC-IV data (as a pandas data frame) for hospital admissions diagnosed with sepsis.
- MIMIC-IV tables merged include dictionary of ICD-9 and ICD-10 codes, diagnoses table, admissions table, patients table, and ICU stays table.

```
def get_sepsis_raw_data(archive_and_download=False) -> pd.DataFrame:
  Read, filter, merge, and return (as a pandas DataFrame) MIMIC-IV data for patients diagnosed with sepsis.
  # Read dictionary of ICD diagnosis codes and filter to include codes which long title includes 'sepsis'.
  # Afterward, drop long title column and drop duplicates.
  df = pandas_read_csv('d_icd_diagnoses.csv')
  df = df[df.apply(lambda x: 'sepsis' in x[LONG_TITLE_KEY], axis=1)]
  df.drop(columns=[LONG_TITLE_KEY], inplace=True)
  df.drop duplicates(inplace=True)
  # Merge filtered 'sepsis' ICD codes with diagnoses ICD table.
  # MIMIC-IV contains both ICD-9 and ICD-10, thus we need to merge on both code and version.
  # Afterward, drop code and version columns and drop duplicates.
  df = df.merge(pandas_read_csv('diagnoses_icd.csv'), on=[ICD_CODE_KEY, ICD_VERSION_KEY], how='inner')
  df.drop(columns=[ICD_CODE_KEY, ICD_VERSION_KEY, SEQ_NUM_KEY], inplace=True)
  df.drop_duplicates(inplace=True)
  # Merge with admissions table on subject id and hospital admission id.
  # Afterward, drop columns which are not needed and drop duplicates.
  df = df.merge(pandas_read_csv('admissions.csv'), on=[SUBJECT_ID_KEY, HADM_ID_KEY], how='inner')
  df.drop(columns=[DISCHTIME_KEY, DEATHTIME_KEY, ADMIT_PROVIDER_ID_KEY, DISCHARGE_LOCATION_KEY, LANGUAGE_KEY,
                    EDREGTIME KEY.
                   EDOUTTIME_KEY], inplace=True)
  df.drop_duplicates(inplace=True)
  # Merge with patients table on subject id.
  # Afterward, drop columns which are not needed and drop duplicates.
  df = df.merge(pandas_read_csv('patients.csv'), on=[SUBJECT_ID_KEY], how='inner')
  df.drop(columns=[DOD_KEY, ANCHORE_YEAR_GROUP_KEY], inplace=True)
  df.drop duplicates(inplace=True)
  # Merge with ICU stays table on subject id and hospital admission id.
  # Afterward, drop columns which are not needed and drop duplicates,
  df = df.merge(pandas_read_csv('icustays.csv'), on=[SUBJECT_ID_KEY, HADM_ID_KEY], how='inner')
  df.drop(columns=[LAST_CAREUNIT_KEY, INTIME_KEY, OUTTIME_KEY, LOS_KEY, STAY_ID_KEY], inplace=True)
  df.drop_duplicates(inplace=True)
  df.reset_index(drop=True, inplace=True)
```

- Second half of helper method to get raw sepsis data is shown on the right.
- Usually complete blood count (CBC) tests are used to track the progression of sepsis. We would like to include these in our data as these could be helpful features in mortality prediction. To be more specific, results for hematocrit, platelet count, and hemoglobin.
- One issue is MIMIC-IV lab events table is large. Even with Google Colab Pro high-ram, trying to load all lab events data we run out of memory. The workaround is to load and filter lab events data in **chunks**.

```
# A complete blood count (CBC) is a blood test usually used as a marker for sepsis.
# We would like to merge data (so far) with lab events associated with CBC.
# To keep things simple, we will treat lab events with labels 'hematocrit', 'platelet count', and 'hemoglobin' as CBC
cbc_tests = {'hematocrit', 'platelet count', 'hemoglobin'}
# Read dictionary of lab event items, filter by blood (fluid) and hematology (category), and filter to include item ids
d_lab_items = pandas_read_csv('d_labitems.csv')
d_lab_items = d_lab_items[(d_lab_items[FLUID_KEY] == 'Blood') & (d_lab_items[CATEGORY_KEY] == 'Hematology')]
d_lab_items = d_lab_items[d_lab_items.apply(lambda x: str(x[LABEL_KEY]).lower().strip() in cbc_tests, axis=1)]
d_lab_items.drop(columns=[FLUID_KEY, CATEGORY_KEY], inplace=True)
d lab items.drop duplicates(inplace=True)
d_lab_items.reset_index(drop=True, inplace=True)
# Unique set of subject ids and hospital admission ids
subject_hadm_ids = df[[SUBJECT_ID_KEY, HADM_ID_KEY]].drop_duplicates().reset_index(drop=True)
# Thus, the workaround is to load and process lab events table in chunks.
chunks = list()
for chunk in pandas_read_csv('labevents.csv', low_memory=False, chunksize=10 ** 7):
    # Drop columns which are not needed from lab events chunk
        columns=[LABEVENT_ID_KEY, VALUE_KEY, VALUEUOM_KEY, FLAG_KEY, REF_RANGE_LOWER_KEY, REF_RANGE_UPPER_KEY,
                 SPECIMEN_ID_KEY, ORDER_PROVIDER_ID_KEY, STORETIME_KEY, COMMENTS_KEY], inplace=True)
    # Filter chunk (by merging on lab item id) to include only CBC lab events
    chunk = chunk.merge(d_lab_items, on=[ITEMID_KEY], how='inner')
    chunk.drop(columns=[ITEMID_KEY], inplace=True)
    # Filter chunk (by merging on subject id and hospital admission id) to exclude non-sepsis lab events
    chunk = chunk.merge(subject_hadm_ids, on=[SUBJECT_ID_KEY, HADM_ID_KEY], how='inner')
    chunk.sort_values(by=[SUBJECT_ID_KEY, HADM_ID_KEY, CHARTTIME_KEY], inplace=True)
    # Group chunk by subject id and hospital admission id reduce to median value
    chunk = chunk.groupby([SUBJECT_ID_KEY, HADM_ID_KEY, LABEL_KEY])[VALUENUM_KEY].median().to_frame().reset_index()
    chunks.append(chunk)
# Finally, concat all chunks and merge with cumulative dataset
df = df.merge(pd.concat(chunks), on=[SUBJECT_ID_KEY, HADM_ID_KEY], how='inner')
df.drop_duplicates(subset=[SUBJECT_ID_KEY, HADM_ID_KEY, LABEL_KEY], inplace=True)
df.reset_index(drop=True, inplace=True)
```

