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#### Prerequisite

Methods to split the dataset into folds & form training, validation sets:

```
def split(df: pd.DataFrame, folds=5):
    df = df.sample(frac=1, random_state=7).reset_index(drop=True)
    num = len(df) // folds
    left = len(df) % folds
    df_folds = []
    prev = 0
    for i in range(folds):
        length = num + (left > 0)
        df_ = df.iloc[prev: prev + length].copy().reset_index(drop=True)
        df_folds.append(df_)
        prev += length
        left -= 1
    return df_folds
def form_train_val(folds, val_fold):
    train_folds = [folds[i] for i in range(len(folds)) if i ≠ val_fold]
    train_df = pd.concat(train_folds).reset_index(drop=True)
    val_df = folds[val_fold].copy()
    return train_df, val_df
```

Q1.

Dataset: Abalone

#### Preprocessing:

- 1. The dataset contained no missing values.
- 2. The categorical feature 'Sex' was one-hot encoded.
- 3. Before regression, data is always standardized.

a)

The regression class standardizes data based on the input parameter & uses fit method of sklearn to find the coefficients and intercept. During prediction, the test data is first standardized w.r.t to the training set and then predicted using linear regression equation.

The standardization method is also implemented for all self-implemented classes in the further parts of the assignment.

```
class Regression:
   def __init__(self, normalise):
        self.normalise = normalise # Gaussian Normalisation
   def fit(self, X: pd.DataFrame, y: pd.Series):
       if self.normalise:
            self.mean = X.mean()
self.std = X.std()
            X = (X - self.mean) / self.std
       lr = LinearRegression()
       lr.fit(X, y)
        self.w = lr.coef_
        self.b = lr.intercept_
   def predict(self, X_test: pd.DataFrame):
        if self.normalise:
            X_test = (X_test - self.mean) / self.std
       y_pred = (X_test * self.w).sum(axis=1) + self.b
        return np.array(y_pred)
```

b)

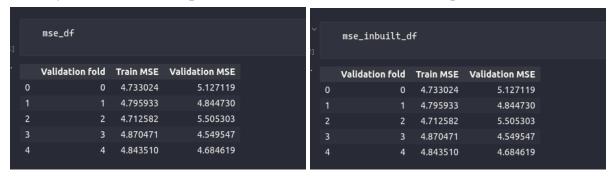
#### MSE function:

```
def MSE(y_actual, y_pred, inbuilt=False):
    if inbuilt:
        return metrics.mean_squared_error(y_actual, y_pred)
    else:
        assert (len(y_actual) = len(y_pred))
        diff = (y_actual - y_pred) ** 2
        return diff.sum() / len(y_actual)
```

### Training:

```
mse_df = {'Validation fold': [], 'Train MSE': [], 'Validation MSE': []}
mse_inbuilt_df = {'Validation fold': [], 'Train MSE': [], 'Validation MSE': []}
for val_fold in range(len(folds)):
     train_df, val_df = form_train_val(folds, val_fold)
     lr = None
     model_filename = f'Weights/1/mse-{val_fold}.sav'
     if os.path.exists(model_filename):
          lr = joblib.load(model_filename)
          lr = Regression(normalise=True)
          lr.fit(train_df[feature_cols], train_df[out_col])
joblib.dump(lr, model_filename)
     train_mse = MSE(train_df[out_col], lr.predict(train_df[feature_cols]))
val_mse = MSE(val_df[out_col], lr.predict(val_df[feature_cols]))
     train_mse_inbuilt = MSE(train_df[out_col], lr.predict(train_df[feature_cols]), inbuilt=True)
     val_mse_inbuilt = MSE(val_df[out_col], lr.predict(val_df[feature_cols]), inbuilt=True)
     mse_df['Validation fold'].append(val_fold)
mse_df['Train MSE'].append(train_mse)
     mse_df['Validation MSE'].append(val_mse)
     mse_inbuilt_df['Validation fold'].append(val_fold)
mse_inbuilt_df['Train MSE'].append(train_mse_inbuilt)
     mse_inbuilt_df['Validation MSE'].append(val_mse_inbuilt)
mse_df = pd.DataFrame(mse_df)
mse_inbuilt_df = pd.DataFrame(mse_inbuilt_df)
```

The MSE on train and validation set using self MSE implementation & sklearn MSE implementation is given below: (The results exactly match)



