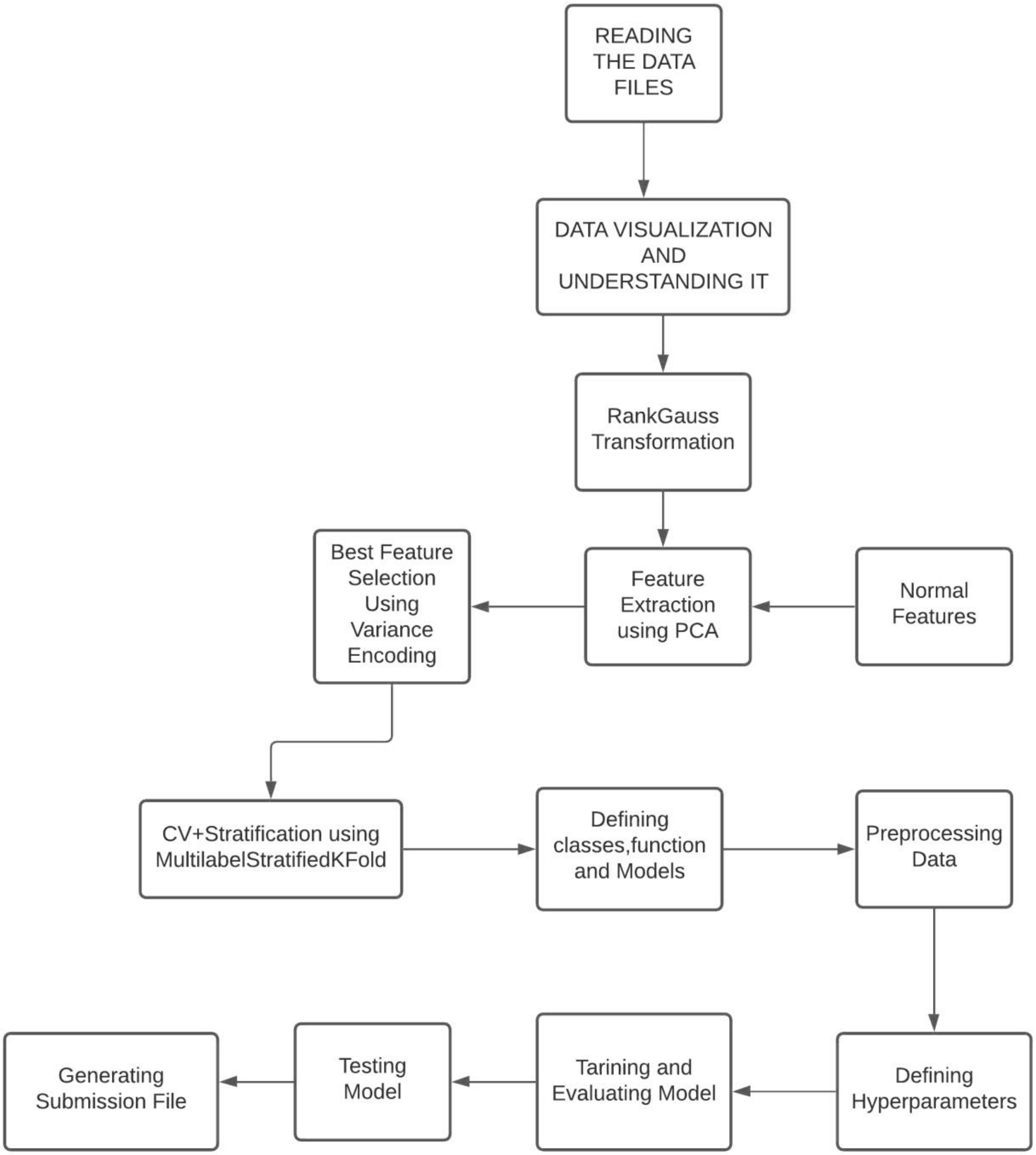
“[ENPM808A] FINAL PROJECT”

Introduction to Machine Learning

PROJECT REPORT

NEVIL PATEL:- 116897068

PROJECT PIPELINE


READING THE DATA FILES
DATA VISUALIZATION AND UNDERSTANDING IT
RankGauss Transformation
Best Feature Selection Using Variance Encoding
Feature Extraction using PCA
Normal Features
CV+Stratification using MultilabelStratifiedKFold
Defining classes,function and Models
Preprocessing Data
Generating Submission File
Testing Model
Tarining and Evaluating Model
Defining Hyperparameters

KAGGLE MOA COMPETITION

The Connectivity Map, a project within the Broad Institute of MIT and Harvard, the Laboratory for Innovation Science at Harvard (LISH), and the NIH Common Funds Library of Integrated Network-Based Cellular Signatures (LINCS), present this challenge with the goal of advancing drug development through improvements to MoA prediction algorithms.

What is the Mechanism of Action (MoA) of a drug? And why is it important?

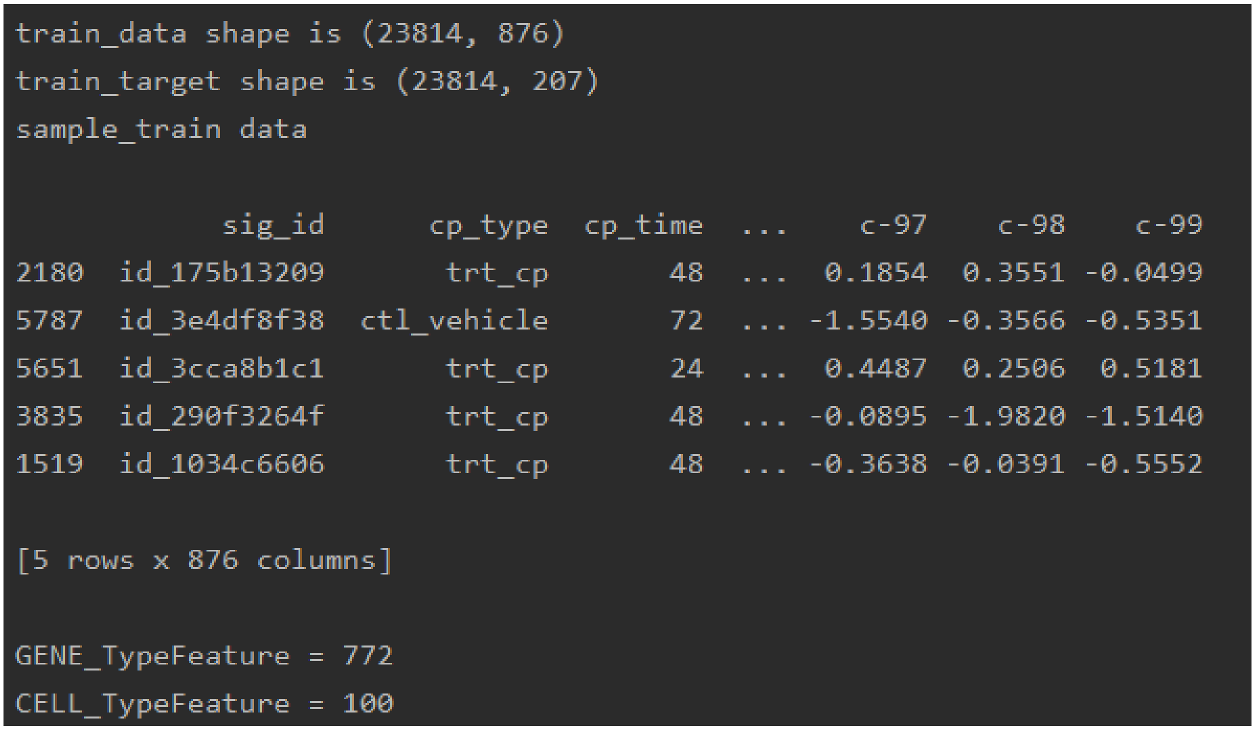
In the past, scientists derived drugs from natural products or were inspired by traditional remedies. Very common drugs, such as paracetamol, known in the US as acetaminophen, were put into clinical use decades before the biological mechanisms driving their pharmacological activities were understood. Today, with the advent of more powerful technologies, drug discovery has changed from the serendipitous approaches of the past to a more targeted model based on an understanding of the underlying biological mechanism of a disease. In this new framework, scientists seek to identify a protein target associated with a disease and develop a molecule that can modulate that protein target. As a shorthand to describe the biological activity of a given molecule, scientists assign a label referred to as mechanism-of-action or MoA for short.

READING MOA DATASET

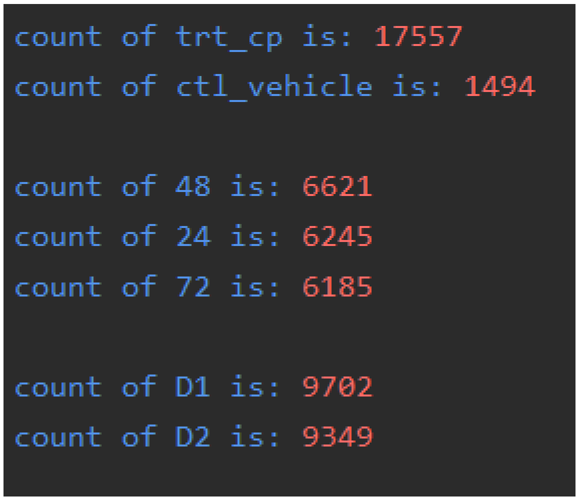
train_features.csv: Features for the training set. Features g- signify gene expression data, and c- signify cell viability data. cp_type indicates samples treated with a compound (cp_vehicle) or with a control perturbation (ctrl_vehicle); control perturbations have no MoAs; cp_time and cp_dose indicate treatment duration (24, 48, 72 hours) and dose (high or low).
cp_type (categorical): Samples treated with a compound or with a control perturbation. Categories include "trt_cp" and "ctl_vehicle", respectively. There is no MoA for "ctl_vehicle".
cp_time (categorical): Treatment duration in hours. Categories include 24, 48, and 72 hours.
cp_dose (categorical): Drug dose. Categories include "D1", "D2" for low and high dose, respectively.
g-[0-771] (continous): Gene expression data - a measure of activation in a given gene after the drug is applied.
c-[0-99] (continous): Cell viability. Basically count of live cells after the drug is applied.
train_targets_scored.csv: The binary MoA targets that are scored. There are 206 MoA targets.
test_features.csv: Features for the test data. We must predict the probability of each scored MoA for each row in the test data.

You might have your data in .csv files or SQL tables. Maybe Excel files. Or .tsv files. Or something else. But the goal is the same in all cases. If you want to analyze that data using **Pandas**, the first step will be to read it into a data structure that's compatible with pandas. There are two types of data structures in pandas: **Series** and **DataFrames**. Our project had the type dataFrames.

DATA UNDERSTANDING AND VISUALIZATION:-

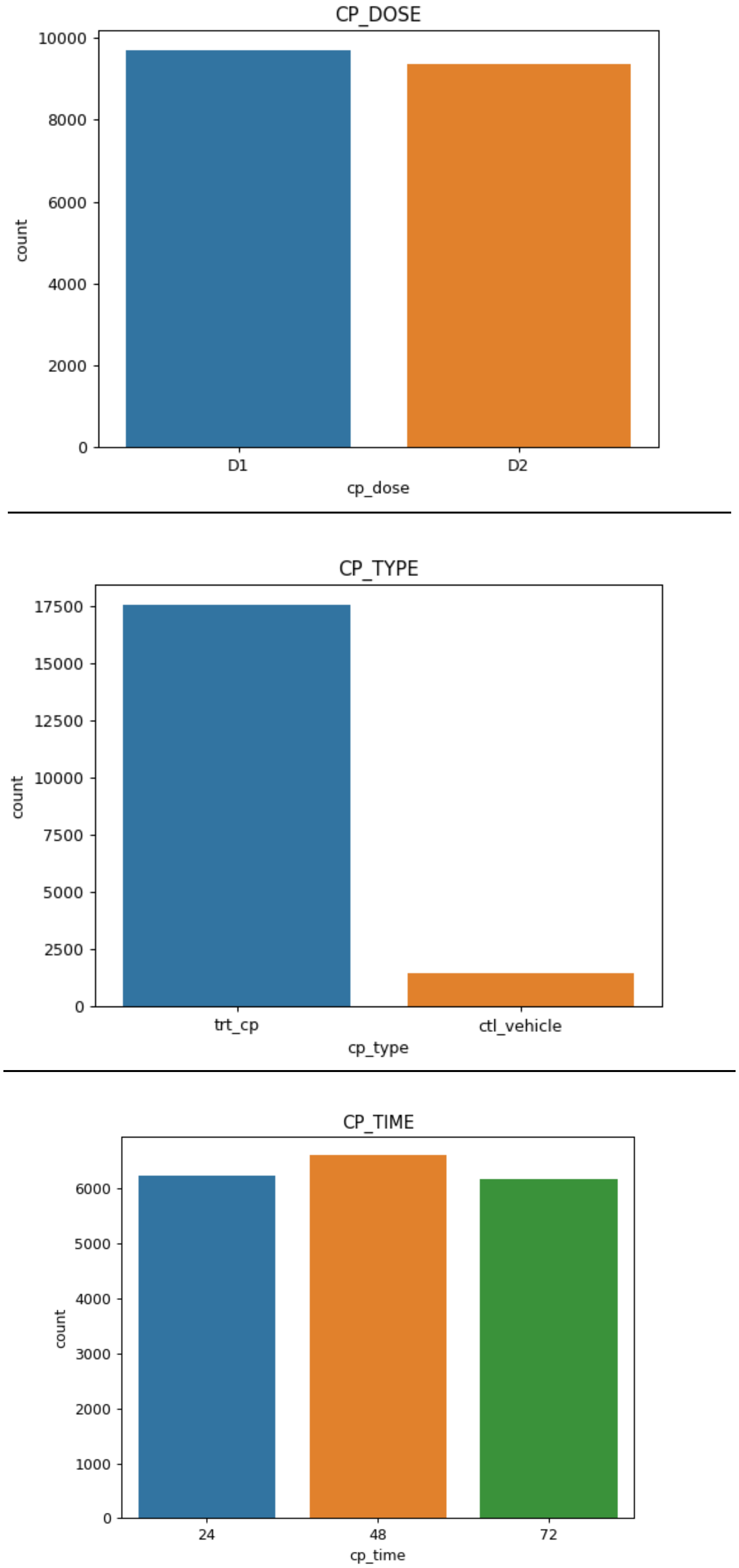


```
train_data shape is (23814, 876)
train_target shape is (23814, 207)
sample_train data

            sig_id      cp_type  cp_time  ...     c-97    c-98    c-99
2180  id_175b13209       trt_cp       48  ...   0.1854  0.3551 -0.0499
5787  id_3e4df8f38  ctl_vehicle       72  ...  -1.5540 -0.3566 -0.5351
5651  id_3cca8b1c1       trt_cp       24  ...   0.4487  0.2506  0.5181
3835  id_290f3264f       trt_cp       48  ...  -0.0895 -1.9820 -1.5140
1519  id_1034c6606       trt_cp       48  ...  -0.3638 -0.0391 -0.5552

[5 rows x 876 columns]

GENE_TypeFeature = 772
CELL_TypeFeature = 100
```

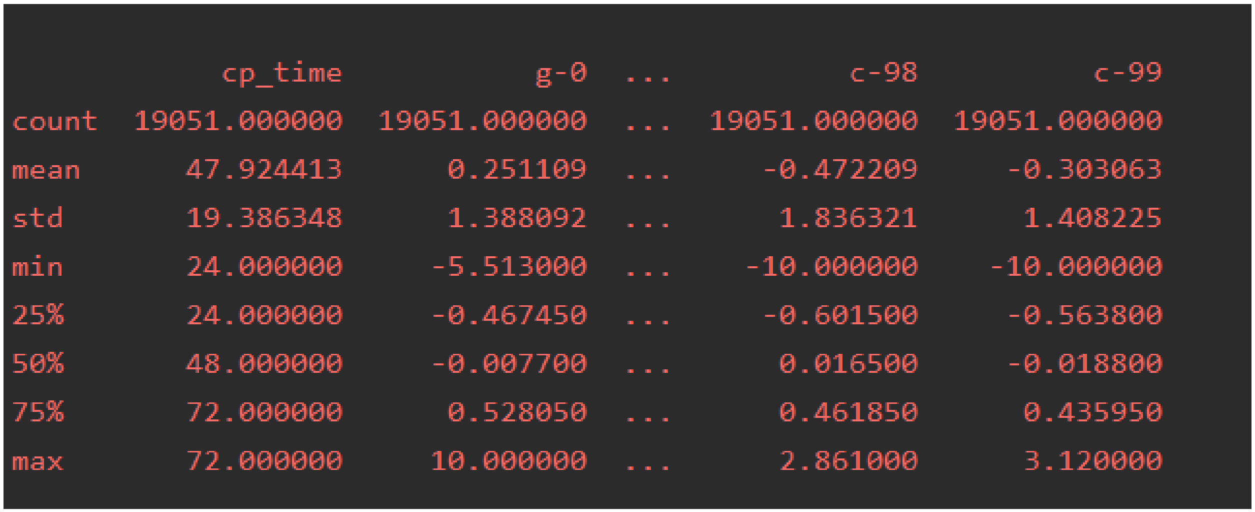


```
count of trt_cp is: 17557
count of ctl_vehicle is: 1494

count of 48 is: 6621
count of 24 is: 6245
count of 72 is: 6185

count of D1 is: 9702
count of D2 is: 9349
```