- Below shows execution of previous helper method to load MIMIC-IV raw sepsis data
- This will take several minutes due to the fact lab events table is very large

seps	sepsis_raw_data = get_sepsis_raw_data(archive_and_download=False) sepsis_raw_data.info() sepsis_raw_data.head()															
Range	eIndex: 232		DataFrame'> , 0 to 23236 lumns): Non-Null Count													
8 1 2 3 4 5 6 7 8 9 10 11 12 13 14 dtype menor	subject_id hadm_id admittime admission_ admission_ insurance marital_st race hospital_e gender anchor_age anchor_yea first_care label valuenum es: float64 ry usage: 2	type location atus xpire_flag r unit (1), int64(23237 non-null	int64 int64 object object object object object int64 object int64 object object float64	admission_location	i nsurance	marital_status	race	hospital_expire_fl	ag gen	der anchor	_age	anchor <u>v</u> ear	first_careumit	label	valu
0	10597253	26837795	2173-04- 14 14:59:00	URGENT	PHYSICIAN REFERRAL	Medicaid	MARRIED	ASIAN - CHINESE					2170	Medical/Surgical Intensive Care Unit (MICU/SICU)	Hematocrit	
1	10597253	26837795	2173-04- 14 14:59:00	URGENT	PHYSICIAN REFERRAL	Medicaid	MARRIED	ASIAN - CHINESE				26	2170	Medical/Surgical Intensive Care Unit (MICU/SICU)	Hemoglobin	
2	10597253	26837795	2173-04- 14 14:59:00	URGENT	PHYSICIAN REFERRAL	Medicaid	MARRIED	ASIAN - CHINESE					2170	Medical/Surgical Intensive Care Unit (MICU/SICU)	Platelet Count	
3	11331147	26958979	2142-05- 14 09:39:00	URGENT	PHYSICIAN REFERRAL	Medicaid	SINGLE	ASIAN - CHINESE		0	F	43	2142	Medical/Surgical Intensive Care Unit (MICU/SICU)	Hematocrit	

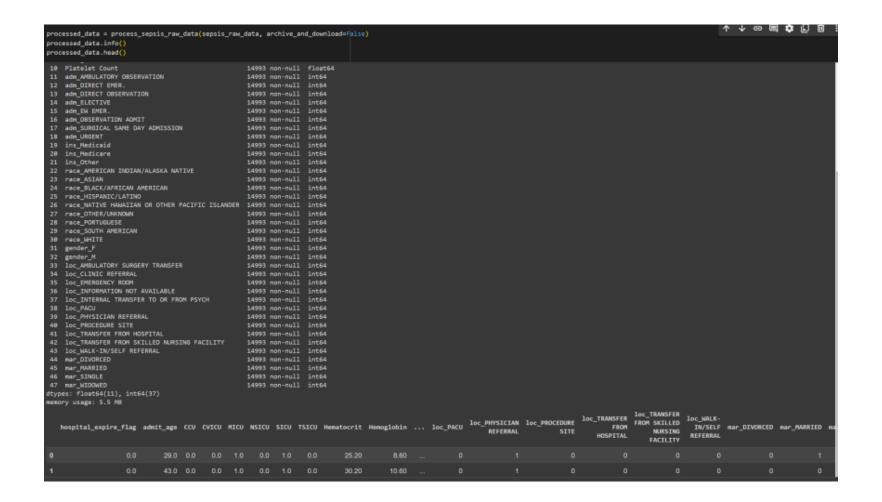
- Helper method (first half) shown on the right is used to processed previously fetched raw sepsis data and create features out of it.
- At a high level:
 - Age at admission is calculated
 - Race and first care unit column values are simplified
 - CBC lab event results become separate columns
 - Categorical columns become onehot encoded

```
process_sepsis_raw_data(raw_data: pd.DataFrame, archive_and_download=False) -> pd.DataFrame
Featurize sepsis raw data. At a high-level
   Age at admission is calculated
   Race column are simplified to ASIAN, WHITE, HISPANIC, BLACK, and OTHER/UNKNOWN
   First care units are simplified to MICU, SICU, NSICU, CCU, and TSIO
   CBC lab event results become separate columns
   Categorical columns, i.e. race, insurance, gender, etc., are one-hot encoded
# create copy of raw sepsis data
df = raw_data.copy()
# Convert admit time to date time and calculate age at admission using MIMIC-IV
df[ADMITTIME_KEY] = pd.to_datetime(df[ADMITTIME_KEY])
df[ADMIT_AGE_KEY] = (df[ADMITTIME_KEY].dt.year - df[ANCHOR_YEAR_KEY]) + df[ANCHOR_AGE_KEY]
df.drop(columns=[ADMITTIME_KEY, ANCHOR_YEAR_KEY, ANCHOR_AGE_KEY], inplace=True)
# Replace race values with simplified values
df[RACE_KEY].replace(regex=r'^ASIAN\D*', value='ASIAN', inplace=True)
df[RACE_KEY].replace(regex=r'~WHITE\D*', value='WHITE', inplace=True)
df[RACE_KEY].replace(regex=r'^HISPANIC\D"', value='HISPANIC\LATINO', inplace=True)
df[RACE_KEY].replace(regex=r'^BLACK\D'', value='BLACK/AFRICAN AMERICAN', inplace=True)
df[RACE_KEY].replace(
     'UNABLE TO OBTAIN', 'OTHER', 'PATIENT DECLINED TO ANSWER', 'UNKNOWN', 'MULTIPLE RACE/ETHNICITY'],
    value='OTHER/UNKNOWN', inplace=True)
df[FIRST_CAREUNIT_KEY].replace(regex=r'^Medical/Surgical\0+', value='MICU,SICU', inplace=True)
df[FIRST_CAREUNIT_KEY].replace(regex=r'^Medical\D*', value='MICU', inplace=True)
df[FIRST_CAREUNIT_KEY].replace(regex=r'^Neuro\D*', value='NSICU', inplace=True)
df[FIRST_CAREUNIT_KEY].replace(regex=r'^Cardiac\D*', value='CVICU', inplace=True)
df[FIRST_CAREUNIT_KEY].replace(regex=r'^Coronary\D+', value='CCU', inplace=True)
df[FIRST_CAREUNIT_KEY].replace(regex=r'^Trauma\D*', value='TSICU', inplace=True)
df[FIRST_CAREUNIT_KEY].replace(regex=r'^Surgical\D*', value='SICU', inplace=True)
# For each row in data aggregate ICU sta types into a list, then one-hot encode into separate columns.
df[FIRST_CAREUNIT_KEY] = df[FIRST_CAREUNIT_KEY].str.split(',', expand=False).reset_index(drop=True)
df = df.join(pd.get_dummies(df[FIRST_CAREUNIT_KEY].apply(pd.Series).stack(), dtype=int).groupby(level=0).sum()
             how='outer')
# Drop old unnecessary first care unit column
df.drop(columns=[FIRST_CAREUNIT_KEY], inplace=True)
```