Mean training MSE & mean validation MSE:

c)
Linear regression using normal equations:

```
class NormalEq:
   def __init__(self, normalise):
       self.normalise = normalise # Gaussian Normalisation
   def fit(self, X_df: pd.DataFrame, y_df: pd.Series):
       if self.normalise:
           self.mean = X_df.mean()
           self.std = X_df.std()
           X_df = (X_df - self.mean) / self.std
           X_df = X_df.copy()
       X_{df['\_bias']} = np.ones(len(X_df))
       X = X_df.to_numpy()
       y = np.array(y_df)
       self.w = np.linalg.pinv(X.T @ X) @ (X.T @ y)
   def predict(self, X_test_df: pd.DataFrame):
       if self.normalise:
           X_test_df = (X_test_df - self.mean) / self.std
           X_test_df = X_test_df.copy()
       X_test_df['_bias'] = np.ones(len(X_test_df))
       X_test = X_test_df.to_numpy()
       return X_test @ self.w
```

### Training:

```
mse_ne_df = {'Validation fold': [], 'Train MSE': [], 'Validation MSE': []}
for val_fold in range(len(folds)):
    train_df, val_df = form_train_val(folds, val_fold)
    lr_ne = None
    model_filename = f'Weights/1/mse-ne-{val_fold}.sav'
    if os.path.exists(model_filename):
        lr_ne = joblib.load(model_filename)
    else:
        lr_ne = NormalEq(normalise=True)
        lr_ne.fit(train_df[feature_cols], train_df[out_col])
        joblib.dump(lr_ne, model_filename)

train_mse = MSE(train_df[out_col], lr_ne.predict(train_df[feature_cols]))
    val_mse = MSE(val_df[out_col], lr_ne.predict(val_df[feature_cols]))

mse_ne_df['Validation fold'].append(val_fold)
mse_ne_df['Train MSE'].append(train_mse)
mse_ne_df['Validation MSE'].append(val_mse)
mse_ne_df = pd.DataFrame(mse_ne_df)
```

Training and validation MSE: (The results match with the previous results)

	mse_ne_df		
	Validation fold	Train MSE	Validation MSE
0	0	4.733024	5.127119
1	1	4.795933	4.844730
2	2	4.712582	5.505303
3	3	4.870471	4.549547
4	4	4.843510	4.684619

d)

Training using sklearn linear regression: (explicit standardization is done)

```
mse_sklearn_df = {'Validation fold': [], 'Train MSE': [], 'Validation MSE': []}
for val_fold in range(len(folds)):
    train_df, val_df = form_train_val(folds, val_fold)
    # explicit standardization
    mean_train_df = train_df[feature_cols].mean()
    std_train_df = train_df[feature_cols].std()
    train_df[feature_cols] = (train_df[feature_cols] - mean_train_df) / std_train_df
    val_df[feature_cols] = (val_df[feature_cols] - mean_train_df) / std_train_df

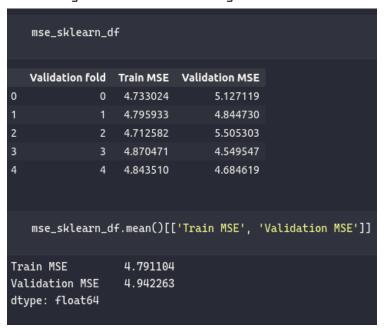
    lr_sklearn = None
    model_filename = f'Weights/1/mse-sklearn-{val_fold}.sav'
    if os.path.exists(model_filename):
        lr_sklearn = joblib.load(model_filename)
    else:
        lr_sklearn = LinearRegression()
        lr_sklearn.fit(train_df[feature_cols], train_df[out_col])
        joblib.dump(lr_sklearn, model_filename)

    train_mse = MSE(train_df[out_col], lr_sklearn.predict(train_df[feature_cols]), inbuilt=True)

    mse_sklearn_df['Validation fold'].append(val_fold)
    mse_sklearn_df['Validation fold'].append(val_fold)
    mse_sklearn_df['Validation MSE'].append(val_mse)

mse_sklearn_df = pd.DataFrame(mse_sklearn_df)
```

MSE using sklearn linear regression.



There is no deviation observed from self implemented linear regression methods.

Q2.

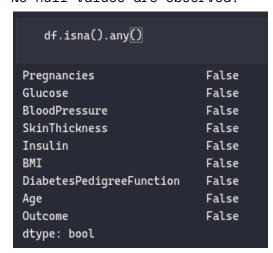
Dataset: Diabetes

### Preprocessing:

- 1. No null values are observed.
- 2. Data is always standardized before regression.