COUNT ON TRAINING DATA

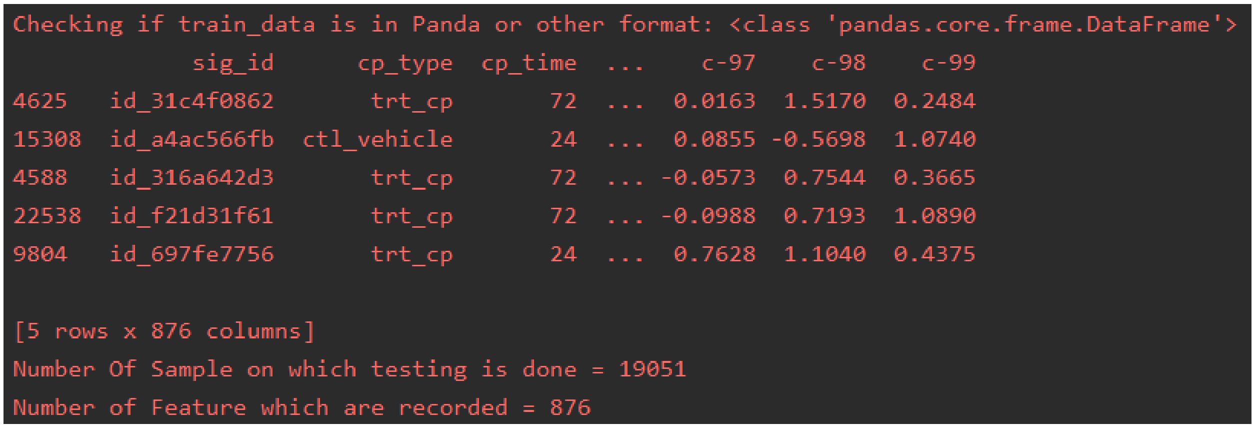


<u>HISTOGRAMS OF THE VALUES OF DOSE,TREATED COMPUND AND TREATMENT TIME</u>



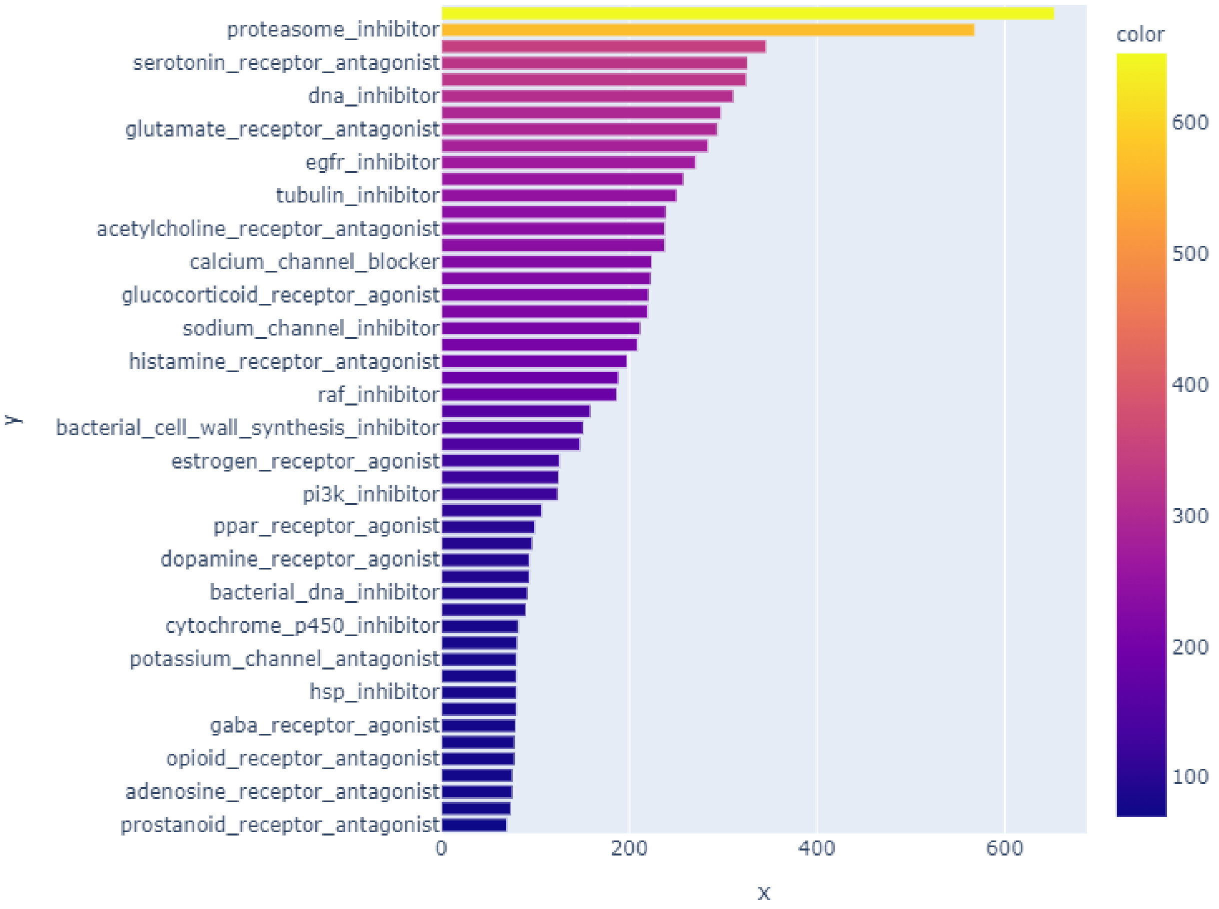
```
           cp_time           g-0  ...           c-98          c-99
count  19051.000000  19051.000000  ...  19051.000000  19051.000000
mean      47.924413      0.251109  ...     -0.472209     -0.303063
std       19.386348      1.388092  ...      1.836321      1.408225
min       24.000000     -5.513000  ...    -10.000000    -10.000000
25%       24.000000     -0.467450  ...     -0.601500     -0.563800
50%       48.000000     -0.007700  ...      0.016500     -0.018800
75%       72.000000      0.528050  ...      0.461850      0.435950
max       72.000000     10.000000  ...      2.861000      3.120000
```

DESCRIPTION OF THE TRAINING DATASET



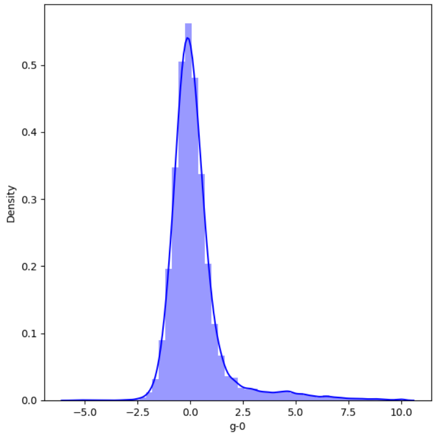
```
Checking if train_data is in Panda or other format: <class 'pandas.core.frame.DataFrame'>
             sig_id      cp_type  cp_time  ...    c-97    c-98    c-99
4625   id_31c4f0862       trt_cp       72  ...  0.0163  1.5170  0.2484
15308  id_a4ac566fb  ctl_vehicle       24  ...  0.0855 -0.5698  1.0740
4588   id_316a642d3       trt_cp       72  ... -0.0573  0.7544  0.3665
22538  id_f21d31f61       trt_cp       72  ... -0.0988  0.7193  1.0890
9804   id_697fe7756       trt_cp       24  ...  0.7628  1.1040  0.4375

[5 rows x 876 columns]
Number Of Sample on which testing is done = 19051
Number of Feature which are recorded = 876
```

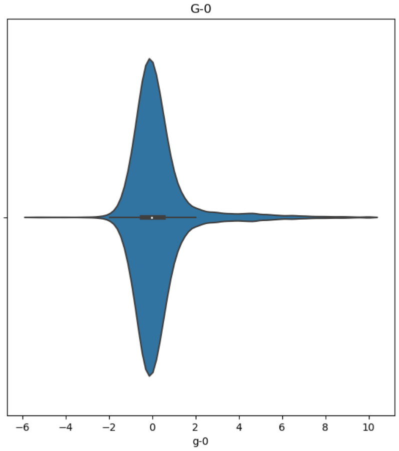
DISPLAYING TRAIN DATA AND IT'S SIZE

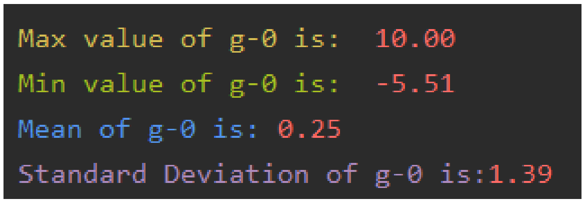


TARGET DATA SCORED

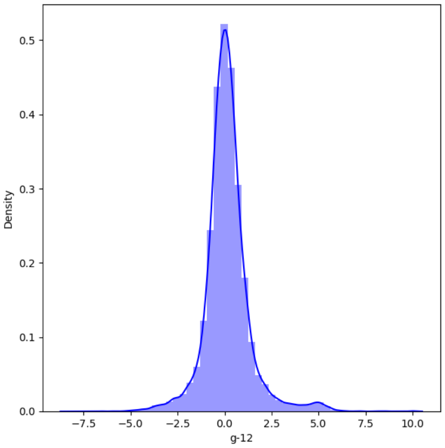
DISPLAYING GENE AND CELL FEATURES(TRAINING DATA)

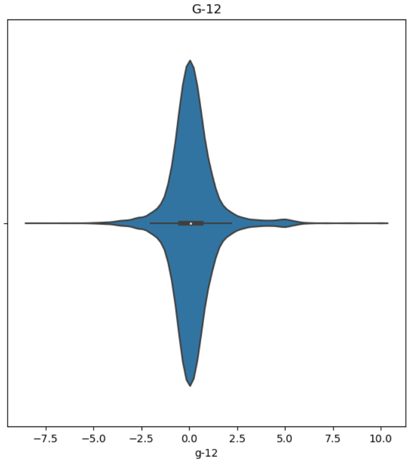


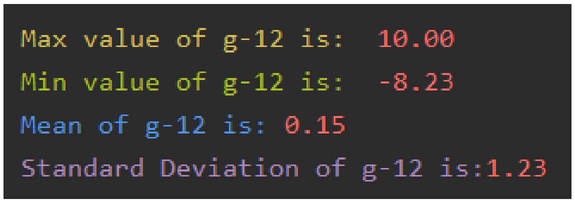




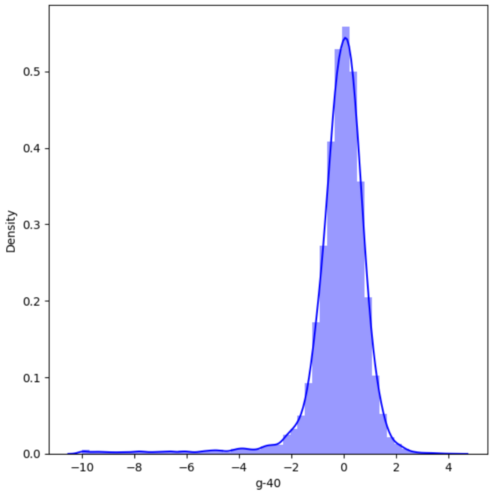
```
Max value of g-0 is:  10.00
Min value of g-0 is:  -5.51
Mean of g-0 is: 0.25
Standard Deviation of g-0 is:1.39
```

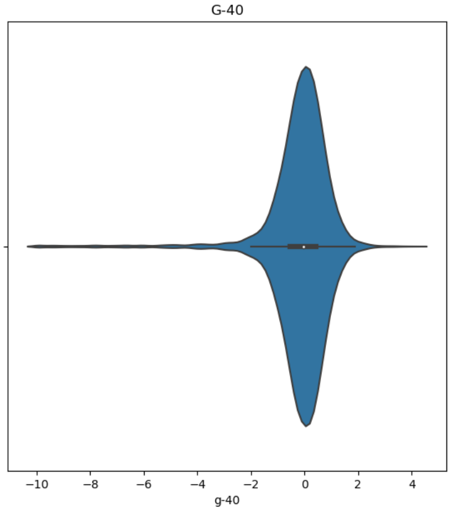


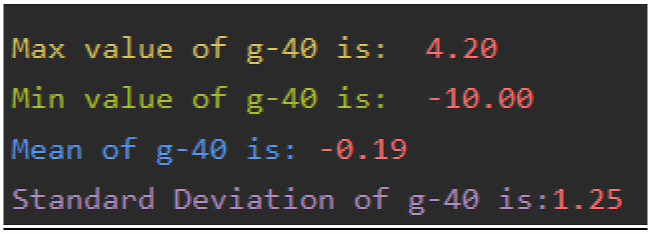




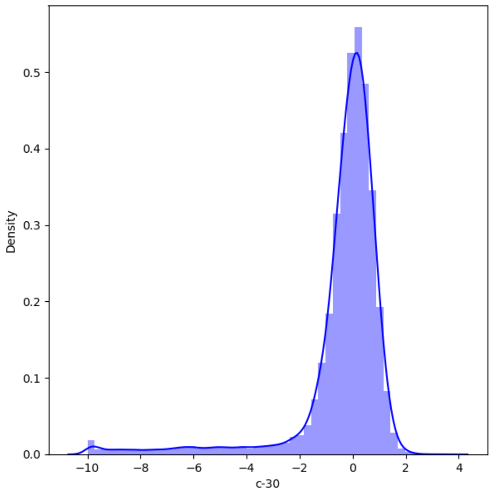
```
Max value of g-12 is:  10.00
Min value of g-12 is:  -8.23
Mean of g-12 is: 0.15
Standard Deviation of g-12 is:1.23
```

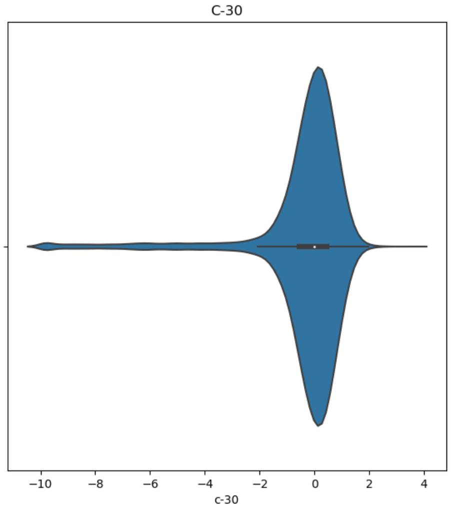


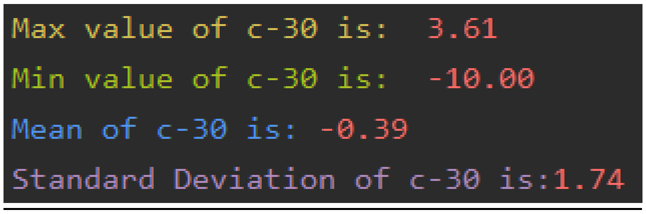




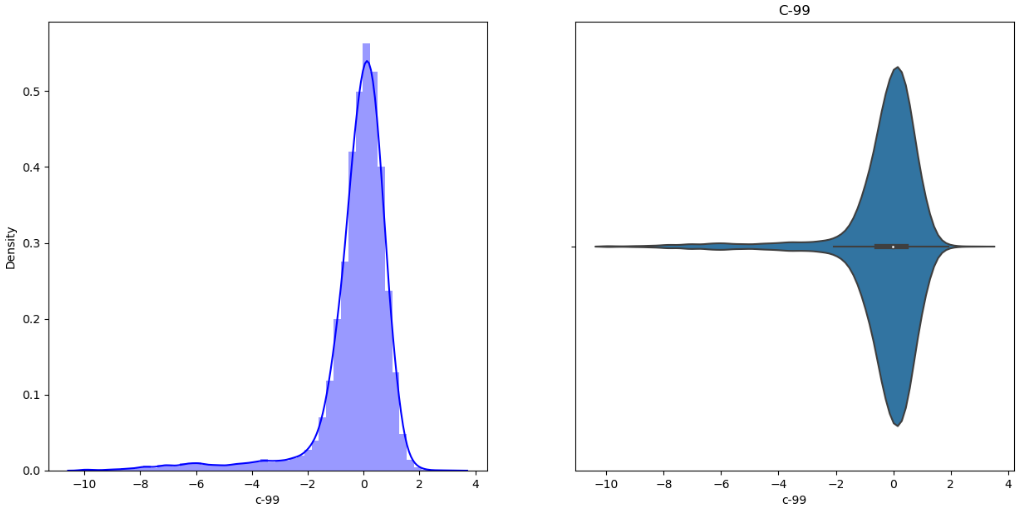
```
Max value of g-40 is:  4.20
Min value of g-40 is:  -10.00
Mean of g-40 is: -0.19
Standard Deviation of g-40 is:1.25
```

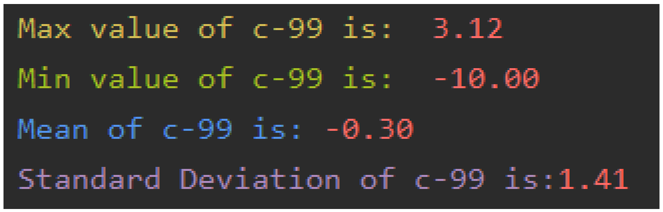






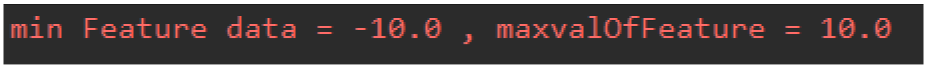
```
Max value of c-30 is:  3.61
Min value of c-30 is:  -10.00
Mean of c-30 is: -0.39
Standard Deviation of c-30 is:1.74
```





```
Max value of c-99 is:  3.12
Min value of c-99 is:  -10.00
Mean of c-99 is: -0.30
Standard Deviation of c-99 is:1.41
```

VISULISATION CONCLUSION(MIN AND MAX VALUE OF FEATURES)



```
min Feature data = -10.0 , maxvalOfFeature = 10.0
```

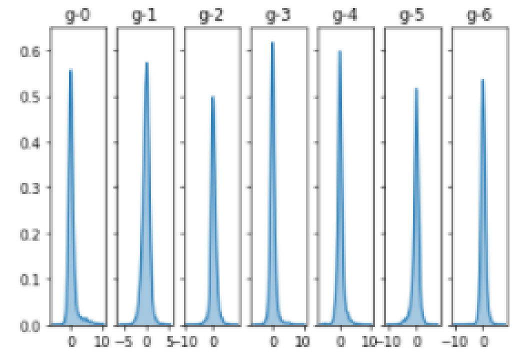
ALL OF THE FEATURES ARE IN RANGE OF -10 TO +10

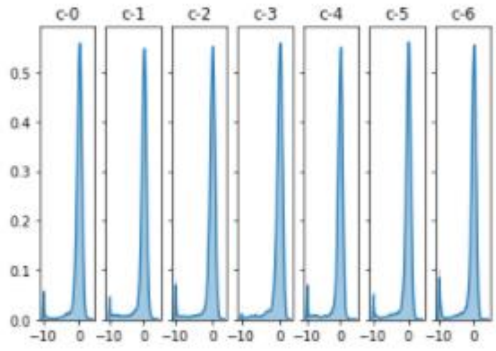
RANKGAUSS TRANSFORMATION:-

Input normalization for gradient-based models such as neural nets is critical. For lightgbm/xgb it does not matter.The best what I found during the past and works straight of the box is "RankGauss". It is based on rank transformation.
This works usually much better than standard mean/std scaler or min/max. Here after checking distributions of g- *and c*- of train and test set. They are spiky distribution rather than normal distribution. Regardless of the train and test, they look be in the same shape. It may be a too simple idea, it appears that the gene expression data and cell viability data can be controlled by the experimenter, so it is safe to assume that these data are independent of each other.Also, since the shape of the distribution is close to normal distribution to begin with, I don't think there is much of a problem if it is forced to be transformed into a Gaussian distribution. We can confirme that the shapes of data got close to the normal distribution. It appears that we were able to transform the distribution of each data to resemble a normal distribution, as intended. So, let's enter the data into the benchmarking method to see the improvement.