- Second half of helper method to process raw sepsis data and create features is shown on the right.
- Only hospital admission rows with lab results for all CBC tests are included.
- Furthermore, duplicate rows and rows with missing values are dropped.

```
# Below code creates separate columns for each CBC lab event result
# First we group by subject id and hospital admission id and aggregate lab event results into a list
tmp = df.groupby([SUBJECT_ID_KEY, HADM_ID_KEY], as_index=False)[[LABEL_KEY, VALUENUM_KEY]].agg(list).reset_index(
# Drop old lab event result columns
df.drop(columns=[LABEL_KEY, VALUENUM_KEY], inplace=True)
# Merge temporary aggregated list of results with data
df = df.merge(tmp, on=[SUBJECT_ID_KEY, HADM_ID_KEY], how='inner')
df = df[df.apply(lambda x: len(x[LABEL KEY]) == 3, axis=1)]
# Split aggregated list of lab event results into separate columns, THen, drop unnecessary columns
df = df.join(pd.DataFrame(df[VALUENUM_KEY].to_list(), columns=df.iloc[0][LABEL_KEY]), how='outer')
df.drop(columns=[SUBJECT_ID_KEY, HADM_ID_KEY, LABEL_KEY, VALUENUM_KEY], inplace=True)
# One-hot encode category columns: admission type, insurance, race, gender, admission location, and marital status
prefix_cols = ['adm', 'ins', 'race', 'gender', 'loc', 'mar']
dummy_cols = [ADMISSION_TYPE_KEY, INSURANCE_KEY, RACE_KEY, GENDER_KEY, ADMISSION_LOCATION_KEY, MARITAL_STATUS_KEY]
df = pd.get_dummies(df, prefix=prefix_cols, columns=dummy_cols, dtype=int)
# Drop duplicates, drop rows with NaN, and reset indices
df.drop_duplicates(inplace=True)
df.dropna(inplace=True)
df.reset_index(drop=True, inplace=True)
# (Optional) download resulting pandas DataFrame into a zipped CSV file
if archive and download:
    archive_name = 'processed_data.zip'
   compression_opts = dict(method='zip', archive_name='processed_data.csv')
   df.to_csv(archive_name, index=False, compression=compression_opts)
   files.download(archive_name)
return df
```

Below shows execution of previous helper method to create features from raw sepsis data



Train, validation, and test split

- Helper method on the right is used to rebalance and split data into train, validation, and test splits.
- Rebalancing is done by randomly down-sampling data such that target values, i.e., hospital_expire_flag, are equally distributed for binary classification.
- The split is 70% train, 15% validation, and 15% test.

```
Split featured data into training, validation, and test sets.
# create a copy of featured data
df = data.copy()
# re-balance, by down-sampling, data, such that equal number of hospital_expire_flag==1
hospital expire flag value counts = df[HOSPITAL EXPIRE FLAG KEY].value counts()
minority_class = hospital_expire_flag_value_counts.idxmin()
majority_class = hospital_expire_flag_value_counts.idxmax()
minority_count = hospital_expire_flag_value_counts[minority_class]
majority_indices = df[df[HOSPITAL_EXPIRE_FLAG_KEY] == majority_class].index
# Make use of Numpy to down-sample (in-place) majority indices
sampled_indices = np.random.choice(majority_indices, size=minority_count, replace=False)
sampled indices = pd.Index(sampled indices).union(df[df[HOSPITAL EXPIRE FLAG KEY] == minority class].index)
# update data frame with down-sampled (re-balanced) data
df = df.loc[sampled_indices].reset_index(drop=True)
# split into features and target (i.e., hospital_expire_flag)
hospital_expire_flag = df[HOSPITAL_EXPIRE_FLAG_KEY].values
features = df.drop(columns=[HOSPITAL EXPIRE FLAG KEY])
# scale features using standard scaler
features = pd.DataFrame(scaler.fit_transform(features), columns=features.columns)
x_tr, x_va, y_tr, y_va = train_test_split(features, hospital_expire_flag, test_size=test_size)
# further split test data into a validation set of equal size
x_va, x_te, y_va, y_te = train_test_split(x_va, y_va, test_size=0.5)
# return train, validation, and test splits
return x_tr, x_va, x_te, y_tr, y_va, y_te
```

- We now define a random binary classifier (shown on right) as a baseline.
- The end goal is to eventually train a neural network that performs better than random guessing.
- This random binary classifier learns the probability distribution of classes from the training data. And during inference, it randomly samples from such learned distribution.

```
class RandomBaselineClassifier(BaseEstimator, ClassifierMixin):
    """
    Random baseline classifier.

def __init__(self):
    self.labels_ = None
    self.probs_ = None

def fit(self, x, y):
    """"

    Fit the model. Save the labels and probability distribution across all classes.
    """
    x, y = check_X_y(x, y)
    self.labels_, self.probs_ = np.unique(y, return_counts=True)
    self.probs_ = self.probs_ / self.probs_.sum()
    return self

def predict(self, x):
    """"

    Predict the labels for the given data, making use of the probability distribution across all classes.
    """
    check_is_fitted(self)
    return np.random.choice(self.labels_, size=len(x), p=self.probs_)
```

- But first, shown on the right is a simple helper method to print results.
- We'll store result metrics for multiple models inside a dictionary.
- Some of the metrics we'll explore further (and print) include AUC (ROC) score, F1 score, precision score, recall score, and accuracy.

```
def print_model_results(model_name: str, result_metrics: dict):
    """
    Print model results (from dictionary).
    """
    if result_metrics is None:
        result_metrics = dict()
    print(model_name)
    print(f'AUC (ROC) score:\t{result_metrics.get("AUC (ROC)", dict()).get(model_name, None)}')
    print(f'F1 score:\t\t{result_metrics.get("F1", dict()).get(model_name, None)}')
    print(f'Precision score:\t{result_metrics.get("Precision", dict()).get(model_name, None)}')
    print(f'Recall score:\t\t{result_metrics.get("Recall", dict()).get(model_name, None)}')
    print(f'Accuracy score:\t\t{result_metrics.get("Accuracy", dict()).get(model_name, None)}')
    print(f'Accuracy score:\t\t{result_metrics.get("Accuracy", dict()).get(model_name, None)}')
    print()
```