# a) Analysis:

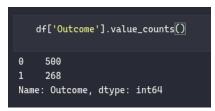
1. No null values are observed.



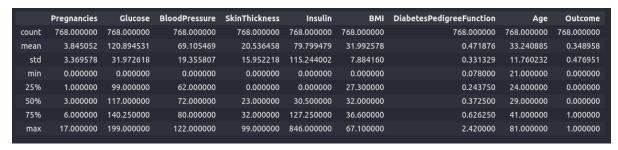
2. No categorical data is observed.



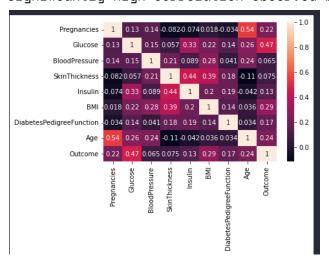
3. There is a 2:1 ratio class imbalance.



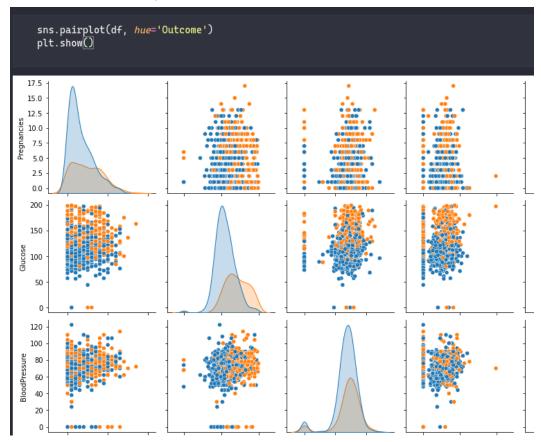
4. Using describe() method of pandas, the following statistics are observed:



5. Correlation heatmap is plotted using seaborn. Maximum correlation of 0.54 and minimum correlation of -0.11 is observed. Overall there is no significantly high correlation observed between the features.



6. A pairplot is also plotted with hue=Outcome using seaborn. A subsection of the plot is shown:



b)
Utility functions: (BCE is binary cross entropy loss)

```
def BCE(y_actual, y_pred):
    return -np.mean(y_actual * np.log(y_pred) + (1 - y_actual) * np.log(1 - y_pred))

def accuracy(y_actual, y_pred):
    return sum([y_pred[i] = y_actual[i] for i in range(len(y_actual))]) / len(y_actual)

def sigmoid(x):
    return 1 / (1 + np.exp(-x))
```

## Class LogRegression:

- 1. Training data and validating data is standardized with training mean and standard deviation.
- 2. Uses Batch Gradient Descent for weight updates
- 3. Utilises Binary Cross Entropy loss as loss criterion (with L2 regularization)

4. Loss function:

```
def loss(self, y_actual, y_pred):
    return BCE(y_actual, y_pred) + self.reg_lambda * np.sum(self.w ** 2)
```

5. Probability function:

```
def prob(self, X):
    return sigmoid(X @ self.w)
```

6. Gradient function:

```
def grad(self, X, y_actual):
    y_pred = self.prob(X)
    gradient = ((y_pred - y_actual) @ X) / self.num_samples + 2 * self.reg_lambda * self.w
    return gradient
```