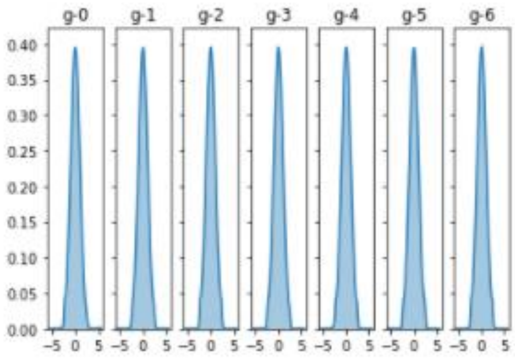
Train Set :

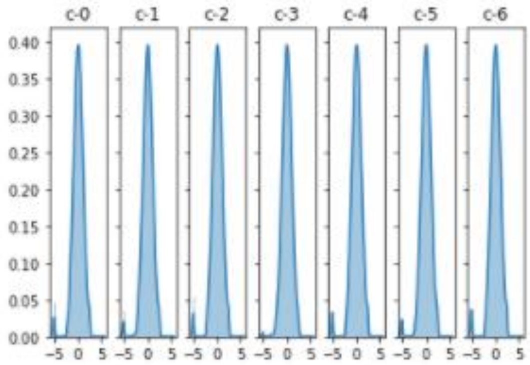
<u>Before</u>





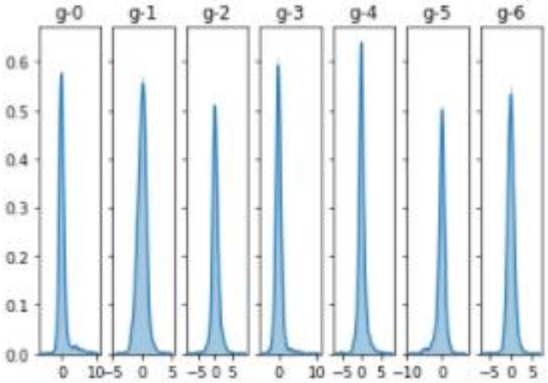
<u>After</u>

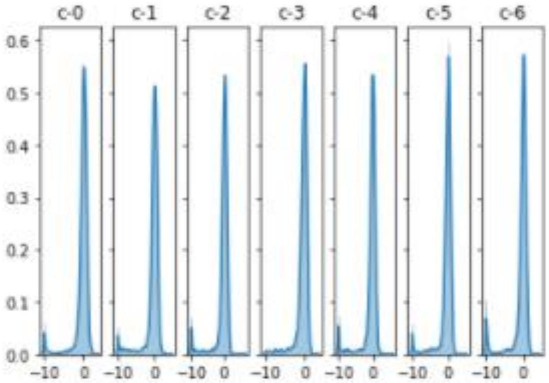




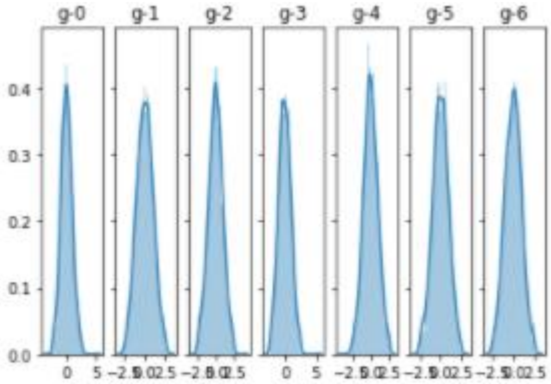
Test Set :

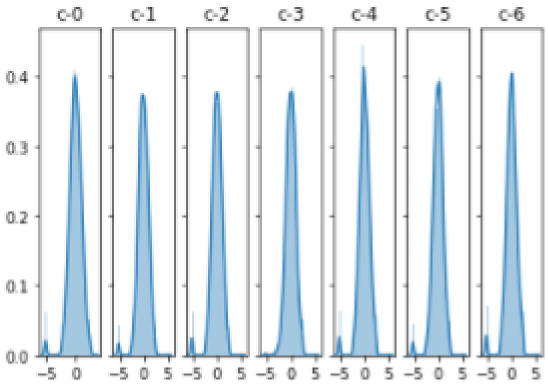
Before





After



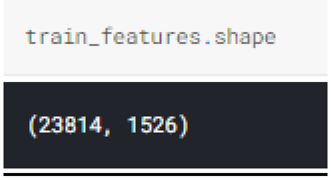


FEATURE EXTRACTION USING PCA AND ADDING TO NORMAL FEATURES:-

Principle Component Analysis (PCA) is a common feature extraction method in data science. Technically, PCA finds the eigenvectors of a covariance matrix with the highest eigenvalues and then uses those to project the data into a new subspace of equal or less dimensions. Practically, PCA converts a matrix of n features into a new dataset of (hopefully) less than n features. That is, it reduces the number of features by constructing a new, smaller number variables which capture a significant portion of the information found in the original features.

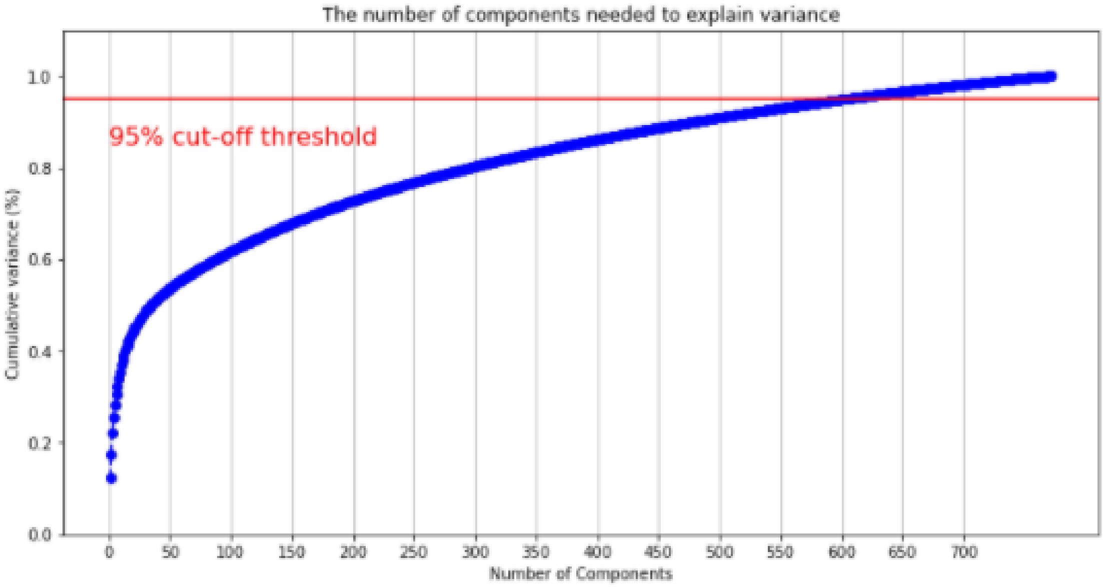
Don’t choose the number of components manually.Instead of that, use the option that allows you to set the variance of the input that is supposed to be explained by the generated components. Remember to scale the data to the range between 0 and 1 before using PCA that is done during RankGauss Transformation. Typically, we want the explained variance to be between 95–99%. **In our MOA case, to get 95% of variance explained we need 600 principal components.**

Size of New train Features after PCA



```
train_features.shape
```

```
(23814, 1526)
```



FEATURE SELECTION USING VARIANCE ENCODING:-

This feature selection algorithm looks only at the features (X), not the desired outputs (y), and can thus be used for unsupervised learning. Variance Threshold is a simple baseline approach to feature selection. It removes all features whose variance doesn't meet some threshold. By default, it removes all zero-variance features, i.e. features that have the same value in all samples.

As an example, suppose that we have a dataset with Boolean features, and we want to remove all features that are either one or zero (on or off) in more than 80% of the samples. Boolean features are Bernoulli random variables, and the variance of such variables is given by

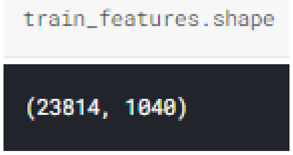
$\mathrm{Var}[X]=p(1-p)$

So we can select using the threshold .8 * (1 - .8):

Here we have used 0.8 as variance threshold.

```
var_thresh = VarianceThreshold(0.8)
```

Size of New train Features after Variance Encoding



```
train_features.shape
```

```
(23814, 1040)
```

CV FOLDS:-

Cross-validation, how I see it, is the idea of minimizing randomness from one split by makings n folds, each fold containing train and validation splits. You train the model on each fold, so you have n models. Then you take average predictions from all models, which supposedly give us more confidence in results. These we will see in following code. I found iterative-stratification package that provides scikit-learn compatible cross validators with stratification for multilabel data.

mskf = MultilabelStratifiedKFold(n_splits=7)

CLASSES AND MODEL(PYTORCH):-

PyTorch is the **fastest growing** Deep Learning framework and it is also used by **Fast.ai** in its MOOC, Deep Learning for Coders and its library.

PyTorch is also very *pythonic*, meaning, it feels more natural to use it if you already are a Python developer.

Besides, using PyTorch may even *improve your health*,

CLASSES:-

DATASET:-

Here the class Dataset is used to convert numpy type data to tensor data format. That's what **from_numpy** is good for. It returns a **CPU/GPU tensor.** If you compare the **types** of both variables, you'll get what you'd expect: numpy.ndarray for the first one and torch.Tensor for the second one.

TRAIN:-

model.train() tells your model that you are training the model. So effectively layers like dropout, batchnorm etc. which behave different on the train and test procedures know what is going on and hence can behave accordingly. Our train function then goes to optimizer, Loss and scheduler.

Adam Optimizer:-

We use one of PyTorch's **optimizers Adam**. An optimizer takes the **parameters** we want to update, the **learning rate** we want to use (and possibly many other hyper-parameters as well!) and **performs the updates** through its **step()** method Besides, we also don't need to zero the gradients one by one anymore. We just invoke the optimizer's **zero_grad()** method and that's it! **Adam** is a replacement optimization algorithm for stochastic gradient descent for training deep learning models. **Adam** combines the best properties of the AdaGrad and RMSProp algorithms to provide an optimization algorithm that can handle sparse gradients on noisy problems.

```
    optimizer = torch.optim.Adam(model.parameters(), lr=LEARNING_RATE, weight_dec
ay=WEIGHT_DECAY)
```

BCE with Logitloss:-

This loss combines a *Sigmoid* layer and the *BCELoss* in one single class. This version is more numerically stable than using a plain *Sigmoid* followed by a *BCELoss* as, by combining the operations into one layer, we take advantage of the log-sum-exp trick for numerical stability.

The unreduced (i.e. with reduction set to 'none') loss can be described as:

$$\ell(x, y) = L = \{l_1, \dots, l_N\}^\top, \quad l_n = -w_n \left[y_n \cdot \log \sigma(x_n) + (1 - y_n) \cdot \log(1 - \sigma(x_n)) \right],$$

N is the batch size. If reduction is not 'none' (default 'mean'), then

$$\ell(x, y) = \begin{cases} \operatorname{mean}(L), & \text{if reduction} = \text{'mean';} \\ \operatorname{sum}(L), & \text{if reduction} = \text{'sum'.} \end{cases}$$

This is used for measuring the error of a reconstruction in for example an auto-encoder. Note that the targets *t[i]* should be numbers between 0 and 1.

```
    loss_fn = nn.BCEWithLogitsLoss()
```

Scheduler:-

It allows dynamic learning rate reducing based on some validation measurements.

```
scheduler = optim.lr_scheduler.OneCycleLR(optimizer=optimizer, pct_start=0.1, div_factor=1e3,
                                              max_lr=1e-2, epochs=EPOCHS, steps_per_epoch=len(trainloader))
```

VALIDATE:-

In machine learning, model validation is referred to as the process where a trained model is evaluated with a testing data set. The testing data set is a separate portion of the same data set from which the training set is derived. The main purpose of using the testing data set is to test the generalization ability of a trained model Model validation is carried out after model training. Together with model training, model validation aims to find an optimal model with the best performance.Here our function Valid_fn does the same task on MOA dataset.

```
 valid_loss, valid_preds = valid_fn(model, loss_fn, validloader, DEVICE)
```

INFERENCE:-

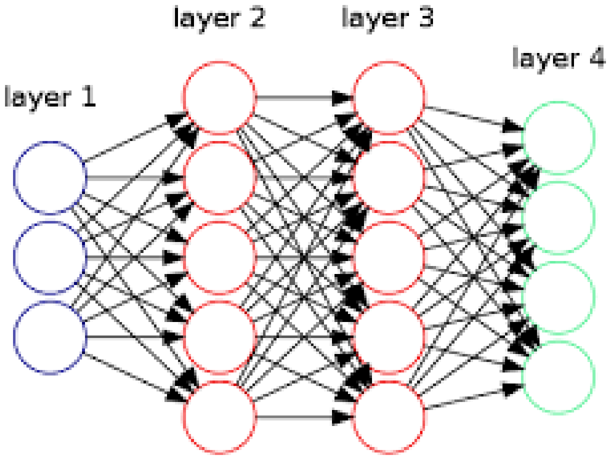
Inference refers to the process of using a trained machine learning algorithm to make a prediction. IoT data can be used as the input to a trained machine learning model, enabling predictions that can guide decision logic on the device, at the edge gateway or elsewhere in the IoT system. Here our function inference_fn predicts the output from the trained model on the train or new dynamic dataset.

```
  predictions = inference_fn(model, testloader, DEVICE)
```

MODEL (Neural Network):-

Multi-label classification involves predicting zero or more class labels. Unlike normal classification tasks where class labels are mutually exclusive, multi-label classification requires specialized machine learning algorithms that support predicting multiple mutually non-exclusive classes or "labels." Deep learning neural networks are an example of an algorithm that natively supports multi-label classification problems. Neural network models for multi-label classification tasks can be easily defined and evaluated using the pytorch deep learning library If the dataset is small, it is good practice to evaluate neural network models repeatedly on the same dataset and report the mean performance across the repeats. This is because of the stochastic nature of the learning algorithm. Additionally, it is good practice to use k-fold cross-validation instead of train/test splits of a dataset to get an unbiased estimate of model performance when making predictions on new data. Again, only if there is not too much data that the process can be completed in a reasonable time. Taking this into account, we will evaluate the MLP model on the multi-output regression task using repeated k-fold cross-validation with 7 folds and 7 repeats.

The MLP model will predict the probability for each class label by default. This means it will predict three probabilities for each sample. These can be converted to crisp class labels by rounding the values to either 0 or 1. We can then calculate the classification accuracy for the crisp class labels. The scores are collected and can be summarized by reporting the mean and standard deviation across all repeats and cross-validation folds. The number of output nodes should match the number of values you want to estimate. For binary classification, you need only one output node. For multiclass classification or multiple regression, you require multiple output nodes. In precise, binary classification using a feedforward neural net is done by computing the activation of a single output node, then checking whether it is larger than some threshold value (commonly 0 or .5). For multiclass classification with a k number of classes, you can calculate the values of k output nodes, then select the index 'i' of the largest value to predict class i..



FEED FORWARD NEURAL NETWORK FOR MULTILABEL CLASSIFICATION

Here in our NN model It does Batch Normalize at every step right from the input features:-1041 than it goes into the hidden layer of network which consist of 2048 neurons. There are 2 identical hidden layers of same size. When the features move from 1st hidden layer to 2nd one we have dropout with low weights below 0.4. In the Last layer we scale the neurons as per the required target i.e. 206

Batch Normalization `self.batch_norm1 = nn.BatchNorm1d(num_features)`
Applies Batch Normalization over a 2D or 3D input (a mini-batch of 1D inputs with optional additional channel dimension)

$$y = \frac{x - \mathrm{E}[x]}{\sqrt{\mathrm{Var}[x] + \epsilon}} * \gamma + \beta$$

The mean and standard-deviation are calculated per-dimension over the mini-batches and \gamma$\gamma$ and \beta$\beta$ are learnable parameter vectors of size C (where C is the input size). By default, the elements of \gamma$\gamma$ are set to 1 and the elements of \beta$\beta$ are set to 0. The standard-deviation is calculated via the biased estimator, equivalent to *torch.var(input, unbiased=False).*

Weight Normalization: `weight_norm(nn.Linear(num_features, hidden_size))`
A Simple Reparameterization to Accelerate Training of Deep Neural Networks. Tim Salimans, Diederik P. Kingma. Download PDF. We present **weight normalization**: a reparameterization of the **weight** vectors in a neural network that decouples the length of those **weight** vectors from their direction.