 Method on the right evaluates following binary classifiers (most from scikit-learn):

- Logistic regression
- Linear support vector machines
- Decision tree classifier
- Random forest classifier
- Gaussian naïve Bayes
- K-neighbors classifier
- Random (baseline) classifier
- Each model is trained on training data and evaluated on test dataset. Result metrics are stored in dictionary and printed to console.

```
evaluate_sklearn_binary_classification_models(x_tr, x_te, y_tr, y_te):
Evaluate sklearn binary classification models.
models = [LogisticRegression(),
          LinearSVC(max iter=5 000),
          DecisionTreeClassifier(),
          RandomForestClassifier(),
          GaussianNB(),
          KNeighborsClassifier(),
          RandomBaselineClassifier()]
# Dictionaries to keep track of multiple metric score for each model
roc_auc_scores = {}
f1_scores = {}
precision_scores = {}
recall scores = {}
accuracy scores = {}
fpr vals = {}
tpr_vals = {}
# Main results dictionary to track all metric scores for each model
result_metrics = {'AUC (ROC)': roc_auc_scores, 'F1': f1_scores, 'Precision': precision_scores,
                   'Recall': recall_scores, 'Accuracy': accuracy_scores, 'fpr': fpr_vals, 'tpr': tpr_vals}
# Train and evaluate each model
for model in models:
    # Fit the model with train data
    model.fit(x tr, y tr)
    # Predict using test data
    y te predictions - model.predict(x te)
    name = str(model).split("(")[0]
    # Calculate and store roc curve
    fpr, tpr, _ = roc_curve(y_te, y_te_predictions)
    fpr_vals[name] = fpr
    tpr_vals[name] - tpr
    roc auc scores[name] = roc auc score(y te, y te predictions)
    f1_scores[name] = f1_score(y_te, y_te_predictions)
    precision scores[name] = precision score(y te, y te predictions)
    recall scores[name] - recall score(y te, y te predictions)
    accuracy_scores[name] = accuracy_score(y_te, y_te_predictions)
    # Print model results
    print_model_results(name, result_metrics)
return result metrics
```

- Below shows execution of evaluating scikit-learn binary classifiers and random (baseline) classifier
- Result metrics are printed to console, but these are visualized and discussed on in slides that follow

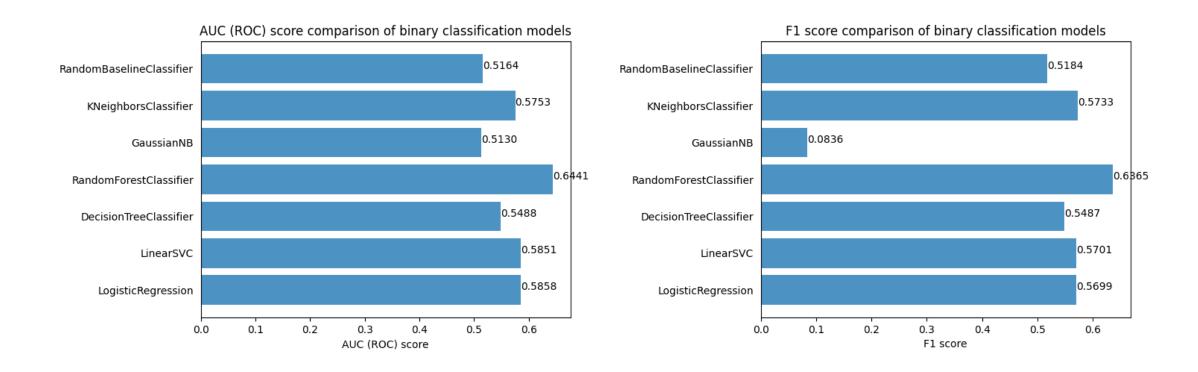
```
results = evaluate_sklearn_binary_classification_models(x_train, x_test, y_train, y_test)
LogisticRegression
F1 score:
Precision score:
                       8.5787692387692388
Recall score:
                       8.5690184049879755
Accuracy score:
/usr/local/lib/python3.10/dist-packages/sklearn/sym/ base.py:1244: ConvergenceWarning: Liblinear failed to converge, increase the number of iterations
 warnings.warn(
LinearSVC
AUC (ROC) score:
                       0.5851336234771818
F1 score:
Precision score:
                       0.5696784073586891
Recall score:
Accuracy score:
DecisionTreeClassifier
AUC (ROC) score:
                       0.5488888371523956
F1 score:
                        0.5486725663716815
                       8.528409090909090909
Precision score:
                       8.5488859884194978
Accuracy score:
RandomForestClassifier
AUC (ROC) score:
                       0.644132452414661
                       0.6261127596439169
Precision score:
Recall score:
                       0.647239263883681
                       0.6440177252584933
Accuracy score:
GaussianNB
                       0.5129800045444218
AUC (ROC) score:
F1 score:
                       0.8835734870317883
Precision score:
Recall score:
KNeighborsClassifier
AUC (ROC) score:
                       0.575269169594323
F1 score:
Precision score:
Recall score:
                       0.593558282208589
                        0.5745937961595273
Accuracy score:
AUC (ROC) score:
                       0.5183553597650514
F1 score:
Precision score:
                       0.4971830985915493
                       0.5414110429447853
Recall score:
                       0.5155096011816839
```