7. Predict function:

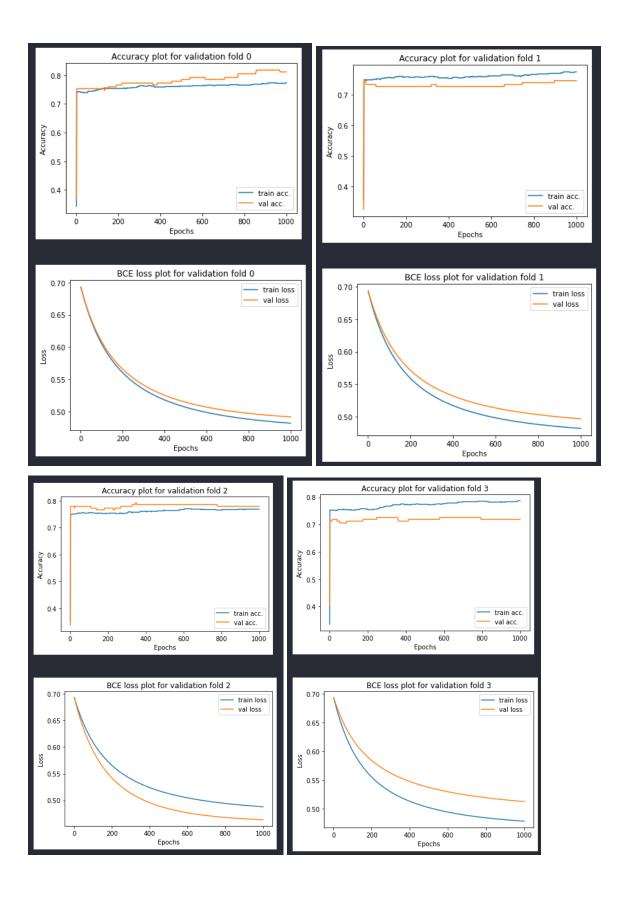
```
def predict(self, X_test):
    if self.normalise:
        | X_test = (X_test - self.mean) / self.std
    else:
        | X_test = X_test.copy()
    X_test['_bias'] = np.ones(len(X_test))
    y_pred = np.array([int((self.w.T @ x) ≥ 0) for x in X_test.to_numpy()])
    return y_pred
```

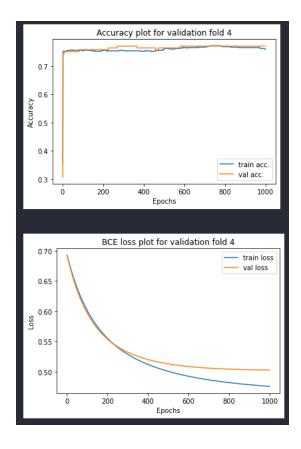
c)

Each fold is run for 1000 epochs with learning rate: 0.01, and lambda: 0. Table representing fold-wise accuracy:

Validation fold	Train Acc.	Validation Acc.
0	0.773616	0.811688
1	0.775244	0.746753
2	0.768730	0.779221
3	0.786992	0.718954
4	0.760976	0.771242

The plots for each fold are given below. It's mainly observed that the training loss starts decreasing with epochs while the validation loss starts gradually decreasing (decreasing with a smaller gradient) with epochs indicating the (slight) loss of generalizability on validation set. W.r.t accuracy, the model has a steep ascent in accuracy in the few first epochs, and then slowly seems to improve both on the test and validation set. No evident overfitting is observed and the model is able to generalize well.





d)

The loss in L2 regularisation takes the form:

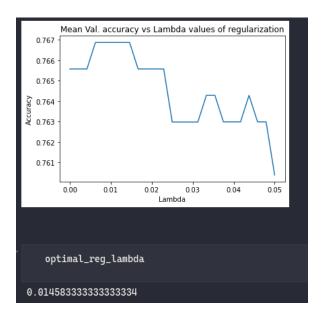
```
def loss(self, y_actual, y_pred):
    return BCE(y_actual, y_pred) + self.reg_lambda * np.sum(self.w ** 2)
```

The gradient in L2 regularisation take the form:

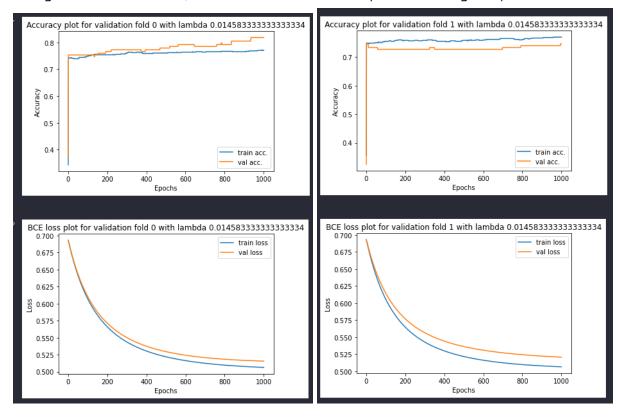
```
def grad(self, X, y_actual):
    y_pred = self.prob(X)
    gradient = ((y_pred - y_actual) @ X) / self.num_samples + 2 * self.reg_lambda * self.w
    return gradient
```