Linearization: `nn.Linear(num_features, hidden_size))`
It is a strategy used in **machine learning** to reduce the dimension with a linear projector. A low-dimensional linear projection of x can separate the values of f if this function remains constant in the direction of a high-dimensional linear space. **nn**. **Linear**(n,m) is a module that creates single layer feed forward network with n inputs and m output. Mathematically, this module is designed to calculate the **linear** equation Ax = b where x is input, b is output, A is weight.

Dense layer : `self.dense1 = nn.utils.weight_norm(nn.Linear(num_features, hidden_size))`
It is the regular deeply connected neural network **layer**. It is most common and frequently used **layer**. **Dense layer** does the below operation on the input and return the output. (self.dense)

Dropout:

```
self.dropout3 = nn.Dropout(0.4)
```

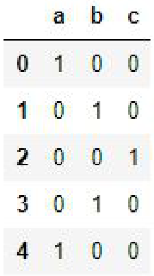
It is a regularization method that approximates training a large number of neural networks with different architectures in parallel. During training, some number of layer outputs are randomly ignored or "*dropped out*." This has the effect of making the layer look-like and be treated-like a layer with a different number of nodes and connectivity to the prior layer. In effect, each update to a layer during training is performed with a different "*view*" of the configured layer. Dropout has the effect of making the training process noisy, forcing nodes within a layer to probabilistically take on more or less responsibility for the inputs.This conceptualization suggests that perhaps dropout breaks-up situations where network layers co-adapt to correct mistakes from prior layers, in turn making the model more robust Dropout simulates a sparse activation from a given layer, which interestingly, in turn, encourages the network to actually learn a sparse representation as a side-effect. As such, it may be used as an alternative to activity regularization for encouraging sparse representations in autoencoder models.

PREPROCESSING DATA:-

_pandas.get_dummies() is used for data manipulation. It converts categorical data into dummy or indicator variables.

```
import pandas as pd
con = pd.Series(list('abcba'))
print(pd.get_dummies(con))
```

Output:

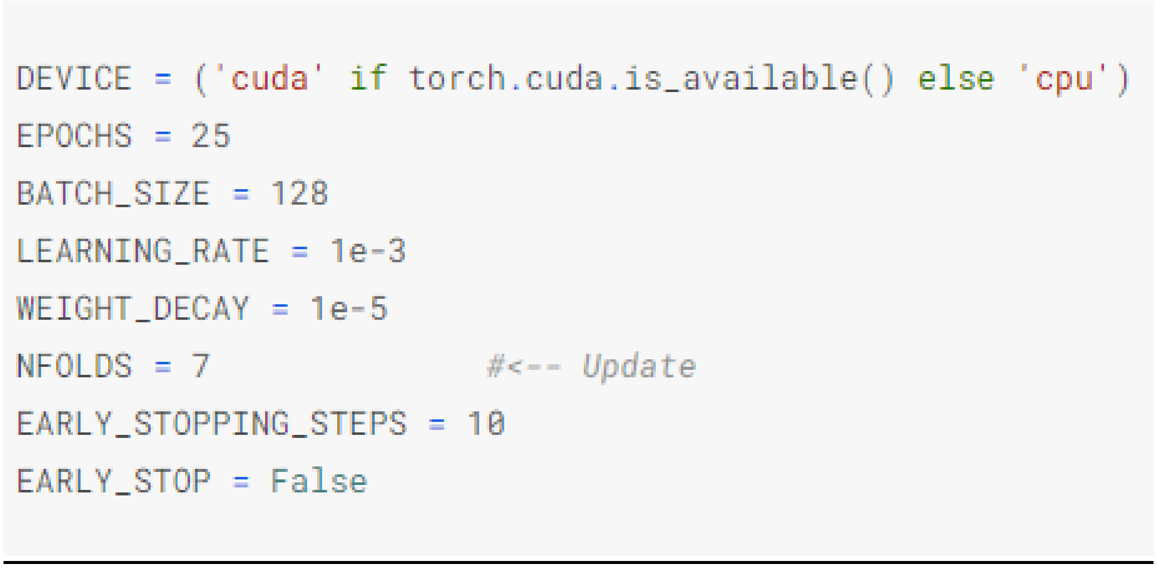


	a	b	c
0	1	0	0
1	0	1	0
2	0	0	1
3	0	1	0
4	1	0	0

```
   data = pd.get_dummies(data, columns=['cp_time','cp_dose'])
```

We did it for the 2 columns cp_time and cp_dose.

CHOOSING HYPERPARAMTERES BASED ON OUR MODEL:-



```
DEVICE = ('cuda' if torch.cuda.is_available() else 'cpu')
EPOCHS = 25
BATCH_SIZE = 128
LEARNING_RATE = 1e-3
WEIGHT_DECAY = 1e-5
NFOLDS = 7                #<-- Update
EARLY_STOPPING_STEPS = 10
EARLY_STOP = False
```

In machine learning, **hyperparameter optimization** or tuning is the problem of choosing a set of optimal hyperparameters for a learning algorithm. A hyperparameter is a parameter whose value is used to control the learning process. By contrast, the values of other parameters (typically node weights) are learned.

The same kind of machine learning model can require different constraints, weights or learning rates to generalize different data patterns. These measures are called hyperparameters, and have to be tuned so that the model can optimally solve the machine learning problem. Hyperparameter optimization finds a tuple of hyperparameters that yields an optimal model which minimizes a predefined loss function on given independent data.[1] The objective function takes a tuple of hyperparameters and returns the associated loss.[1] Cross-validation is often used to estimate this generalization performance.[2]

Epoch:-

It is a term used in machine learning and indicates the number of passes of the entire training dataset the machine learning algorithm has completed. Datasets are usually grouped into batches (especially when the amount of data is very large). Some people use the term iteration loosely and refer to putting one batch through the model as an iteration.

If the batch size is the whole training dataset then the number of epochs is the number of iterations. For practical reasons, this is usually not the case. Many models are created with more than one epoch. The general relation where dataset size is *d*, number of epochs is *e*, number of iterations is *i*, and batch size is *b* would be $d*e = i*b$. We choose epochs=128 because a model should run to train is based on many parameters related to both the data itself and the goal of the model, and while there have been efforts to turn this process into an algorithm and deep understanding of the data. Here we have decided the epoch and batch size according to the model and data visualization. We got good output and results after trial and error with many other model epochs and batch size

The learning rate :-

It is a hyperparameter that controls how much to change the model in response to the estimated error each time the model weights are updated. Choosing the learning rate is challenging as a value too small may result in a long training process that could get stuck, whereas a value too large may result in learning a sub-optimal set of weights too fast or an unstable training process. The learning rate may be the most important hyperparameter when configuring your neural network. Therefore it is vital to know how to investigate the effects of the learning rate on model performance and to build an intuition about the dynamics of the learning rate on model behavior. Here we have used a general learning rate for multilabel classification problem and it worked out for our dataset. By increasing the learning rate te system showed too much of loss and by decreasing the rate it became slower. So based on that we have generalized our learning rate. We also decided our learning rate on the factos such as :- How large learning rates result in unstable training and tiny rates result in a failure to train, Momentum can accelerate training and learning rate schedules can help to converge the optimization process, Adaptive learning rates can accelerate training and alleviate some of the pressure of choosing a learning rate and learning rate schedule.

Early Stopping:-

It is a form of regularization used to avoid overfitting when training a learner with an iterative method, such as gradient descent. Such methods update the learner so as to make it better fit the training data with each iteration. Up to a point, this improves the learner's performance on data outside of the training set. Past that point, however, improving the learner's fit to the training data comes at the expense of increased generalization error. Early stopping rules provide guidance as to how many iterations can be run before the learner begins to over-fit. Early stopping rules have been employed in many different machine learning methods, with varying amounts of theoretical foundation.

Weight Decay:-

Generally a wd = 0.00001 works pretty well. However, the folks at fastai have been a little conservative in this respect. Hence the default value of weight decay in fastai is actually 0.00001 . The reason to choose this value is because if you have too much weight decay, then no matter how much you train, the model never quite fits well enough whereas if you have too little weight decay, you can still train well, you just have to stop a little bit early.

N folds:-Here N folds is defined as the number of times the model will do training Iteration in order to average CV loss.

TRAINING FUNCTION:-

MULTIFOLD TRAINING FUNCTION = N * SINGLEFOLD TRAINING FUNCTION

SINGLE FOLD TRAINING FUNCTION :-

It follows the pipeline as given below. This is a generalized pytorch training function pipeline

- Pre-Processing raw train and test data.
- Converting it into tensor format.
- Defining Neural net model function, optimizer, scheduler, early stopping and loss.
- Iterating over epochs and training the model by passing the defined parameters by using Train and validation function.
- Saving the Validation and Train Loss in a list while training.
- Separating Minimum Losses in a list called as Best Losses.
- After iterations end it moves to evaluate the Train model on Test set by using Inference func.
- Once that is done the function return out of fold predictions and Test set predictions

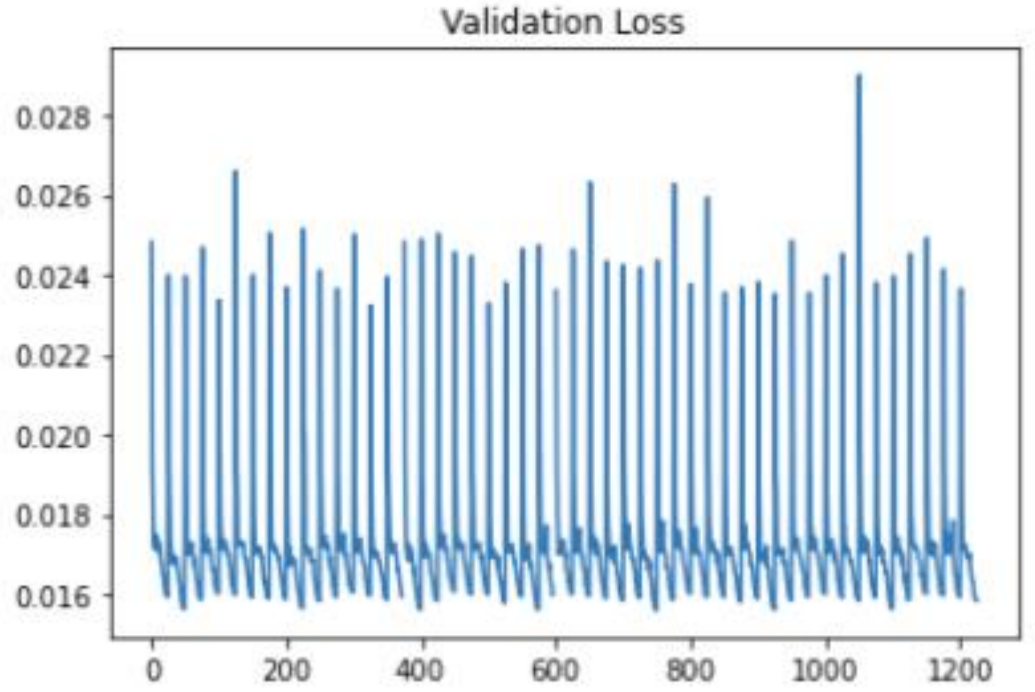
Here Number of Seed is used to repeat the steps given above in order to minimize the CV Log loss and to average it on multiple seeds.

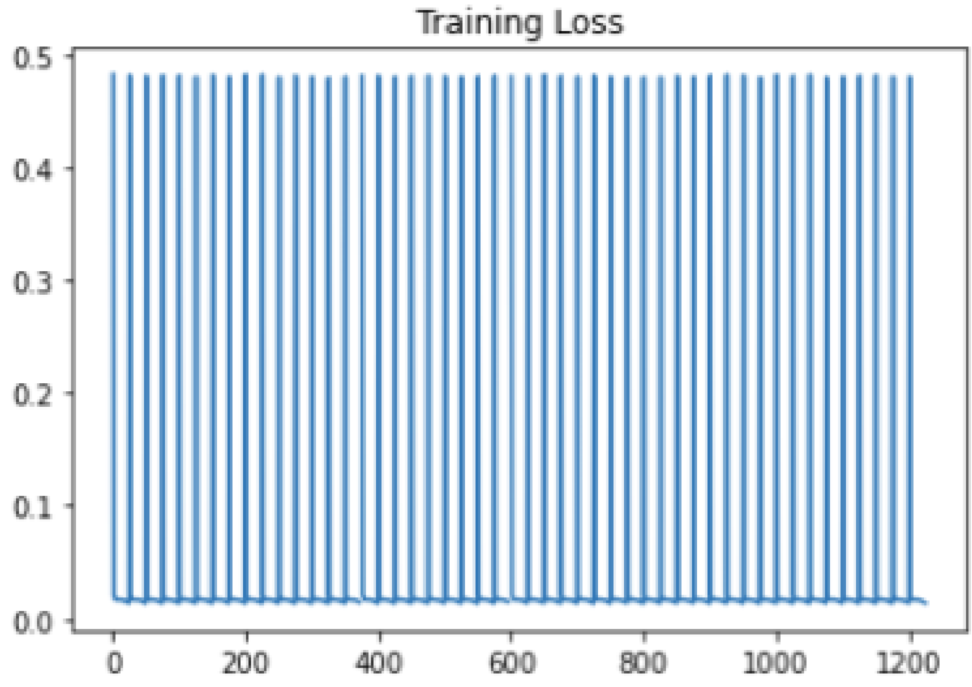
CALCULATING CV LOG LOSS:-

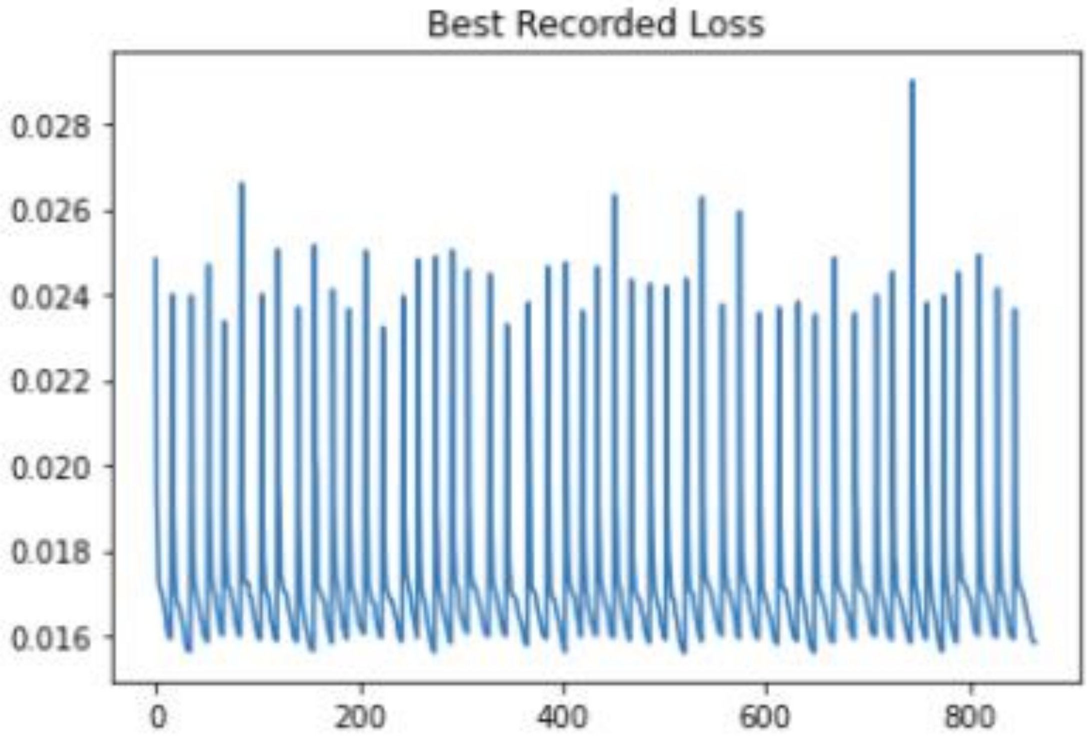
This is the loss function used in (multinomial) logistic regression and extensions of it such as neural networks, defined as the negative log-likelihood of a logistic model that returns y_pred probabilities for its training data y_true. The log loss is only defined for two or more labels. For a single sample with true label yt in {0,1} and estimated probability yp that yt = 1, the log loss is

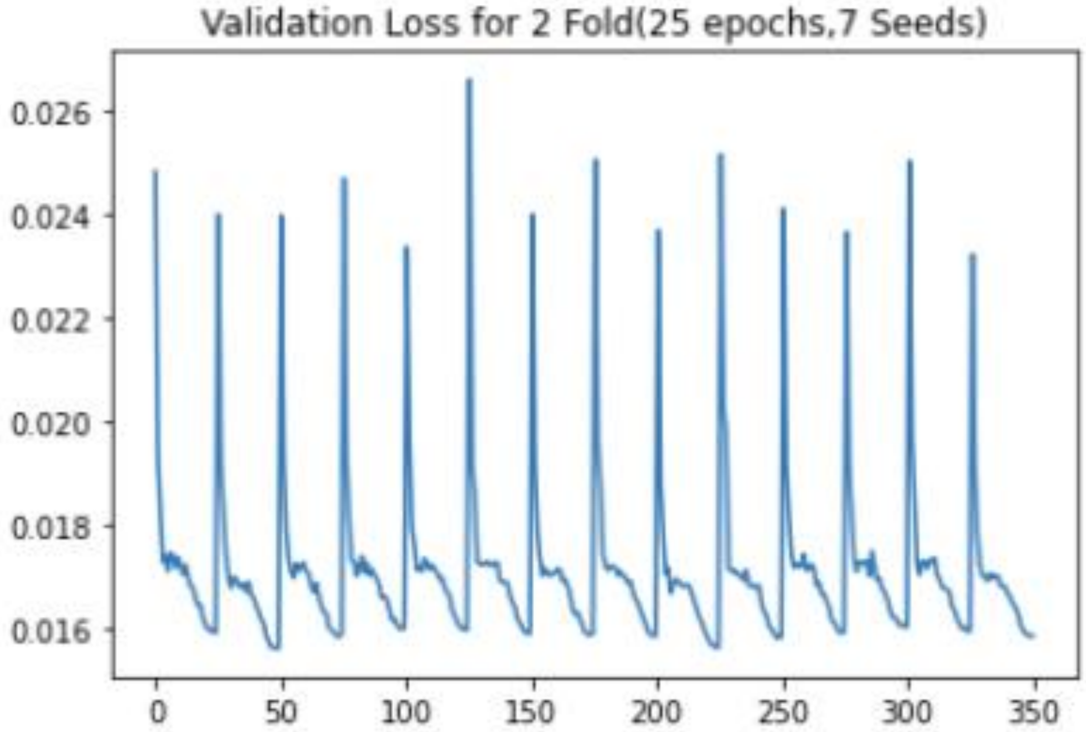
$-\log P(yt|yp) = -(yt \log(yp) + (1 - yt) \log(1 - yp))$