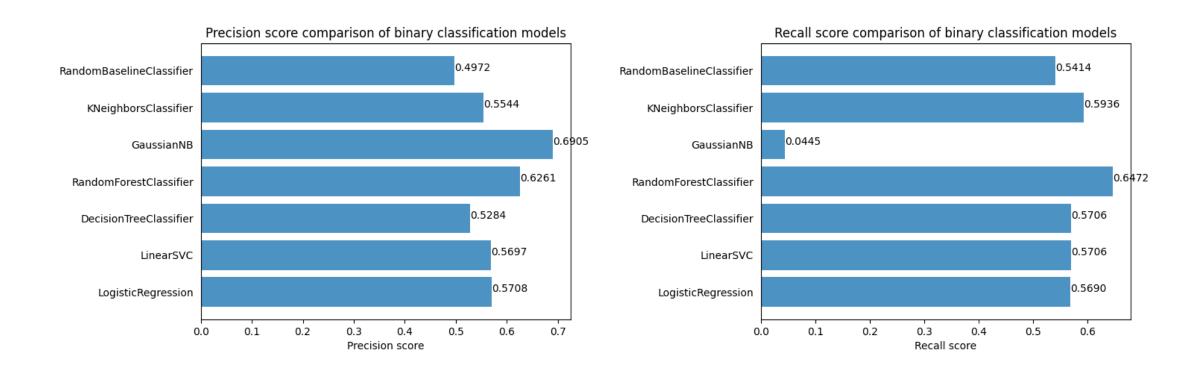
Scikit-learn and random baseline binary

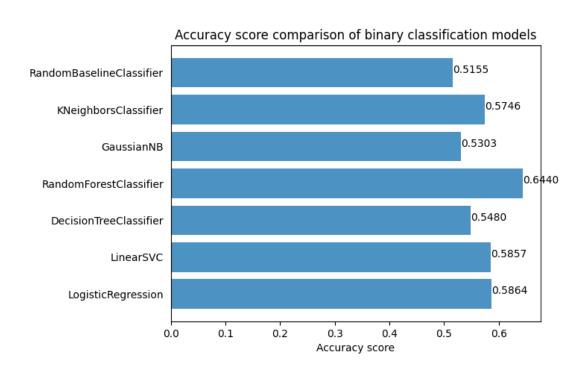
classifiers

- Method on the right visualizes result metrics (stored in dictionary).
- For each evaluation metric a horizontal bar plot is created.
- Horizontal bar for neural network (in future slides) is colored red for easy comparison.
- In the slides that follow are these plots.

```
save_and_download_figure(fig_name: str, download: bool):
  Save and download figure.
  if download:
      plt.savefig(fig_name, bbox_inches='tight')
      files.download(fig_name)
ef visualize_result_metrics(result_metrics: dict, download: bool):
  Visualize result metrics.
  # for each evaluation metric create a horizontal bar graph
  for eval_name in result_metrics:
      # skip fpr/tpr, these are separately used to plot ROC curve
      if eval_name in {'fpr', 'tpr'}:
      # plot in horizontal bar graph all scores for the given metric
      scores = result_metrics[eval_name]
      fig, ax = plt.subplots()
      ind = range(len(scores))
      ax.barh(ind, list(scores.values()), align='center', alpha=0.8)
      # Add metric score to the end of bar graph
      for i in range(len(scores)):
          score = list(scores.values())[i]
          plt.text(score, i, "{:0.4f}".format(score), ha='left')
      # Set x-axis labels, y-axis labels, and title
      ax.set_yticks(ind)
      ax.set_yticklabels(scores.keys())
      ax.set_xlabel(f'{eval_name} score')
      ax.tick_params(left=False, top=False, right=False)
      ax.set_title(f'{eval_name} score comparison of binary classification models')
      # Color red bar graph for NeuralNetwork
      models = list(scores.keys())
      neural_network_index = models.index('NeuralNetwork') if 'NeuralNetwork' in models else None
      if neural_network_index is not None:
          ax.get_children()[neural_network_index].set_color('r')
      # (optional) save and download the figure
      fig_name = f'{eval_name}_{neural_network_index}.png'
      save and download figure(fig name, download)
      plt.show()
      print()
```







Key insights:

- Random forest classifier performs best at mortality prediction overall. With an accuracy of ~0.644.
- Random (baseline) classifier performs the worst overall (as expected), with ~0.5155 accuracy and ~0.5164 AUC (ROC).

- Now, we will build, train, and evaluate a very simple PyTorch neural network.
- First, we need to define a device. This is helpful if running on a GPU. However, GPU is not required.
- On the right is implementation of a very simple neural network. It takes as input:
 - input_size The number of features in the training data.
 - hidden_layer_size The number of neurons in the hidden layer.
- The architecture of this neural network is very simple: a single hidden layer followed by a single neuron and a sigmoid layer. Between these we make use of dropout (20%) for regularization and a leaky ReLu function (for non-linearity).

```
class NeuralNetwork(nn.Module):
    Neural Network model.
    def __init__(self, input_size, hidden_layer_size):
        Initialize Neural Network model. Input size is the number of features,
        hidden layer size is the number of neurons in the hidden layer.
        super().__init__()
        self.sequential = nn.Sequential(
            nn.Dropout(0.2),
            nn.Linear(input_size, hidden_layer_size),
            nn.LeakyReLU(),
            nn.Dropout(0.2),
            nn.Linear(hidden_layer_size, 1),
            nn.Sigmoid()
    def forward(self, x):
        Forward pass.
        return self.sequential(x)
```

- Before proceeding, we need to define a custom dataset wrapper object, shown on the right.
- Data, features and labels, are stored as PyTorch tensors (float) to device.

```
class CustomDataset(Dataset):
   Custom dataset class.
   def __init__(self, x, y):
        Initialize CustomDataset class.
       self.x = torch.tensor(x.values).float().to(device)
       self.y = torch.tensor(y).float().unsqueeze(-1).to(device)
       self.length = self.x.shape[0]
   def __getitem__(self, idx):
        Get item.
       return self.x[idx], self.y[idx]
   def __len__(self):
        Get size of dataset.
       return self.length
```

- On the right we define helper methods to train and evaluate neural network a single epoch.
- At a high-level, train loop makes a model prediction, calculates the loss, and performs one step of back propagation. A running loss over the training data is computed and returned.
- The evaluation loop returns the loss of model prediction over all validation dataset.

```
train loop(dataloader: DataLoader, model: nn.Module, loss fn, optimizer):
  Single epoch train loop.
  # Aggregate running loss for single epoch train loop
  running loss = 0.0
  # set model to train mode
  # iterate over all data in batches
  for _, (x, y) in enumerate(dataloader):
      # make model prediction
      pred = model(x)
      loss = loss_fn(pred, y)
      # perform one step of back propagation
      loss.backward()
      optimizer.step()
      # zero (reset) gradient
      optimizer.zero grad()
      # update running loss
      running_loss += loss.item() * x.size(0)
  return running loss / len(dataloader.dataset)
ef eval_loop(dataloader: DataLoader, model: nn.Module, loss_fn):
  Single epoch validation evaluation.
  # set model to eval mode
  model.eval()
  # with no gradient, calculate loss function of model prediction on all data
  with torch.no grad():
      (x, y) = next(iter(dataloader))
      pred = model(x)
      return loss_fn(pred, y).item()
```