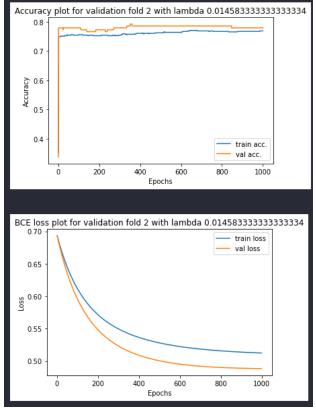
For finding optimal lambda, a grid search is performed over 25 values in linspace (0  $\rightarrow$  0.05). The metric to decide the optimality of lambda is the highest mean validation accuracy over all folds. The plot for mean validation accuracy vs lambdas is given below along with the choice of optimal lambda:

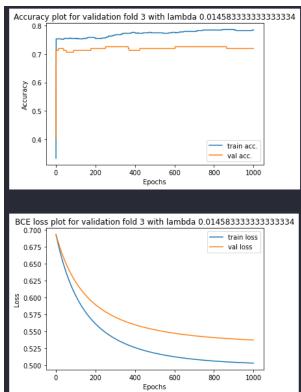
There are multiple values (specifically 0.006 → 0.014) where highest mean validation accuracy is observed. The lambda with the highest value among the highest mean validation accuracy is chosen to demonstrate the effect of choice of lambda on the model in later experiments.

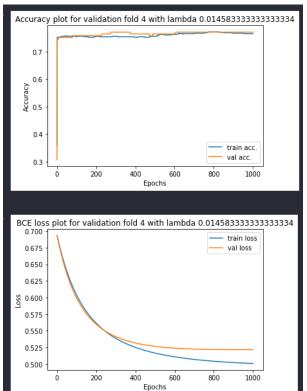


Using lambda=0.014583, the above tables and plots are again plotted.









log_reg_lambda_df			
	Validation fold	Train Acc.	Validation Acc.
0	0	0.770358	0.818182
1	1	0.770358	0.746753
2	2	0.768730	0.779221
3	3	0.783740	0.718954
4	4	0.765854	0.771242

### Performance comparison:

Comparing the mean training and validation accuracy of regularised and unregularised models.

Unregularised:

```
log_reg_df.mean()[['Train Acc.', 'Validation Acc.']]

Train Acc. 0.773111

Validation Acc. 0.765572

dtype: float64
```

#### Regularised:

```
log_reg_lambda_df.mean()[['Train Acc.', 'Validation Acc.']]

Train Acc. 0.771808

Validation Acc. 0.766870
dtype: float64
```

In the unregularised model, a slightly higher training accuracy is observed w.r.t to regularised model although a slightly lower validation accuracy is observed w.r.t to the regularised model. This indicates a higher extent of generalizability in the regularised model.

Comparing the mean distance of weights from origin in both the models:

```
mean_dist_unregularized = np.mean([np.sum(x.w ** 2) for x in log_reg_models])
mean_dist_regularized = np.mean([np.sum(x.w ** 2) for x in log_reg_olambda_models])
mean_dist_unregularized, mean_dist_regularized

(1.4866829173322713, 1.1995173286141736)
```

The mean weight distance in the unregularised model is higher than the mean weight distance of the regularised model indicating lower weight values in the regularised model.

e)

Sklearn results with unregularised model:

Model used:

Validation fold	Train Acc.	Validation Acc.
0	0.734528	0.720779
1	0.701954	0.701299
2	0.705212	0.733766
3	0.744715	0.679739
4	0.725203	0.725490

Sklearn results with regularised model:

Model used:

```
log_reg = LogisticRegression(penalty='l2', random_state=7)
```

```
log_reg_l2_sklearn_df.mean()[['Train Acc.', 'Validation Acc.']]

violog_reg_l2_sklearn_df.mean()[['Train Acc.', 'Validation Acc.']]

violog_reg_l2_sklearn_df.mean()[['Train Acc.', 'Validation Acc.']]

violog_reg_l2_sklearn_df.mean()[['Train Acc.', 'Validation Acc.']]
```

log_reg_l2_sk √ 0.7s	learn_df	
Validation fold	Train Acc.	Validation Acc.
0	0.734528	0.720779
1	0.705212	0.701299
2	0.705212	0.733766
3	0.746341	0.679739
4	0.725203	0.732026

Self-implemented logistic regression outperforms sklearn's implementation. This can arise due to multiple reasons, primarily hyperparameter tuning (self implemented model runs for 1000 epochs while sklearn's logistic model runs for maximum 100 epochs) & difference in convergence algorithms.