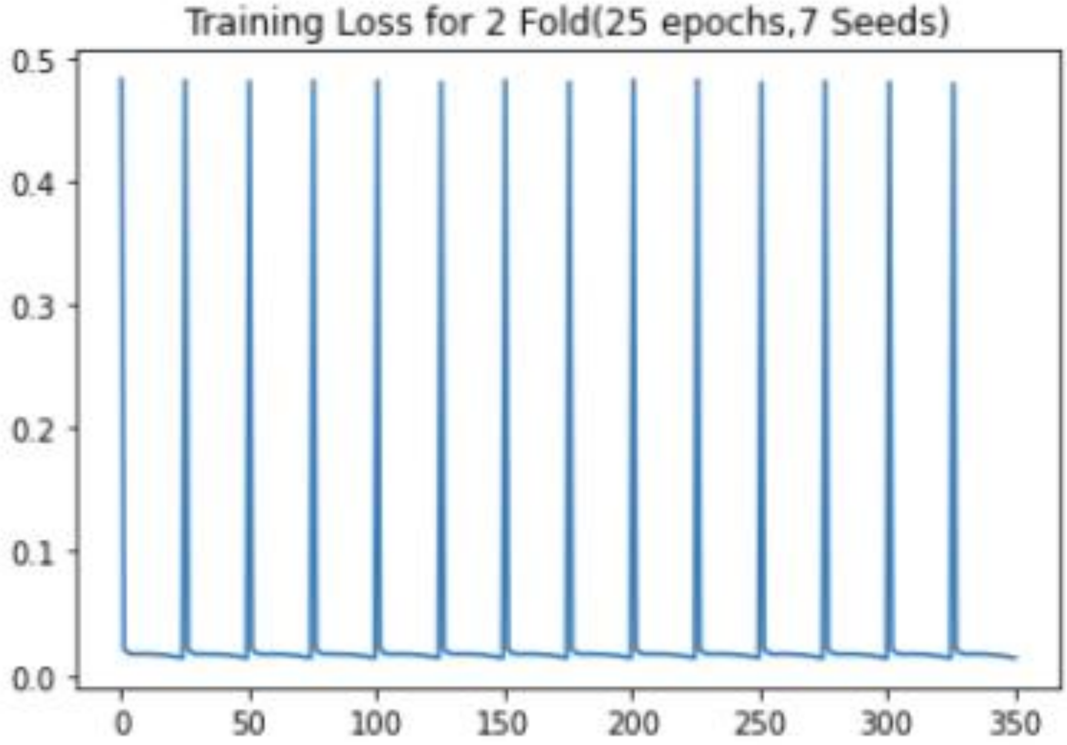
LEARNING AND VALIDATION CURVES:- (Loss vs (Seed*Epoch*Folds))

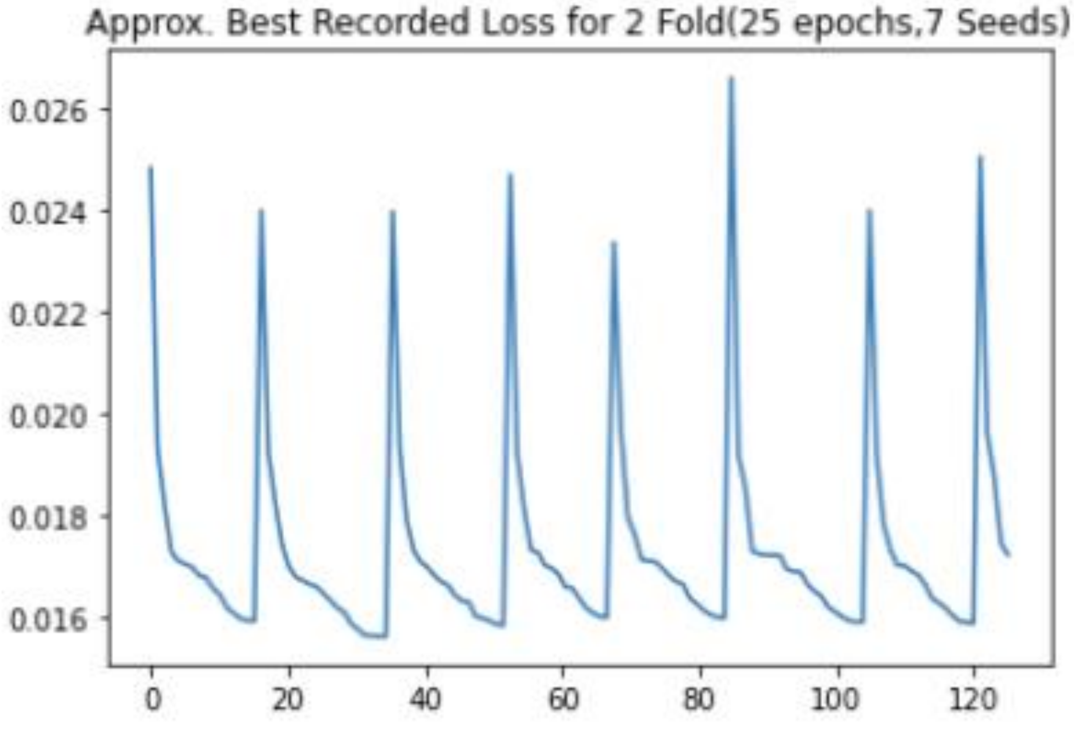





Best Recorded Loss
0.028
0.026
0.024
0.022
0.020
0.018
0.016
0
200
400
600
800


Validation Loss for 2 Fold(25 epochs,7 Seeds)
0.026
0.024
0.022
0.020
0.018
0.016
0
50
100
150
200
250
300
350


Training Loss for 2 Fold(25 epochs,7 Seeds)
0.5
0.4
0.3
0.2
0.1
0.0
0
50
100
150
200
250
300
350


Approx. Best Recorded Loss for 2 Fold(25 epochs,7 Seeds)
0.026
0.024
0.022
0.020
0.018
0.016
0
20
40
60
80
100
120

GENERATING PREDICTION FILE:-

Here we will merge the prediction and the test target and align that data with the proper heading into the submission.csv

SUBMITTING AND OBTAINING SCORE:-

Here For every `sig_id` you will be predicting the probability that the sample had a positive response for each `<MoA>` target. For NN `sig_id` rows and MM `<MoA>` targets, you will be making N×MN×M predictions. Submissions are scored by the log loss:

$$\text{score} = -\frac{1}{M}\sum_{m=1}^{M}\frac{1}{N}\sum_{i=1}^{N}\left[y_{i,m}\log(\hat{y}_{i,m}) + (1-y_{i,m})\log(1-\hat{y}_{i,m})\right]$$

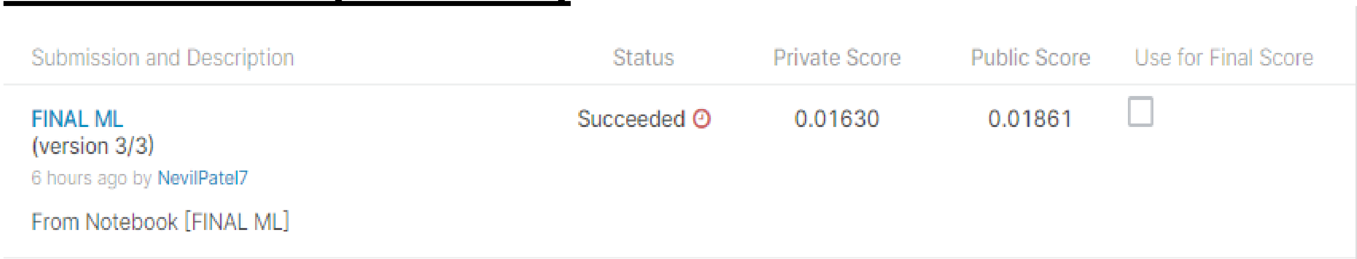
where:

- NN is the number of `sig_id` observations in the test data (i=1,…,Ni=1,…,N)
- MM is the number of scored MoA targets (m=1,…,Mm=1,…,M)
- y^i,my^i,m is the predicted probability of a positive `MoA` response for a `sig_id`
- yi,myi,m is the ground truth, 1 for a positive response, 0 otherwise
- log()log() is the natural (base e) logarithm

Note: the actual submitted predicted probabilities are replaced with max(min(p,1−10−15),10−15)max(min(p,1−10−15),10−15). A smaller log loss is better.

Number of Folds	CV Log Loss
1	0.1323
3	0.0737
4	0.0625
5	0.0239
7	0.01456
9	0.05627

FINAL SCORE(Folds = 7)



Submission and Description	Status	Private Score	Public Score	Use for Final Score
FINAL ML (version 3/3) 6 hours ago by NevilPatel7 From Notebook [FINAL ML]	Succeeded	0.01630	0.01861	□

REFERENCES:-

https://data36.com/pandas-tutorial-1-basics-reading-data-files-dataframes-data-selection/

https://pytorch.org/docs/stable/generated/torch.nn.BCEWithLogitsLoss.html

https://pytorch.org/docs/stable/optim.html

https://link.springer.com/referenceworkentry/10.1007%2F978-1-4419-9863-7_233#:~:text=Definition,the%20training%20set%20is%20derived.

https://datascience.stackexchange.com/questions/40275/multi-class-neural-networks-different-features

https://machinelearningmastery.com/dropout-for-regularizing-deep-neural-networks/

https://www.geeksforgeeks.org/python-pandas-get_dummies-method/#:~:text=get_dummies()%20is%20used%20for,into%20dummy%20or%20indicator%20variables

https://www.kaggle.com/

CODE:-

MoA DATA VISUALIZATION:-

```
import numpy as np  # linear algebra
import pandas as pd  # data processing, CSV file I/O (e.g. pd.read_csv)
from sklearn.model_selection import train_test_split
import matplotlib.pyplot as plt
import plotly.express as px
import random
import seaborn as sns
from colorama import Fore, Back, Style

y_ = Fore.YELLOW
r_ = Fore.RED
g_ = Fore.GREEN
b_ = Fore.BLUE
m_ = Fore.MAGENTA
sr_ = Style.RESET_ALL

def plotCounterPlot(feature):
    plt.figure(dpi=90)
    sns.countplot(train_data[feature])
    counts = train_data[feature].value_counts()
    for i in range(len(counts)):
        print(f"{b_}count of {counts.index[i]} is: {r_}{counts.values[i]}")


def plotDistribution(feature, color):
    plt.figure(figsize=(15,7))
    plt.subplot(121)
    sns.distplot(train_data[feature],color=color)
    plt.subplot(122)
    sns.violinplot(train_data[feature])
    print("{}Max value of {} is: {} {:.2f} \n{}Min value of {} is: {} {:.2f}\n{}Mean of {} is: {}{:.2f}\n{}Standard Deviation of {} is:{}{:.2f}"\

.format(y_,feature,r_,train_data[feature].max(),g_,feature,r_,train_data[feature].min(),b_,feature,r_,train_data[feature].mean(),m_,feature,r_,train_data[feature].std()))
# Input data files are available in the Kaggle/input/lish-moa

train_data = pd.read_csv('Kaggle/input/lish-moa/train_features.csv')
train_target = pd.read_csv('Kaggle/input/lish-moa/train_targets_scored.csv')

print('train_data shape is {}'.format(train_data.shape))
print("train_target shape is {}".format(train_target.shape))

#From Above , it seems number of data is 2E4, which is avergage number. The main things to note
#here is that: a) Number of features is 876, which is quite large. b) Number of labels for single data
```

```
#prediction is 207, which is also above average.


train_data, test_data , train_target, test_target  =
train_test_split(train_data,train_target, test_size=0.2)


print("sample_train data\n")
print(train_data.head())
print("")


NGTypeFeature = sum(train_data.columns.to_series().str.contains('g-') == True )
NCTypeFeature = sum(train_data.columns.to_series().str.contains('c-') == True )

print("GENE_TypeFeature = {} \nCELL_TypeFeature = {}".format(NGTypeFeature ,
NCTypeFeature))

plotCounterPlot('cp_type')
plt.title("CP_TYPE")
# plt.show()
print("")

plotCounterPlot('cp_time')
plt.title("CP_TIME")
# plt.show()
print("")

plotCounterPlot('cp_dose')
plt.title("CP_DOSE")
# plt.show()
print("")

print(train_data.describe())

print("Checking if train_data is in Panda or other format:
{}".format((type(train_data))))

print(train_data.head())

NDataRow , NDataCol = train_data.shape
print("Number Of Sample on which testing is done = {}  \nNumber of Feature which are
recorded = {}".format(NDataRow,NDataCol))

df = train_target.iloc[:,1:].sum(axis=0).sort_values(ascending=True)[-50:]
fig = px.bar(x=df.values,y = df.index,color=df.values)
fig.show()

plotDistribution("g-0" , "blue")
plt.title("G-0")

plotDistribution("g-12" , "blue")
plt.title("G-12")

plotDistribution("g-20" , "blue")
```

```
plt.title("G-20")

plotDistribution("g-40" , "blue")
plt.title("G-40")

plotDistribution("g-60" , "blue")
plt.title("G-60")

plotDistribution("c-30" , "blue")
plt.title("C-30")

plotDistribution("c-60" , "blue")
plt.title("C-60")

plotDistribution("c-99" , "blue")
plt.title("C-99")
plt.show()

minValOfFeature = min(train_data.min(axis = 1))
maxValOfFeature = max (train_data.iloc[: , 4:].max(axis = 1))
print("min Feature data = {} , maxvalOfFeature = {}".format(minValOfFeature ,
maxValOfFeature))
```

MoA Machine Learning Pipeline CODE:-

final-ml (1)

December 15, 2020

[74]:
```
# This Python 3 environment comes with many helpful analytics libraries␣
↪installed
# It is defined by the kaggle/python Docker image: https://github.com/kaggle/
↪docker-python
# For example, here's several helpful packages to load

import numpy as np # linear algebra
import pandas as pd # data processing, CSV file I/O (e.g. pd.read_csv)

# Input data files are available in the read-only "../input/" directory
# For example, running this (by clicking run or pressing Shift+Enter) will list␣
↪all files under the input directory

import os
for dirname, _, filenames in os.walk('/kaggle/input'):
    for filename in filenames:
        print(os.path.join(dirname, filename))

# You can write up to 20GB to the current directory (/kaggle/working/) that␣
↪gets preserved as output when you create a version using "Save & Run All"
# You can also write temporary files to /kaggle/temp/, but they won't be saved␣
↪outside of the current session
```

```
/kaggle/input/iterativestratification/.travis.yml
/kaggle/input/iterativestratification/setup.cfg
/kaggle/input/iterativestratification/LICENSE
/kaggle/input/iterativestratification/.gitignore
/kaggle/input/iterativestratification/README.md
/kaggle/input/iterativestratification/setup.py
/kaggle/input/iterativestratification/tests/test_ml_stratifiers.py
/kaggle/input/iterativestratification/tests/__init__.py
/kaggle/input/iterativestratification/iterstrat/ml_stratifiers.py
/kaggle/input/iterativestratification/iterstrat/__init__.py
/kaggle/input/lish-moa/train_targets_scored.csv
/kaggle/input/lish-moa/sample_submission.csv
/kaggle/input/lish-moa/train_drug.csv
/kaggle/input/lish-moa/train_targets_nonscored.csv
```

```
/kaggle/input/lish-moa/train_features.csv
/kaggle/input/lish-moa/test_features.csv
```

[75]:

```
import sys
sys.path.append('../input/iterativestratification')
from iterstrat.ml_stratifiers import MultilabelStratifiedKFold

import numpy as np
import random
import pandas as pd
import matplotlib.pyplot as plt
import os
import copy
import seaborn as sns

from sklearn import preprocessing
from sklearn.metrics import log_loss
from sklearn.preprocessing import StandardScaler
from sklearn.decomposition import PCA

import torch
import torch.nn as nn
import torch.nn.functional as F
import torch.optim as optim

import warnings
warnings.filterwarnings('ignore')

from sklearn.preprocessing import QuantileTransformer
```

1 Reading the Data Files

[76]:

```
os.listdir('../input/lish-moa')

train_features = pd.read_csv('../input/lish-moa/train_features.csv')
train_targets_scored = pd.read_csv('../input/lish-moa/train_targets_scored.csv')
train_targets_nonscored = pd.read_csv('../input/lish-moa/
 ↪train_targets_nonscored.csv')

test_features = pd.read_csv('../input/lish-moa/test_features.csv')
sample_submission = pd.read_csv('../input/lish-moa/sample_submission.csv')
```

2 *RankGauss on Train & Test Data Set*

[77]:

```
GENES = [col for col in train_features.columns if col.startswith('g-')]
CELLS = [col for col in train_features.columns if col.startswith('c-')]



for col in (GENES + CELLS):

    transformer = QuantileTransformer(n_quantiles=100,random_state=0,␣
 ↪output_distribution="normal")
    vec_len = len(train_features[col].values)
    vec_len_test = len(test_features[col].values)
    raw_vec = train_features[col].values.reshape(vec_len, 1)
    transformer.fit(raw_vec)

    train_features[col] = transformer.transform(raw_vec).reshape(1, vec_len)[0]
    test_features[col] = transformer.transform(test_features[col].values.
 ↪reshape(vec_len_test, 1)).reshape(1, vec_len_test)[0]
```