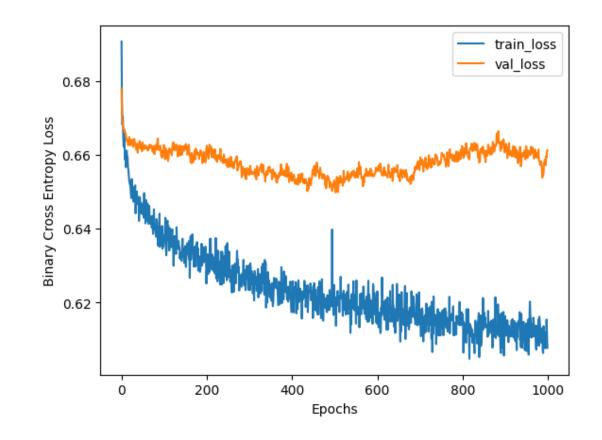
- Putting all previous helper methods together, the train method on the right performs the end-2-end training of the neural network.
- Train method takes as input the model to train, a training data loader, a validation data loader, and multiple hyperparameters such as number of epochs, the loss function, and an optimizer.
- We'll train for 1000 epochs using a batch size of 64.
- Adam optimizer and binary cross entropy loss are used for training.

```
train(epochs: int, tr_dataloader: DataLoader, model: nn.Module, loss_fn, optimizer, va_dataloader: DataLoader)
    Main train method. For a number of epochs, train and eval loops are called on neural network model and
    train/validation datasets. Train and validation losses returned as a result
    train_losses = []
    val_losses = []
    for t in range(epochs):
        print(f"Epoch: {t + 1}", end='\t')
        # Call train loop and append resulting loss
        train_loss = train_loop(tr_dataloader, model, loss_fn, optimizer)
        train_losses.append(train_loss)
        print(f"Train loss: {train_loss}", end='\t')
        # Call evaluation loop and append resulting loss
        val_loss = eval_loop(va_dataloader, model, loss_fn)
        val_losses.append(val_loss)
        print(f"Val loss: {val_loss}")
        print()
    # Return losses as pandas DataFrame
    return pd.DataFrame({'train_loss': train_losses, 'val_loss': val_losses})
 Hyperparameters, number of epochs to train and batch size to use for training
EPOCHS = 1 000
BATCH_SIZE = 64
# Create data loaders for training, validation, and test datasets.
 Make use of batching only for training data.
train_dataloader = DataLoader(CustomDataset(x_train, y_train), batch_size=BATCH_SIZE)
val_dataloader = DataLoader(CustomDataset(x_val, y_val), batch_size=len(x_val))
test_dataloader = DataLoader(CustomDataset(x_test, y_test), batch_size=len(x_test))
# Create Neural Network model with hidden layer size equal to 64
neural_network = NeuralNetwork(input_size=x_train.shape[-1], hidden_layer_size=64).to(device)
# We'll make use of Adam optimizer
adam_optimizer = torch.optim.Adam(neural_network.parameters())
 # We'll make use of binary cross entropy loss function for training
bce loss = nn.BCELoss()
```

 Running end-2-end training of neural network takes a minute or two. Train and validation losses are printed for each epoch (screenshot on right) and returned at the end.

```
losses = train(EPOCHS, train_dataloader, neural_network, bce_loss, adam_optimizer, val_dataloader
                Train loss: 0.6907873664596962 Val loss: 0.6780612468719482
Epoch: 1
                Train loss: 0.6742603828863596 Val loss: 0.6717148423194885
Epoch: 3
                Train loss: 0.6682193287194766 Val loss: 0.6690405011177063
                Train loss: 0.6703828369919874 Val loss: 0.6683736443519592
Epoch: 5
               Train loss: 0.6650036905553731 Val loss: 0.6672652959823608
Epoch: 6
                Train loss: 0.6622134472865107 Val loss: 0.6669309139251709
Epoch: 7
                Train loss: 0.666801398043961
Epoch: 8
                Train loss: 0.6631036534256531 Val loss: 0.6660763621330261
Epoch: 9
                Train loss: 0.6587122350954764 Val loss: 0.6661960482597351
Epoch: 10
                Train loss: 0.6606766650720145 Val loss: 0.6661266088485718
Epoch: 11
               Train loss: 0.6566901881356892 Val loss: 0.6655481457710266
Epoch: 12
               Train loss: 0.6588460185654279 Val loss: 0.6644909381866455
Epoch: 13
                Train loss: 0.661177255044546 Val loss: 0.6643700003623962
Epoch: 14
               Train loss: 0.6596925163401183 Val loss: 0.6636632680892944
Epoch: 15
               Train loss: 0.6595881200931607 Val loss: 0.6640703678131104
Epoch: 16
                Train loss: 0.6568752959712761 Val loss: 0.6626473665237427
                Train loss: 0.6559406047290219 Val loss: 0.6626899242401123
```

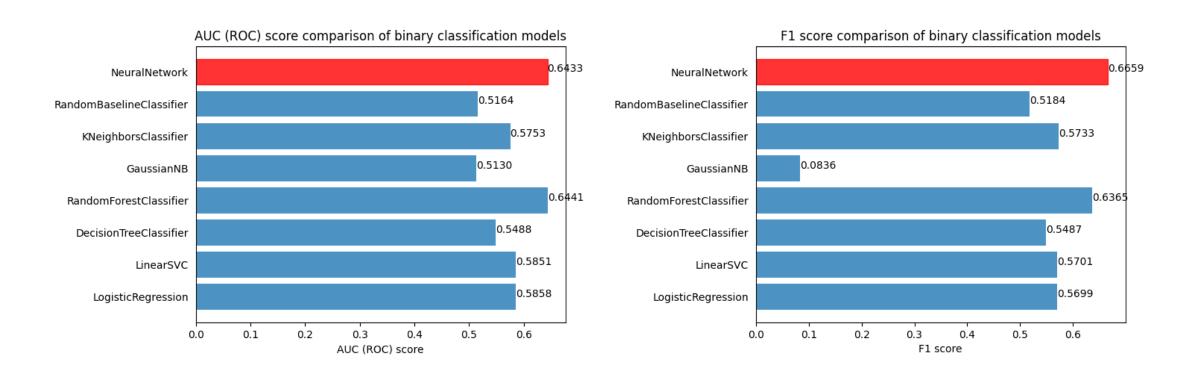
- Plotting train and validation losses after end-2-end training of neural network some observations:
 - Train loss decreases throughout epochs.
 - However, validation loss plateaus around ~0.66.
- We need to be very careful with underfitting on the training data and overfitting on the validation data.