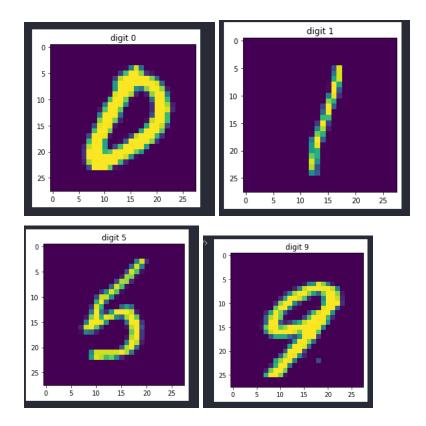
Q3.

Dataset: MNIST (loaded train set using idx2numpy)

orig\_X = idx2numpy.convert\_from\_file('/content/drive/My Drive/Data Colab/ml-pg-assignment-3/train-images.idx3-ubyte')
y = idx2numpy.convert\_from\_file('/content/drive/My Drive/Data Colab/ml-pg-assignment-3/train-labels.idx1-ubyte')

a)

5 instances of each class are visualised using imshow() method of matplotlib. Here are some samples visualisations for reference:



## b)

Logistic regression class is extended to One-vs-One approach. For n classes, n\*(n-1)/2 classifiers are needed where each classifier classifies only between a single pair of classes. At last, a majority vote is taken to determine the output class label. OVO requires dataset bifurcation and is computationally expensive. Each sub logistic classifier standardizes the data & is run for 2000 epochs with lr=0.01 & lambda=0.01. Fit method of OVO logistic classifier:

```
def fit_ovo(self, _X, y, _X_val, y_val, epochs, display):
    if display:
        print('* Fitting OVO models')
    for c1 in range(self.num_classes):
        idx = (y = c1) | (y = c2)
        idx_val = (y_val = c1) | (y_val = c2)
            X_val_c1_c2 = _X[idx]
        X_val_c1_c2 = _X_val[idx_val]
        y_val_c1_c2 = np.array([int(u = c1) for u in y[idx]])
        y_val_c1_c2 = np.array([int(u = c1) for u in y_val[idx_val]])
        self.models[(c1, c2)] = LogRegression_Base()
        self.models[(c1, c2)].fit(X_c1_c2, y_c1_c2, X_val_c1_c2, y_val_c1_c2, epochs)
    if display:
        print(f'> Fitted model {c1}, {c2}')
        print(f'> Acc. train: {accuracy(y_c1_c2, self.models[(c1, c2)].predict(X_c1_c2))}')
        if _X_val is not None:
            print(f'> Acc. val: {accuracy(y_val_c1_c2, self.models[(c1, c2)].predict(X_val_c1_c2))}')
        print('==========')
```

#### Predict method:

```
def predict_ovo(self, X):
    predictions = {}
    for c1 in range(self.num_classes):
        for c2 in range(c1 + 1, self.num_classes):
            p = self.models[(c1, c2)].predict(X)
            predictions[(c1, c2)] = [c1 if u else c2 for u in p]
    y_ = np.array(list(predictions.values()))
    y = np.array([mode(y_[:, i]) for i in range(X.shape[0])])
    return y
```

### Accuracy table:

ovo_df		
Validation fold	Train Acc.	Validation Acc.
0	0.916687	0.911667
1	0.915875	0.916083
2	0.917542	0.909167
3	0.916542	0.915333
4	0.916562	0.913417

### Class-wise train accuracy for each fold:

```
        ovo_classwise_train_df

        ovo_classwise_train_distriction_classwise_train_distriction_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_train_classwise_t
```

#### Class-wise validation accuracy for each fold:

```
ovo_classwise_val_df
        0
                           2
                                    3
                                             4
                                                      5
                                                                6
                                                                                  8
0 0.947099 0.980597 0.887179 0.859873 0.938879 0.898036 0.950764 0.906959 0.839422 0.900931
1 0.962478 0.979577 0.877414 0.874262 0.923736 0.890459 0.955954 0.917534 0.852787
                                                                                     0.913924
 0.950997 0.977528 0.871219 0.867781 0.939523 0.881468 0.957663 0.915294 0.849408
                                                                                     0.877704
 0.959149 0.985765 0.887188 0.876040 0.920455 0.890028 0.965577 0.908272 0.844652
                                                                                     0.904087
4 0.967374 0.978261 0.874062 0.854096 0.934690 0.904982 0.944492 0.908944 0.843911 0.909475
```

c)