3 PCA + Normal Features

[78]:

```
def seed_everything(seed=42):
    random.seed(seed)
    os.environ['PYTHONHASHSEED'] = str(seed)
    np.random.seed(seed)
    torch.manual_seed(seed)
    torch.cuda.manual_seed(seed)
    torch.backends.cudnn.deterministic = True

seed_everything(seed=42)
```

[79]:

```
n_comp = 600  #<--Update

data = pd.concat([pd.DataFrame(train_features[GENES]), pd.
 ↪DataFrame(test_features[GENES])])
data2 = (PCA(n_components=n_comp, random_state=42).fit_transform(data[GENES]))
train2 = data2[:train_features.shape[0]]; test2 = data2[-test_features.shape[0]:
 ↪]

train2 = pd.DataFrame(train2, columns=[f'pca_G-{i}' for i in range(n_comp)])
test2 = pd.DataFrame(test2, columns=[f'pca_G-{i}' for i in range(n_comp)])

# drop_cols = [f'c-{i}' for i in range(n_comp,len(GENES))]
train_features = pd.concat((train_features, train2), axis=1)
```

```
test_features = pd.concat((test_features, test2), axis=1)
```

[80]:

```
n_comp = 50  #<--Update

data = pd.concat([pd.DataFrame(train_features[CELLS]), pd.
 ↪DataFrame(test_features[CELLS])])
data2 = (PCA(n_components=n_comp, random_state=42).fit_transform(data[CELLS]))
train2 = data2[:train_features.shape[0]]; test2 = data2[-test_features.shape[0]:
 ↪]

train2 = pd.DataFrame(train2, columns=[f'pca_C-{i}' for i in range(n_comp)])
test2 = pd.DataFrame(test2, columns=[f'pca_C-{i}' for i in range(n_comp)])

# drop_cols = [f'c-{i}' for i in range(n_comp,len(CELLS))]
train_features = pd.concat((train_features, train2), axis=1)
test_features = pd.concat((test_features, test2), axis=1)
```

[81]:

```
train_features.shape
```

[81]:

```
(23814, 1526)
```

4 BEST FEATURE SELECTION(VARIANCE ENCODING)

[82]:

```
from sklearn.feature_selection import VarianceThreshold


var_thresh = VarianceThreshold(0.8)  #<-- Update
data = train_features.append(test_features)
data_transformed = var_thresh.fit_transform(data.iloc[:, 4:])

train_features_transformed = data_transformed[ : train_features.shape[0]]
test_features_transformed = data_transformed[-test_features.shape[0] : ]


train_features = pd.
 ↪DataFrame(train_features[['sig_id','cp_type','cp_time','cp_dose']].values.
 ↪reshape(-1, 4),\
                              columns=['sig_id','cp_type','cp_time','cp_dose'])

train_features = pd.concat([train_features, pd.
 ↪DataFrame(train_features_transformed)], axis=1)


test_features = pd.
 ↪DataFrame(test_features[['sig_id','cp_type','cp_time','cp_dose']].values.
 ↪reshape(-1, 4),\
                              columns=['sig_id','cp_type','cp_time','cp_dose'])

test_features = pd.concat([test_features, pd.
 ↪DataFrame(test_features_transformed)], axis=1)


train = train_features.merge(train_targets_scored, on='sig_id')
train = train[train['cp_type']!='ctl_vehicle'].reset_index(drop=True)
test = test_features[test_features['cp_type']!='ctl_vehicle'].
 ↪reset_index(drop=True)

target = train[train_targets_scored.columns]

train = train.drop('cp_type', axis=1)
test = test.drop('cp_type', axis=1)
target_cols = target.drop('sig_id', axis=1).columns.values.tolist()

train_features.shape
```

[82]:

```
(23814, 1040)
```

5 CV FOLDS

[83]:

```
folds = train.copy()

mskf = MultilabelStratifiedKFold(n_splits=7)

for f, (t_idx, v_idx) in enumerate(mskf.split(X=train, y=target)):
    folds.loc[v_idx, 'kfold'] = int(f)

folds['kfold'] = folds['kfold'].astype(int)


print(train.shape)
print(folds.shape)
print(test.shape)
print(target.shape)
print(sample_submission.shape)
folds
```

```
(21948, 1245)
(21948, 1246)
(3624, 1039)
(21948, 207)
(3982, 207)
```

```
[83]:             sig_id cp_time cp_dose         0         1         2         3  \
      0      id_000644bb2      24      D1  1.134849  0.907687 -0.416385 -0.966814
      1      id_000779bfc      72      D1  0.119282  0.681738  0.272399  0.080113
      2      id_000a6266a      48      D1  0.779973  0.946463  1.425350 -0.132928
      3      id_0015fd391      48      D1 -0.734910 -0.274641 -0.438509  0.759097
      4      id_001626bd3      72      D2 -0.452718 -0.477513  0.972316  0.970731
      …               …     …       …       …         …         …        …
      21943  id_fff8c2444      72      D1  0.237856 -1.228203  0.218376 -0.365976
      21944  id_fffb1ceed      24      D2  0.209361 -0.022389 -0.235888 -0.796989
      21945  id_fffb70c0c      24      D2 -1.911021  0.587228 -0.588417  1.296405
      21946  id_fffcb9e7c      24      D1  0.816407  0.417618  0.431631  0.300617
      21947  id_ffffdd77b      72      D1 -1.243096  1.567730 -0.269573  1.083636

                    4         5         6  …  trpv_agonist  trpv_antagonist  \
      0     -0.254723 -1.017473 -1.364787  …             0                0
      1      1.205169  0.686517  0.313396  …             0                0
      2     -0.006122  1.492493  0.235577  …             0                0
      3      2.346330 -0.858153 -2.288417  …             0                0
      4      1.463427 -0.869555 -0.375501  …             0                0
      …           …         …         …  …           …              …
      21943 -0.330177  0.569243 -0.150978  …             0                0
      21944 -0.674009  0.919312  0.735603  …             0                0
      21945 -1.002640  0.850589 -0.304313  …             0                0
      21946  1.070346 -0.024189  0.048942  …             0                0
      21947 -0.511235 -2.099634 -1.622462  …             0                0

             tubulin_inhibitor  tyrosine_kinase_inhibitor  \
      0                      0                          0
      1                      0                          0
      2                      0                          0
      3                      0                          0
      4                      0                          0
      …                    …                          …
      21943                  0                          0
      21944                  0                          0
      21945                  0                          0
      21946                  0                          0
      21947                  0                          0

             ubiquitin_specific_protease_inhibitor  vegfr_inhibitor  vitamin_b  \
      0                                          0                0          0
      1                                          0                0          0
      2                                          0                0          0
      3                                          0                0          0
      4                                          0                0          0
      …                                        …                …        …
      21943                                      0                0          0
```

```
21944                                      0               0          0
21945                                      0               0          0
21946                                      0               0          0
21947                                      0               0          0

       vitamin_d_receptor_agonist  wnt_inhibitor  kfold
0                               0              0      5
1                               0              0      0
2                               0              0      6
3                               0              0      0
4                               0              0      4
…                           …            …    …
21943                           0              0      5
21944                           0              0      1
21945                           0              0      5
21946                           0              0      1
21947                           0              0      6

[21948 rows x 1246 columns]
```

6 DEFINING CLASSES(DATASET,TRAIN,VALID,INFERENCE)

[84]:
```python
class MoADataset:
    def __init__(self, features, targets):
        self.features = features
        self.targets = targets

    def __len__(self):
        return (self.features.shape[0])

    def __getitem__(self, idx):
        dct = {
            'x' : torch.tensor(self.features[idx, :], dtype=torch.float),
            'y' : torch.tensor(self.targets[idx, :], dtype=torch.float)
        }
        return dct

class TestDataset:
    def __init__(self, features):
        self.features = features

    def __len__(self):
        return (self.features.shape[0])

    def __getitem__(self, idx):
        dct = {
            'x' : torch.tensor(self.features[idx, :], dtype=torch.float)
        }
        return dct

def train_fn(model, optimizer, scheduler, loss_fn, dataloader, device):
    model.train()
    final_loss = 0

    for data in dataloader:
        optimizer.zero_grad()
        inputs, targets = data['x'].to(device), data['y'].to(device)
#         print(inputs.shape)
        outputs = model(inputs)
        loss = loss_fn(outputs, targets)
        loss.backward()
        optimizer.step()
        scheduler.step()

        final_loss += loss.item()

    final_loss /= len(dataloader)

    return final_loss

def valid_fn(model, loss_fn, dataloader, device):
    model.eval()
    final_loss = 0
    valid_preds = []

    for data in dataloader:
        inputs, targets = data['x'].to(device), data['y'].to(device)
        outputs = model(inputs)
        loss = loss_fn(outputs, targets)

        final_loss += loss.item()
        valid_preds.append(outputs.sigmoid().detach().cpu().numpy())

    final_loss /= len(dataloader)
    valid_preds = np.concatenate(valid_preds)

    return final_loss, valid_preds

def inference_fn(model, dataloader, device):
    model.eval()
    preds = []

    for data in dataloader:
        inputs = data['x'].to(device)

        with torch.no_grad():
            outputs = model(inputs)

        preds.append(outputs.sigmoid().detach().cpu().numpy())

    preds = np.concatenate(preds)

    return preds
```

7 MODEL

[85]:

```
class Model(nn.Module):      # <-- Update
    def __init__(self, num_features, num_targets, hidden_size):
        super(Model, self).__init__()
        self.batch_norm1 = nn.BatchNorm1d(num_features)
        self.dense1 = nn.utils.weight_norm(nn.Linear(num_features, hidden_size))

        self.batch_norm2 = nn.BatchNorm1d(hidden_size)
        self.dropout2 = nn.Dropout(0.4)
        self.dense2 = nn.utils.weight_norm(nn.Linear(hidden_size, hidden_size))

        self.batch_norm3 = nn.BatchNorm1d(hidden_size)
        self.dropout3 = nn.Dropout(0.4)
        self.dense3 = nn.utils.weight_norm(nn.Linear(hidden_size, num_targets))

    def forward(self, x):
        x = self.batch_norm1(x)
        x = F.relu(self.dense1(x))

        x = self.batch_norm2(x)
        x = self.dropout2(x)
        x = F.relu(self.dense2(x))

        x = self.batch_norm3(x)
        x = self.dropout3(x)
        x = self.dense3(x)

        return x
```

8 PREPROCESSING DATA

[86]:
```
def process_data(data):
    data = pd.get_dummies(data, columns=['cp_time','cp_dose'])
    return data

feature_cols = [c for c in process_data(folds).columns if c not in target_cols]
feature_cols = [c for c in feature_cols if c not in ['kfold','sig_id']]
len(feature_cols)
```

[86]:
```
1041
```

9 HYPERPARAMETERS

[87]:
```
DEVICE = ('cuda' if torch.cuda.is_available() else 'cpu')
EPOCHS = 25
BATCH_SIZE = 128
LEARNING_RATE = 1e-3
WEIGHT_DECAY = 1e-5
NFOLDS = 7              #<-- Update
EARLY_STOPPING_STEPS = 10
EARLY_STOP = False

num_features=len(feature_cols)
num_targets=len(target_cols)
hidden_size=2048
```

[88]:
```
# to plot validation loss
train_loss_ = []
# to plot the training loss
valid_loss_ = []
# to plot the best recorded loss
best_loss_ = []
```

10 DEFINING SINGLE AND MULTIFOLD TRAINING FUNCTION

[89]:
```
def run_training(fold, seed):
    global train_loss_
    global valid_loss_
    global best_loss_

    seed_everything(seed)

    train = process_data(folds)
    test_ = process_data(test)
    trn_idx = train[train['kfold'] != fold].index
    val_idx = train[train['kfold'] == fold].index

    train_df = train[train['kfold'] != fold].reset_index(drop=True)
    valid_df = train[train['kfold'] == fold].reset_index(drop=True)

    x_train, y_train  = train_df[feature_cols].values, train_df[target_cols].
↪values
    x_valid, y_valid =  valid_df[feature_cols].values, valid_df[target_cols].
↪values

    train_dataset = MoADataset(x_train, y_train)
    valid_dataset = MoADataset(x_valid, y_valid)
    trainloader = torch.utils.data.DataLoader(train_dataset,␣
↪batch_size=BATCH_SIZE, shuffle=True)
    validloader = torch.utils.data.DataLoader(valid_dataset,␣
↪batch_size=BATCH_SIZE, shuffle=False)

    model = Model(
        num_features=num_features,
        num_targets=num_targets,
        hidden_size=hidden_size,
    )

    model.to(DEVICE)
    optimizer = torch.optim.Adam(model.parameters(), lr=LEARNING_RATE,␣
↪weight_decay=WEIGHT_DECAY)
    scheduler = optim.lr_scheduler.OneCycleLR(optimizer=optimizer, pct_start=0.
↪1, div_factor=1e3,
                                              max_lr=1e-2, epochs=EPOCHS,␣
↪steps_per_epoch=len(trainloader))

    loss_fn = nn.BCEWithLogitsLoss()

    early_stopping_steps = EARLY_STOPPING_STEPS
    early_step = 0

    oof = np.zeros((len(train), target.iloc[:, 1:].shape[1]))
    best_loss = np.inf

    for epoch in range(EPOCHS):

        train_loss = train_fn(model, optimizer,scheduler, loss_fn, trainloader,␣
↪DEVICE)
        train_loss_.append(train_loss)
        print(f"FOLD: {fold}, EPOCH: {epoch}, train_loss: {train_loss}")
        valid_loss, valid_preds = valid_fn(model, loss_fn, validloader, DEVICE)
        valid_loss_.append(valid_loss)
        print(f"FOLD: {fold}, EPOCH: {epoch}, valid_loss: {valid_loss}")

        if valid_loss < best_loss:

            best_loss = valid_loss
            best_loss_.append(best_loss)
            oof[val_idx] = valid_preds
            torch.save(model.state_dict(), f"FOLD{fold}_.pth")

        elif(EARLY_STOP == True):

            early_step += 1
            if (early_step >= early_stopping_steps):
                break


    #--------------------- PREDICTION---------------------
    x_test = test_[feature_cols].values
    testdataset = TestDataset(x_test)
    testloader = torch.utils.data.DataLoader(testdataset, batch_size=BATCH_SIZE, shuffle=False)

    model = Model(
        num_features=num_features,
        num_targets=num_targets,
        hidden_size=hidden_size,

    )

    model.load_state_dict(torch.load(f"FOLD{fold}_.pth"))
    model.to(DEVICE)

    predictions = np.zeros((len(test_), target.iloc[:, 1:].shape[1]))
    predictions = inference_fn(model, testloader, DEVICE)

    return oof, predictions


def run_k_fold(NFOLDS, seed):
    oof = np.zeros((len(train), len(target_cols)))
    predictions = np.zeros((len(test), len(target_cols)))

    for fold in range(NFOLDS):
        oof_, pred_ = run_training(fold, seed)
        predictions += pred_ / NFOLDS
        oof += oof_

    return oof, predictions
```