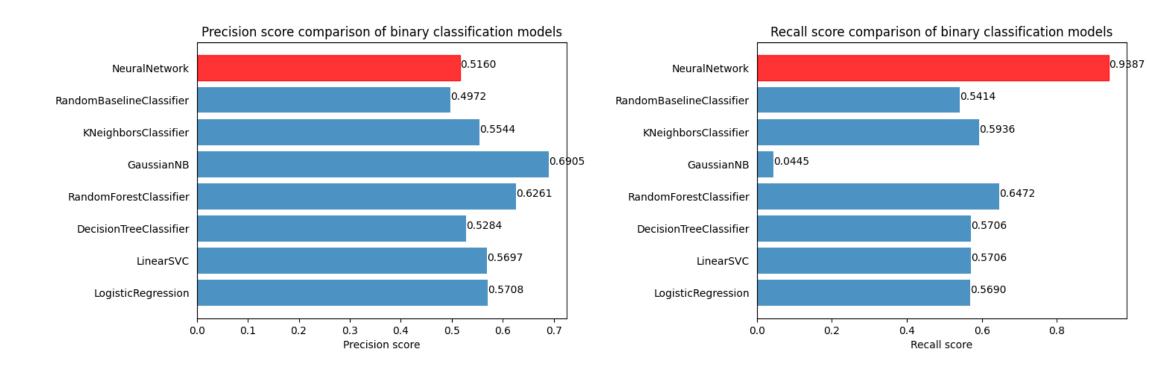


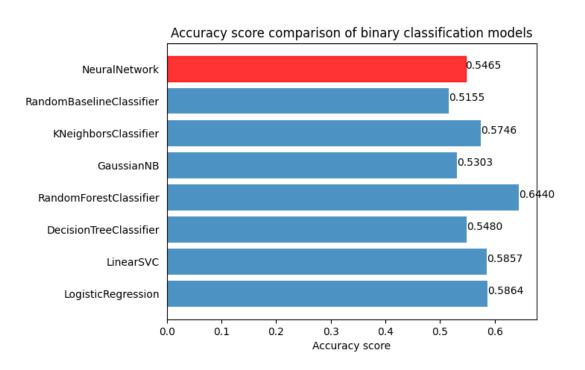
- Helper methods on the right are used to evaluate neural network on test dataset. This includes computing multiple metrics such as AUC (ROC), F1, precision, recall, and accuracy.
- The best threshold is also computed based on ROC curve.

```
metric_score_eval(y_true, y_pred, metric, threshold=None):
Calculate metric score given true and predicted values.
y pred = y pred.squeeze().cpu().detach().numpy()
if threshold is not None:
    y_pred = np.where(y_pred > threshold, 1, 0)
return metric(y_true.squeeze().cpu().detach().numpy(), y_pred)
evaluate neural network(dataloader: Dataloader, model: nn.Module, result metrics: dict):
Evaluate neural network model on test dataset.
if result metrics is None:
    result metrics - {
# set model to eval mode
model.eval()
# with no gradient, calculate loss function of model prediction on all data
with torch.no grad():
    (x, y) - next(iter(dataloader))
    model_name = model.__class__.__name_
    pred - model(x)
    fpr, tpr, thresholds - metric score eval(y, pred, lambda y true, y pred: roc curve(y true, y pred))
    result_metrics['fpr'][model_name] - fpr
    result_metrics['tpr'][model_name] = tpr
    best_threshold - float('inf')
    best_f1_score = float('-inf')
        f1 = metric_score_eval(y, pred, lambda y_true, y_pred: f1_score(y_true, y_pred), threshold=threshold)
            best f1 score - f1
            best threshold = threshold
    result_metrics["AUC (ROC)"][model_name] - metric_score_eval(y, pred, lambda y_true, y_pred: roc_auc_score(y_true, y_pred))
    result metrics["F1"][model name] - best f1 score
    result_metrics["Precision"][model_name] - metric_score_eval(y, pred, lambda y_true, y_pred: precision_score(y_true, y_pred),
                                                                threshold=best_threshold)
    result_metrics["Recall"][model_name] - metric_score_eval(y, pred, lambda y true, y pred: recall_score(y true, y pred),
                                                             threshold=best threshold)
    result metrics["Accuracy"][model name] - metric score eval(y, pred, lambda y true, y pred: accuracy score(y true, y pred),
                                                               threshold-best threshold)
    print model results(model name, result metrics)
 # return result metrics dictionary
return result metrics
```

- Evaluating neural network metrics are printed to console and stored in existing results dictionary.
- In next slides we plot and compare all models, including this trained neural network.







Key insights:

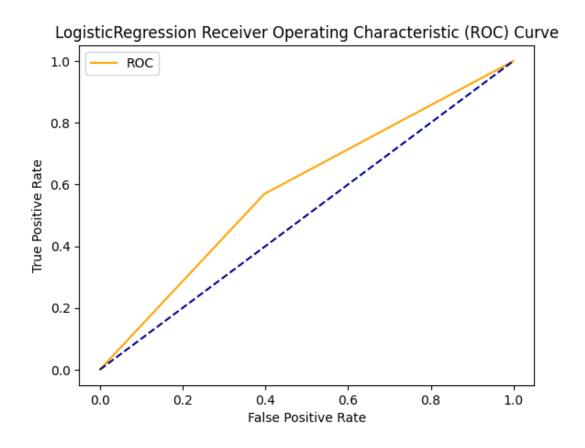
- Trained neural network performs better than random guessing.
- However, random forest classifier still performs better at mortality prediction compared to neural network with regards to accuracy.
- Neural network outperforms all other models on recall but underperforms on precision.

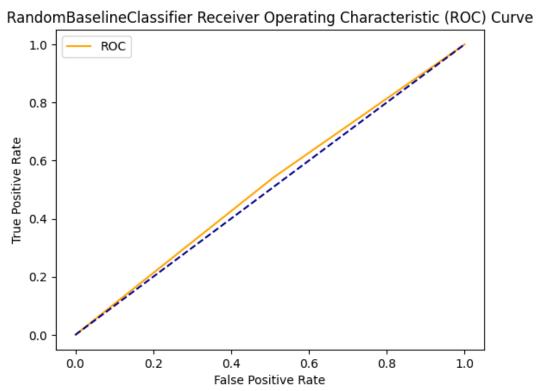
- In last few slides we will plot ROC curves for all models.
- Code (shown on the right)
 comes from
 https://jovian.com/vipul0036vi
 pul/how-to-find-optimal threshold-for-binary classification-roc-curve

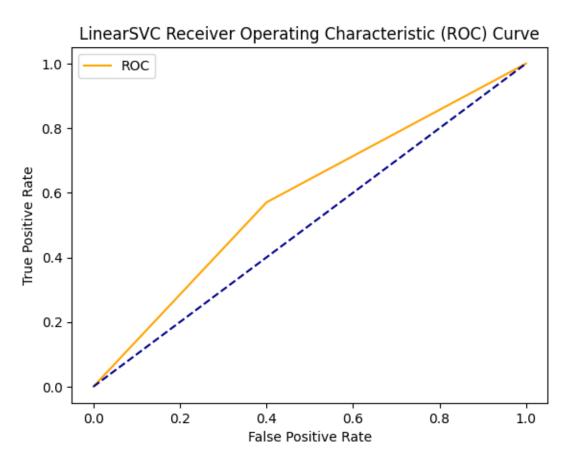
```
plot_roc_curve(model_name: str, fpr, tpr, download: bool):
 Plots a ROC curve given the false positive rate (fpr) and true positive rate (tpr) of a model.
  Code from https://jovian.com/vipul0036vipul/how-to-find-optimal-threshold-for-binary-classification-roc-curve
  plt.plot(fpr, tpr, color='orange', label='ROC')
 plt.plot([0, 1], [0, 1], color='darkblue', linestyle='--')
 plt.xlabel('False Positive Rate')
 plt.ylabel('True Positive Rate')
 plt.title(f'{model_name} Receiver Operating Characteristic (ROC) Curve')
 plt.legend()
 fig_name = f'{model_name}_roc_curve.png'
  save and download figure(fig name, download)
of plot_all_roc_curves(result_metrics: dict, download: bool):
 Plots all ROC curves.
 for model_name in set(result_metrics['fpr'].keys()).union(set(result_metrics['tpr'].keys()));
     plot roc curve(model name, result metrics['fpr'][model name], result metrics['tpr'][model name],
                     download=download)
     print()
```

Key insights:

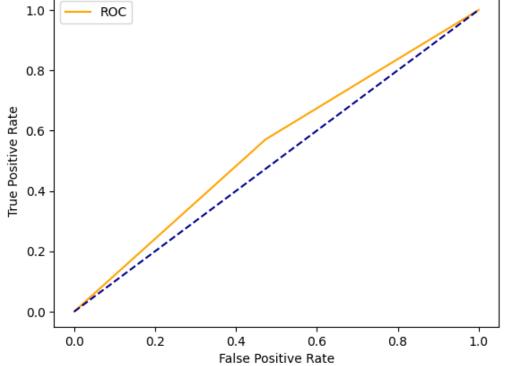
ROC for random classifier is as expected

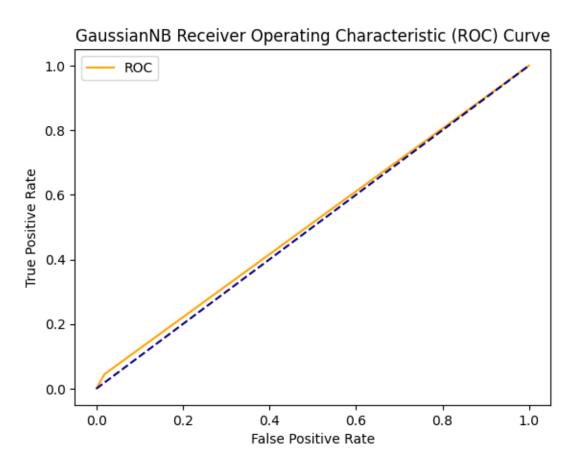








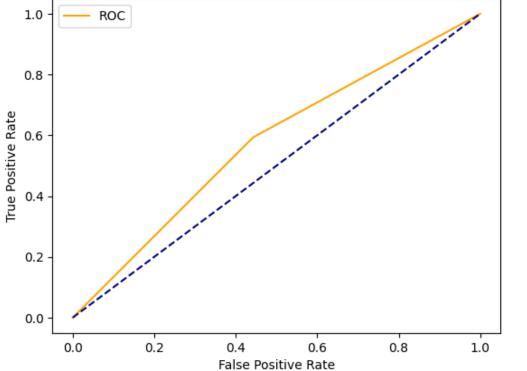




Key insights:

 Gaussian naïve Bayes, which performed the worst, has similar a ROC as random

guessing KNeighborsClassifier Receiver Operating Characteristic (ROC) Curve

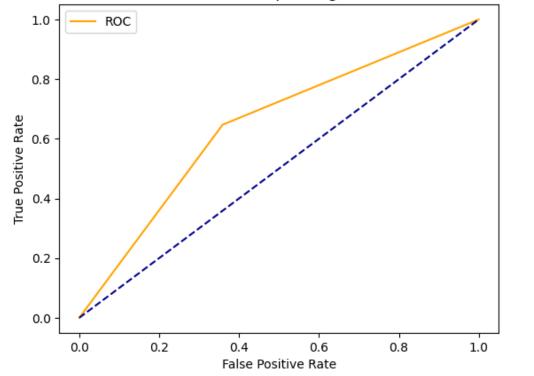


NeuralNetwork Receiver Operating Characteristic (ROC) Curve 1.0 ROC 0.8 True Positive Rate 0.6 0.4 0.2 0.0 0.2 0.6 0.8 1.0 0.0 0.4 False Positive Rate

Key insights:

 ROC for neural network and random forest classifier are similar. But there is still a lot of room for improvement.

RandomForestClassifier Receiver Operating Characteristic (ROC) Curve



Learnings and future work

- Some things learned:
 - Mortality prediction on MIMIC-IV (framed as binary classification) is difficult.
 - We see a very simple neural network does perform better than a random classifier. However, there is still a lot of room for improvement.
- Future work / enhancements include:
 - Making use of data augmentation to train better performing model.
 - Play with different model architectures and training hyperparameters.
 Though we need to be careful not to overfit on the training data.
 - Make use of additional features for the training data. For example, more lab event results, prescribed medications, etc.