11 TRAINING AND TESTING

[90]:

```
# Averaging on multiple SEEDS

SEED = [0, 1, 2, 3 ,4, 5 ,6]  #<-- Update
oof = np.zeros((len(train), len(target_cols)))
predictions = np.zeros((len(test), len(target_cols)))

for seed in SEED:

    oof_, predictions_ = run_k_fold(NFOLDS, seed)
    oof += oof_ / len(SEED)
    predictions += predictions_ / len(SEED)

train[target_cols] = oof
test[target_cols] = predictions
```

```
FOLD: 0, EPOCH: 0, train_loss: 0.48232868185811706
FOLD: 0, EPOCH: 0, valid_loss: 0.024814292937517166
FOLD: 0, EPOCH: 1, train_loss: 0.02107173926672157
FOLD: 0, EPOCH: 1, valid_loss: 0.019315823763608932
FOLD: 0, EPOCH: 2, train_loss: 0.018996933551163088
FOLD: 0, EPOCH: 2, valid_loss: 0.018227280303835868
FOLD: 0, EPOCH: 3, train_loss: 0.01764812731013006
FOLD: 0, EPOCH: 3, valid_loss: 0.017300846874713897
FOLD: 0, EPOCH: 4, train_loss: 0.017051006686322544
FOLD: 0, EPOCH: 4, valid_loss: 0.017407792396843435
FOLD: 0, EPOCH: 5, train_loss: 0.01694557220250571
FOLD: 0, EPOCH: 5, valid_loss: 0.017122614867985247
FOLD: 0, EPOCH: 6, train_loss: 0.016944134151753113
FOLD: 0, EPOCH: 6, valid_loss: 0.017487628497183324
FOLD: 0, EPOCH: 7, train_loss: 0.01701711434997669
FOLD: 0, EPOCH: 7, valid_loss: 0.017396538332104684
FOLD: 0, EPOCH: 8, train_loss: 0.01705438644327477
FOLD: 0, EPOCH: 8, valid_loss: 0.01718995697796345
FOLD: 0, EPOCH: 9, train_loss: 0.017072569477517587
FOLD: 0, EPOCH: 9, valid_loss: 0.017394925542175768
FOLD: 0, EPOCH: 10, train_loss: 0.01707026385860581
FOLD: 0, EPOCH: 10, valid_loss: 0.017227504588663577
```

```
FOLD: 0, EPOCH: 11, train_loss: 0.017071871802869704
FOLD: 0, EPOCH: 11, valid_loss: 0.01705886472016573
FOLD: 0, EPOCH: 12, train_loss: 0.01694477510442134
FOLD: 0, EPOCH: 12, valid_loss: 0.017242863439023495
FOLD: 0, EPOCH: 13, train_loss: 0.016834985806929822
FOLD: 0, EPOCH: 13, valid_loss: 0.017002611085772515
FOLD: 0, EPOCH: 14, train_loss: 0.016744794343046997
FOLD: 0, EPOCH: 14, valid_loss: 0.01683291345834732
FOLD: 0, EPOCH: 15, train_loss: 0.01654451344871805
FOLD: 0, EPOCH: 15, valid_loss: 0.016795877888798712
FOLD: 0, EPOCH: 16, train_loss: 0.016415288507127437
FOLD: 0, EPOCH: 16, valid_loss: 0.016584612652659415
FOLD: 0, EPOCH: 17, train_loss: 0.016158162020653687
FOLD: 0, EPOCH: 17, valid_loss: 0.016459527127444744
FOLD: 0, EPOCH: 18, train_loss: 0.015874763348830395
FOLD: 0, EPOCH: 18, valid_loss: 0.01646276954561472
FOLD: 0, EPOCH: 19, train_loss: 0.015568107081463143
FOLD: 0, EPOCH: 19, valid_loss: 0.016209116987884045
FOLD: 0, EPOCH: 20, train_loss: 0.01523009328437703
FOLD: 0, EPOCH: 20, valid_loss: 0.016090518794953823
FOLD: 0, EPOCH: 21, train_loss: 0.01476657761222854
FOLD: 0, EPOCH: 21, valid_loss: 0.015992887131869794
FOLD: 0, EPOCH: 22, train_loss: 0.01439099450956802
FOLD: 0, EPOCH: 22, valid_loss: 0.015996361672878264
FOLD: 0, EPOCH: 23, train_loss: 0.014070984020474412
FOLD: 0, EPOCH: 23, valid_loss: 0.015950537137687206
FOLD: 0, EPOCH: 24, train_loss: 0.01391883668344037
FOLD: 0, EPOCH: 24, valid_loss: 0.015938356928527356
FOLD: 1, EPOCH: 0, train_loss: 0.48164497100475695
FOLD: 1, EPOCH: 0, valid_loss: 0.023990048542618752
FOLD: 1, EPOCH: 1, train_loss: 0.02125996716168462
FOLD: 1, EPOCH: 1, valid_loss: 0.01925745338201523
FOLD: 1, EPOCH: 2, train_loss: 0.018982065341048907
FOLD: 1, EPOCH: 2, valid_loss: 0.01826371282339096
FOLD: 1, EPOCH: 3, train_loss: 0.017765485656251308
FOLD: 1, EPOCH: 3, valid_loss: 0.017435449585318567
FOLD: 1, EPOCH: 4, train_loss: 0.017055268855575397
FOLD: 1, EPOCH: 4, valid_loss: 0.01700600393116474
FOLD: 1, EPOCH: 5, train_loss: 0.016884893774479427
FOLD: 1, EPOCH: 5, valid_loss: 0.01680383525788784
FOLD: 1, EPOCH: 6, train_loss: 0.01696788412550477
FOLD: 1, EPOCH: 6, valid_loss: 0.01700858797878027
FOLD: 1, EPOCH: 7, train_loss: 0.01697442078722172
FOLD: 1, EPOCH: 7, valid_loss: 0.01698469549417496
FOLD: 1, EPOCH: 8, train_loss: 0.017057943442950443
FOLD: 1, EPOCH: 8, valid_loss: 0.01684837684035301
FOLD: 1, EPOCH: 9, train_loss: 0.01707357317082533
FOLD: 1, EPOCH: 9, valid_loss: 0.01681532885879278
```

```
FOLD: 1, EPOCH: 10, train_loss: 0.01701134249415933
FOLD: 1, EPOCH: 10, valid_loss: 0.016884175315499305
FOLD: 1, EPOCH: 11, train_loss: 0.01702892197435405
FOLD: 1, EPOCH: 11, valid_loss: 0.016736076734960078
FOLD: 1, EPOCH: 12, train_loss: 0.016938764728656432
FOLD: 1, EPOCH: 12, valid_loss: 0.016910760439932348
FOLD: 1, EPOCH: 13, train_loss: 0.01684195919557899
FOLD: 1, EPOCH: 13, valid_loss: 0.01666232731193304
FOLD: 1, EPOCH: 14, train_loss: 0.016781124767853695
FOLD: 1, EPOCH: 14, valid_loss: 0.016613694317638875
FOLD: 1, EPOCH: 15, train_loss: 0.01656384022944436
FOLD: 1, EPOCH: 15, valid_loss: 0.016481956504285335
FOLD: 1, EPOCH: 16, train_loss: 0.01639245954171127
FOLD: 1, EPOCH: 16, valid_loss: 0.016348120048642157
FOLD: 1, EPOCH: 17, train_loss: 0.01613922528669137
FOLD: 1, EPOCH: 17, valid_loss: 0.016200663335621358
FOLD: 1, EPOCH: 18, train_loss: 0.015877455656676472
FOLD: 1, EPOCH: 18, valid_loss: 0.016118471100926398
FOLD: 1, EPOCH: 19, train_loss: 0.015539707844050564
FOLD: 1, EPOCH: 19, valid_loss: 0.01588365714997053
FOLD: 1, EPOCH: 20, train_loss: 0.015128381315897516
FOLD: 1, EPOCH: 20, valid_loss: 0.015780030451714992
FOLD: 1, EPOCH: 21, train_loss: 0.014706411139190603
FOLD: 1, EPOCH: 21, valid_loss: 0.015661385916173456
FOLD: 1, EPOCH: 22, train_loss: 0.014258321748450905
FOLD: 1, EPOCH: 22, valid_loss: 0.015657323598861694
FOLD: 1, EPOCH: 23, train_loss: 0.013933191392697445
FOLD: 1, EPOCH: 23, valid_loss: 0.015643304996192455
FOLD: 1, EPOCH: 24, train_loss: 0.01374531992185278
FOLD: 1, EPOCH: 24, valid_loss: 0.015640568807721137
FOLD: 2, EPOCH: 0, train_loss: 0.4808451424093068
FOLD: 2, EPOCH: 0, valid_loss: 0.02396875739097595З
FOLD: 2, EPOCH: 1, train_loss: 0.021134131657732588
FOLD: 2, EPOCH: 1, valid_loss: 0.019332114979624747
FOLD: 2, EPOCH: 2, train_loss: 0.019023318502570497
FOLD: 2, EPOCH: 2, valid_loss: 0.01792460974305868
FOLD: 2, EPOCH: 3, train_loss: 0.017661144095314604
FOLD: 2, EPOCH: 3, valid_loss: 0.017341603264212607
FOLD: 2, EPOCH: 4, train_loss: 0.017108005756626323
FOLD: 2, EPOCH: 4, valid_loss: 0.017110489681363104
FOLD: 2, EPOCH: 5, train_loss: 0.016865184917082998
FOLD: 2, EPOCH: 5, valid_loss: 0.017000625021755696
FOLD: 2, EPOCH: 6, train_loss: 0.016894768467363045
FOLD: 2, EPOCH: 6, valid_loss: 0.017267115898430347
FOLD: 2, EPOCH: 7, train_loss: 0.017013532413663914
FOLD: 2, EPOCH: 7, valid_loss: 0.017131545171141623
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FOLD: 1, EPOCH: 10, valid_loss: 0.016825353875756264
FOLD: 1, EPOCH: 11, train_loss: 0.01704934801348821
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FOLD: 1, EPOCH: 12, valid_loss: 0.016858120150864124
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FOLD: 1, EPOCH: 13, valid_loss: 0.016760229282081127
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FOLD: 1, EPOCH: 21, valid_loss: 0.01571882378309965
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FOLD: 1, EPOCH: 22, valid_loss: 0.01569646816700697
FOLD: 1, EPOCH: 23, train_loss: 0.01396188179829291
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FOLD: 1, EPOCH: 24, train_loss: 0.013796968829064142
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FOLD: 2, EPOCH: 0, valid_loss: 0.025146274119615553
FOLD: 2, EPOCH: 1, train_loss: 0.020991972882021852
FOLD: 2, EPOCH: 1, valid_loss: 0.02022985689342022
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FOLD: 0, EPOCH: 19, valid_loss: 0.016219929270446302
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FOLD: 0, EPOCH: 20, valid_loss: 0.01607202023267746
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FOLD: 0, EPOCH: 23, valid_loss: nan
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FOLD: 3, EPOCH: 21, train_loss: 0.014708973416665784
FOLD: 3, EPOCH: 21, valid_loss: 0.016116833351552486
FOLD: 3, EPOCH: 22, train_loss: 0.014291971206006145
FOLD: 3, EPOCH: 22, valid_loss: 0.01604284904897213
FOLD: 3, EPOCH: 23, train_loss: 0.01397979850595703
FOLD: 3, EPOCH: 23, valid_loss: 0.016011085473001004
FOLD: 3, EPOCH: 24, train_loss: 0.013815053592936522
FOLD: 3, EPOCH: 24, valid_loss: 0.01601501151919365
FOLD: 4, EPOCH: 0, train_loss: 0.4814382762249027
FOLD: 4, EPOCH: 0, valid_loss: 0.024914344623684883
FOLD: 4, EPOCH: 1, train_loss: 0.021361648973052195
FOLD: 4, EPOCH: 1, valid_loss: 0.0193980748206377
FOLD: 4, EPOCH: 2, train_loss: 0.01892429678289055
FOLD: 4, EPOCH: 2, valid_loss: 0.01807621240615845
FOLD: 4, EPOCH: 3, train_loss: 0.017710748255303523
FOLD: 4, EPOCH: 3, valid_loss: 0.017391298189759253
FOLD: 4, EPOCH: 4, train_loss: 0.017085795987676195
FOLD: 4, EPOCH: 4, valid_loss: 0.017147911451756953
FOLD: 4, EPOCH: 5, train_loss: 0.01685315921117051
FOLD: 4, EPOCH: 5, valid_loss: 0.017055432088673116
FOLD: 4, EPOCH: 6, train_loss: 0.016976427312205437
FOLD: 4, EPOCH: 6, valid_loss: 0.017009622342884542
```

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FOLD: 4, EPOCH: 7, train_loss: 0.016933950215426027
FOLD: 4, EPOCH: 7, valid_loss: 0.017158462963998318
FOLD: 4, EPOCH: 8, train_loss: 0.017022862352532187
FOLD: 4, EPOCH: 8, valid_loss: 0.017318418174982073
FOLD: 4, EPOCH: 9, train_loss: 0.01705175664174516
FOLD: 4, EPOCH: 9, valid_loss: 0.017287997528910637
FOLD: 4, EPOCH: 10, train_loss: 0.016970691486534212
FOLD: 4, EPOCH: 10, valid_loss: 0.016964208111166956
FOLD: 4, EPOCH: 11, train_loss: 0.016943717198002906
FOLD: 4, EPOCH: 11, valid_loss: 0.017264471501111985
FOLD: 4, EPOCH: 12, train_loss: 0.016905814263538845
FOLD: 4, EPOCH: 12, valid_loss: 0.01703455775976181
FOLD: 4, EPOCH: 13, train_loss: 0.016825945325651948
FOLD: 4, EPOCH: 13, valid_loss: 0.01702758491039276
FOLD: 4, EPOCH: 14, train_loss: 0.016757222063535332
FOLD: 4, EPOCH: 14, valid_loss: 0.01686743963509798
FOLD: 4, EPOCH: 15, train_loss: 0.01653239261485687
FOLD: 4, EPOCH: 15, valid_loss: 0.016775177568197252
FOLD: 4, EPOCH: 16, train_loss: 0.016369672016981914
FOLD: 4, EPOCH: 16, valid_loss: 0.016644030027091503
FOLD: 4, EPOCH: 17, train_loss: 0.016129688708251027
FOLD: 4, EPOCH: 17, valid_loss: 0.016494632251560688
FOLD: 4, EPOCH: 18, train_loss: 0.01589710402878977
FOLD: 4, EPOCH: 18, valid_loss: 0.016339619494974613
FOLD: 4, EPOCH: 19, train_loss: 0.01558316388756645
FOLD: 4, EPOCH: 19, valid_loss: 0.016252162493765356
FOLD: 4, EPOCH: 20, train_loss: 0.015173551879924576
FOLD: 4, EPOCH: 20, valid_loss: 0.016077344305813313
FOLD: 4, EPOCH: 21, train_loss: 0.014750995673239231
FOLD: 4, EPOCH: 21, valid_loss: 0.016080063804984092
FOLD: 4, EPOCH: 22, train_loss: 0.014366832479429083
FOLD: 4, EPOCH: 22, valid_loss: 0.016005329862236975
FOLD: 4, EPOCH: 23, train_loss: 0.014000736170632093
FOLD: 4, EPOCH: 23, valid_loss: 0.015978044904768465
FOLD: 4, EPOCH: 24, train_loss: 0.013829051802048877
FOLD: 4, EPOCH: 24, valid_loss: 0.015968659184873103
FOLD: 5, EPOCH: 0, train_loss: 0.4802205621638671
FOLD: 5, EPOCH: 0, valid_loss: 0.02413658283650875
FOLD: 5, EPOCH: 1, train_loss: 0.02126514426350188
FOLD: 5, EPOCH: 1, valid_loss: 0.019291314631700515
FOLD: 5, EPOCH: 2, train_loss: 0.01904139505559895
FOLD: 5, EPOCH: 2, valid_loss: 0.018079844638705253
FOLD: 5, EPOCH: 3, train_loss: 0.017673574711139103
FOLD: 5, EPOCH: 3, valid_loss: 0.01754952758550644
FOLD: 5, EPOCH: 4, train_loss: 0.01707403847098756
FOLD: 5, EPOCH: 4, valid_loss: 0.017020833753049372
FOLD: 5, EPOCH: 5, train_loss: 0.016875136092457235
FOLD: 5, EPOCH: 5, valid_loss: 0.017544100135564802
```

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FOLD: 5, EPOCH: 6, train_loss: 0.016861857966754306
FOLD: 5, EPOCH: 6, valid_loss: 0.017278988882899284
FOLD: 5, EPOCH: 7, train_loss: 0.01700489751386399
FOLD: 5, EPOCH: 7, valid_loss: 0.017168056443333624
FOLD: 5, EPOCH: 8, train_loss: 0.01706573140940496
FOLD: 5, EPOCH: 8, valid_loss: 0.017130962535738946
FOLD: 5, EPOCH: 9, train_loss: 0.017041101608247983
FOLD: 5, EPOCH: 9, valid_loss: 0.017088485285639762
FOLD: 5, EPOCH: 10, train_loss: 0.017026309031663703
FOLD: 5, EPOCH: 10, valid_loss: 0.01712613705545664
FOLD: 5, EPOCH: 11, train_loss: 0.017002666229698933
FOLD: 5, EPOCH: 11, valid_loss: 0.017003004290163517
FOLD: 5, EPOCH: 12, train_loss: 0.016979180574163692
FOLD: 5, EPOCH: 12, valid_loss: 0.01709418583661318
FOLD: 5, EPOCH: 13, train_loss: 0.016843714079737258
FOLD: 5, EPOCH: 13, valid_loss: 0.01783735156059265
FOLD: 5, EPOCH: 14, train_loss: 0.016679469413649874
FOLD: 5, EPOCH: 14, valid_loss: 0.016959945634007455
FOLD: 5, EPOCH: 15, train_loss: 0.016565393016603935
FOLD: 5, EPOCH: 15, valid_loss: 0.01680417448282242
FOLD: 5, EPOCH: 16, train_loss: 0.016330036436061877
FOLD: 5, EPOCH: 16, valid_loss: 0.016605207063257695
FOLD: 5, EPOCH: 17, train_loss: 0.016166272794916517
FOLD: 5, EPOCH: 17, valid_loss: 0.016463107392191888
FOLD: 5, EPOCH: 18, train_loss: 0.01583819335237855
FOLD: 5, EPOCH: 18, valid_loss: 0.016459889747202396
FOLD: 5, EPOCH: 19, train_loss: 0.015510343008858412
FOLD: 5, EPOCH: 19, valid_loss: 0.016218247637152673
FOLD: 5, EPOCH: 20, train_loss: 0.01512312514669433
FOLD: 5, EPOCH: 20, valid_loss: 0.016065676957368852
FOLD: 5, EPOCH: 21, train_loss: 0.014708964477236174
FOLD: 5, EPOCH: 21, valid_loss: 0.01603235591202974
FOLD: 5, EPOCH: 22, train_loss: 0.014291144869461352
FOLD: 5, EPOCH: 22, valid_loss: 0.015965398848056794
FOLD: 5, EPOCH: 23, train_loss: 0.013965516325821277
FOLD: 5, EPOCH: 23, valid_loss: 0.015956440903246404
FOLD: 5, EPOCH: 24, train_loss: 0.013813428726478094
FOLD: 5, EPOCH: 24, valid_loss: 0.015930245742201806
FOLD: 6, EPOCH: 0, train_loss: 0.480280967365925
FOLD: 6, EPOCH: 0, valid_loss: 0.023650210872292517
FOLD: 6, EPOCH: 1, train_loss: 0.021199466711303003
FOLD: 6, EPOCH: 1, valid_loss: 0.019135429859161376
FOLD: 6, EPOCH: 2, train_loss: 0.018989772630893454
FOLD: 6, EPOCH: 2, valid_loss: 0.017774301692843438
FOLD: 6, EPOCH: 3, train_loss: 0.017688723483762773
FOLD: 6, EPOCH: 3, valid_loss: 0.01734578989446163
FOLD: 6, EPOCH: 4, train_loss: 0.01713540465856085
FOLD: 6, EPOCH: 4, valid_loss: 0.01712867643684149
```
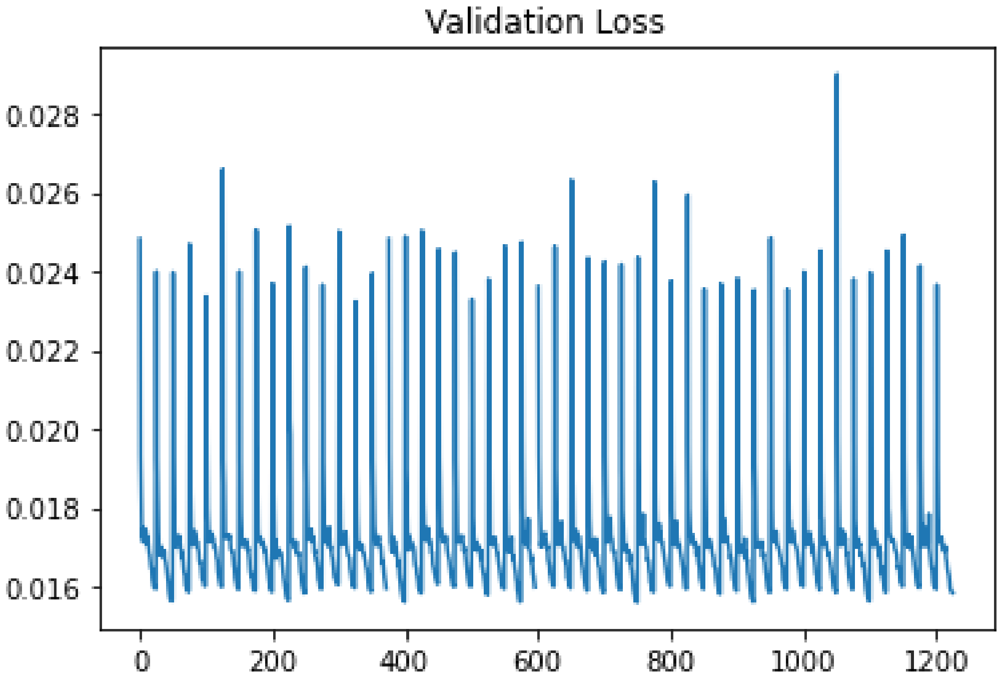
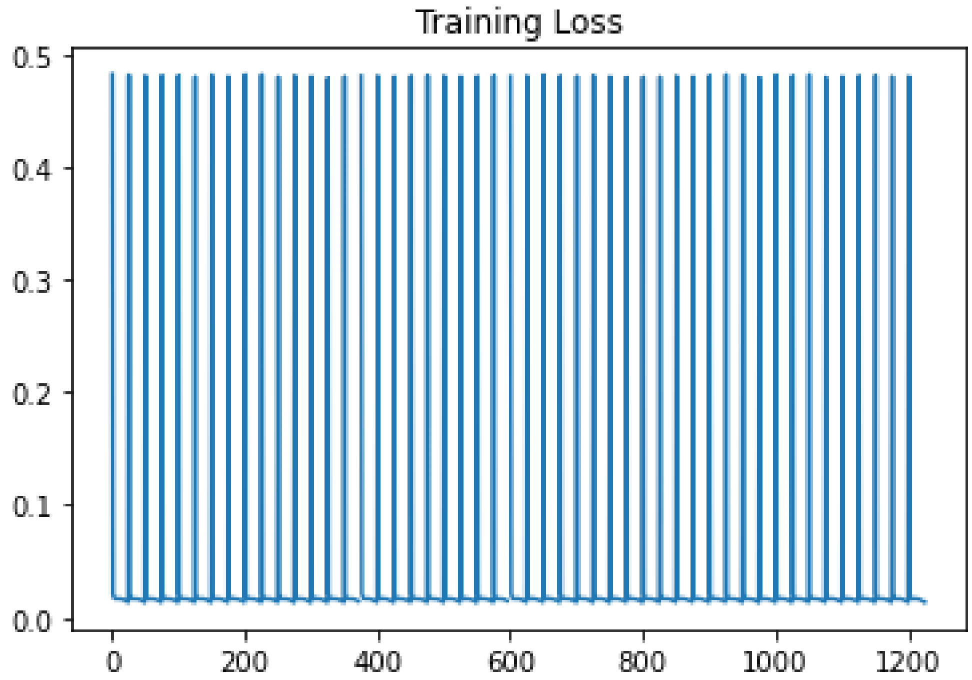

```
FOLD: 6, EPOCH: 5, train_loss: 0.016926547778504237
FOLD: 6, EPOCH: 5, valid_loss: 0.01710812121629715
FOLD: 6, EPOCH: 6, train_loss: 0.0170036763282252
FOLD: 6, EPOCH: 6, valid_loss: 0.017142675705254077
FOLD: 6, EPOCH: 7, train_loss: 0.017026163301855125
FOLD: 6, EPOCH: 7, valid_loss: 0.01723992347717285
FOLD: 6, EPOCH: 8, train_loss: 0.017082421558902782
FOLD: 6, EPOCH: 8, valid_loss: 0.01707722622901201
FOLD: 6, EPOCH: 9, train_loss: 0.017043254129132445
FOLD: 6, EPOCH: 9, valid_loss: 0.01698746148496866
FOLD: 6, EPOCH: 10, train_loss: 0.017063623471629052
FOLD: 6, EPOCH: 10, valid_loss: 0.01691389985382557
FOLD: 6, EPOCH: 11, train_loss: 0.01701099362832551
FOLD: 6, EPOCH: 11, valid_loss: 0.016918593309819697
FOLD: 6, EPOCH: 12, train_loss: 0.016962517496375812
FOLD: 6, EPOCH: 12, valid_loss: 0.016884964928030967
FOLD: 6, EPOCH: 13, train_loss: 0.016819300206035982
FOLD: 6, EPOCH: 13, valid_loss: 0.017013469077646733
FOLD: 6, EPOCH: 14, train_loss: 0.016720949387063786
FOLD: 6, EPOCH: 14, valid_loss: 0.01670393142849207
FOLD: 6, EPOCH: 15, train_loss: 0.01657447481185806
FOLD: 6, EPOCH: 15, valid_loss: 0.01661783494055271
FOLD: 6, EPOCH: 16, train_loss: 0.016433359244141448
FOLD: 6, EPOCH: 16, valid_loss: 0.016441736556589603
FOLD: 6, EPOCH: 17, train_loss: 0.016177555254730237
FOLD: 6, EPOCH: 17, valid_loss: 0.016382538452744483
FOLD: 6, EPOCH: 18, train_loss: 0.01592019636842872
FOLD: 6, EPOCH: 18, valid_loss: 0.01630394671112299
FOLD: 6, EPOCH: 19, train_loss: 0.015576305495080899
FOLD: 6, EPOCH: 19, valid_loss: 0.016181243360042574
FOLD: 6, EPOCH: 20, train_loss: 0.01525749311763413
FOLD: 6, EPOCH: 20, valid_loss: 0.015973382778465748
FOLD: 6, EPOCH: 21, train_loss: 0.014793983508585667
FOLD: 6, EPOCH: 21, valid_loss: 0.01592020835727453
FOLD: 6, EPOCH: 22, train_loss: 0.01439013465174607
FOLD: 6, EPOCH: 22, valid_loss: 0.01586281456053257
FOLD: 6, EPOCH: 23, train_loss: 0.014098920555291126
FOLD: 6, EPOCH: 23, valid_loss: 0.015853472501039505
FOLD: 6, EPOCH: 24, train_loss: 0.013911979653093279
FOLD: 6, EPOCH: 24, valid_loss: 0.015843976363539694
```

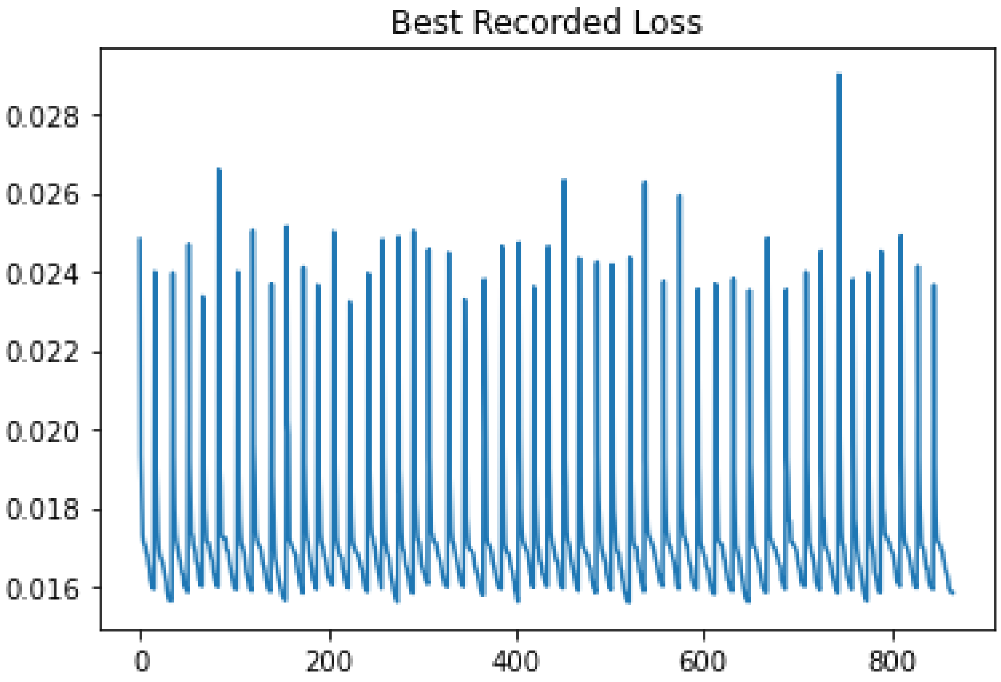
[99]:

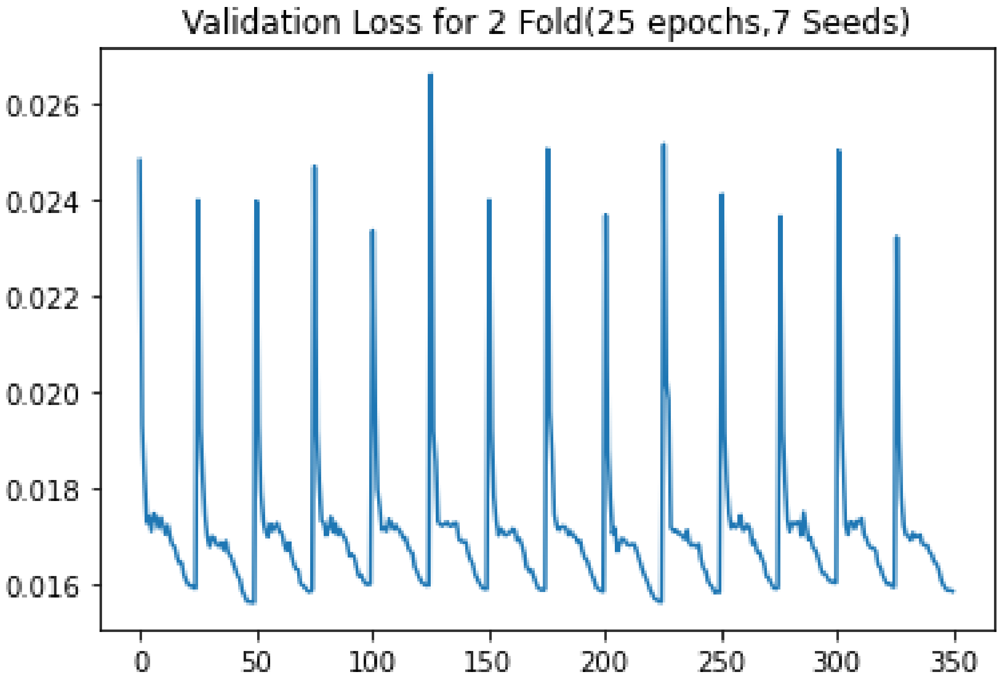
```
import matplotlib.pyplot as plt
import numpy as np
x = np.linspace(0,1225,1225);
plt.title("Validation Loss")
plt.plot(x,valid_loss_)
plt.show()
```

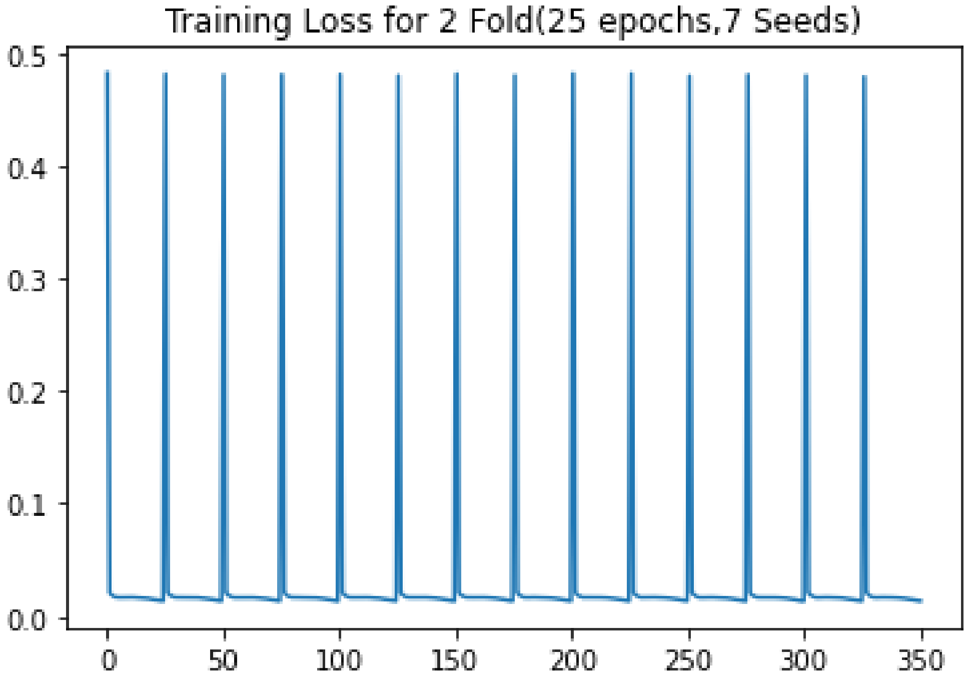
```
x = np.linspace(0,1225,1225);
plt.title("Training Loss")
plt.plot(x,train_loss_)
plt.show()

x = np.linspace(0,865,865);
plt.title("Best Recorded Loss")
plt.plot(x,best_loss_)
plt.show()

x = np.linspace(0,350,350);
plt.title("Validation Loss for 2 Fold(25 epochs,7 Seeds)")
plt.plot(x,valid_loss_[:350])
plt.show()

x = np.linspace(0,350,350);
plt.title("Training Loss for 2 Fold(25 epochs,7 Seeds)")
plt.plot(x,train_loss_[:350])
plt.show()

x = np.linspace(0,125,125);
plt.title("Approx. Best Recorded Loss for 2 Fold(25 epochs,7 Seeds)")
plt.plot(x,best_loss_[:125])
plt.show()
```

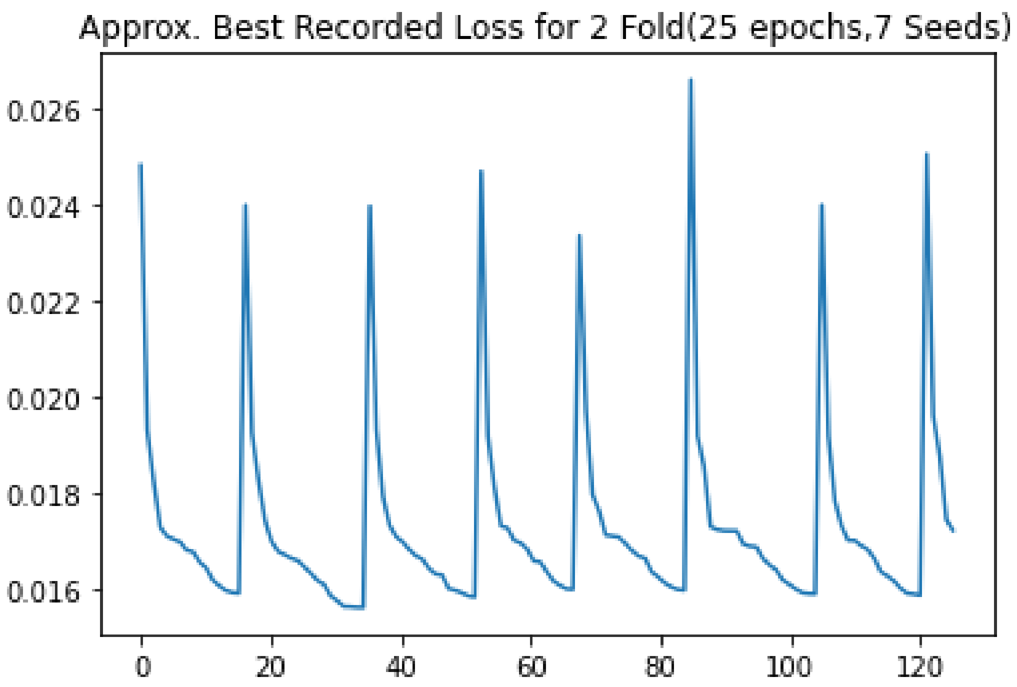



Training Loss
0.5
0.4
0.3
0.2
0.1
0.0
0
200
400
600
800
1000
1200


Best Recorded Loss
0.028
0.026
0.024
0.022
0.020
0.018
0.016
0
200
400
600
800


Validation Loss for 2 Fold(25 epochs,7 Seeds)
0.026
0.024
0.022
0.020
0.018
0.016
0
50
100
150
200
250
300
350


Training Loss for 2 Fold(25 epochs,7 Seeds)
0.5
0.4
0.3
0.2
0.1
0.0
0
50
100
150
200
250
300
350



12 CALCULATING LOG LOSS

[92]:

```
valid_results = train_targets_scored.drop(columns=target_cols).
 ↪merge(train[['sig_id']+target_cols], on='sig_id', how='left').fillna(0)



y_true = train_targets_scored[target_cols].values
y_pred = valid_results[target_cols].values

score = 0
for i in range(len(target_cols)):
    score_ = log_loss(y_true[:, i], y_pred[:, i])
    score += score_ / target.shape[1]

print("CV log_loss: ", score)
```

```
CV log_loss:  0.014467723033458807
```

13 GENERATING SUBMISSION FILE

[93]:

```
sub = sample_submission.drop(columns=target_cols).
 ↪merge(test[['sig_id']+target_cols], on='sig_id', how='left').fillna(0)
sub.to_csv('submission.csv', index=False)
sub.shape
```

```
[93]: (3982, 207)
```