Logistic regression class is extended to the One-vs-Rest approach. For n classes, n classifiers are needed where each classifier classifies between a class and all the rest classes. At last, the class with the highest positive probability is taken. OVR is relatively computationally efficient but suffers from class imbalance. Each sub logistic classifier standardizes that data & is run for 2000 epochs with lr=0.01 & lambda=0.01. Fit method of OVR logistic classifier:

Predict method of OVR logistic classifier:

```
def predict_ovr(self, X):
    prob = []
    for c in range(self.num_classes):
        prob.append(self.models[c].predict_prob(X))
    prob_ = np.array(prob)
    y = np.array([np.argmax(prob_[:, i]) for i in range(X.shape[0])])
    return y
```

Accuracy table:

```
      ovr_df

      Validation fold
      Train Acc.
      Validation Acc.

      0
      0.860979
      0.862250

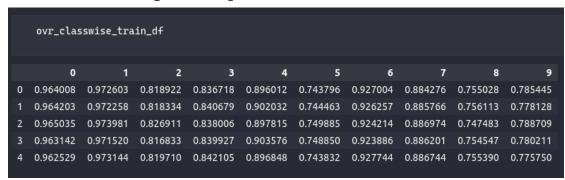
      1
      0.861437
      0.858583

      2
      0.862688
      0.852833

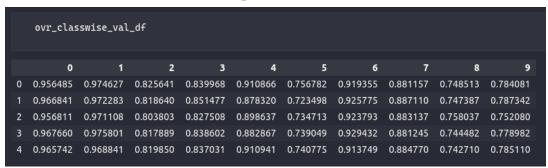
      3
      0.861417
      0.858417

      4
      0.860833
      0.860333
```

Class-wise training accuracy for each fold:



Class-wise validation accuracy for each fold:



There are some classes with lower accuracies such as 5, 8, 3 (in both 0V0 and 0VR) indicating the difficulty in classification for these classes.

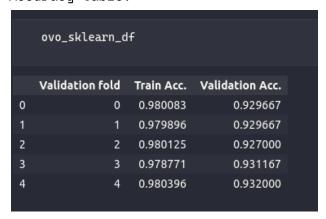
### d)

Comparison with sklearn implementation. Dataset is explicitly standardized before classification.

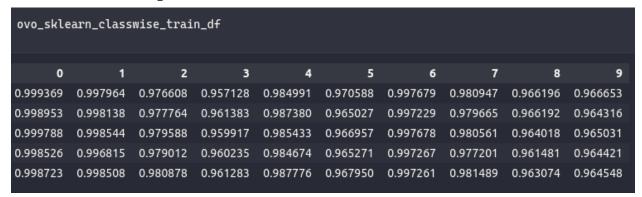
Using OneVsOneClassifier:

Model used: (Max iters=750 to ensure convergence)

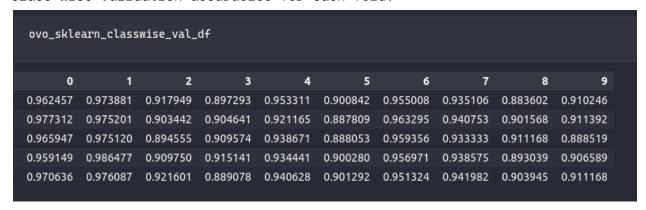
Accuracy table:



Class Wise training accuracies for each fold:



Class Wise validation accuracies for each fold:



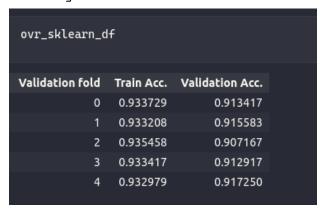
Sklearn's OVO implementation outperforms self implementation in training accuracy showcasing better convergence, although slightly better performance in validation showcasing similar generalizability of models.

Using OneVsRestClassifier:

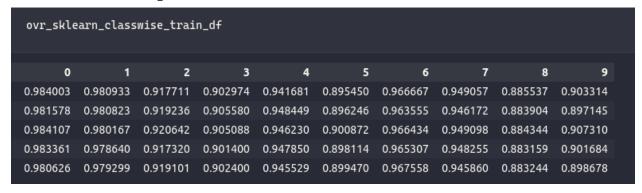
Model used: (Max iters=750 to ensure convergence)

lr = OneVsRestClassifier(LogisticRegression(*max\_iter*=750, *random\_state*=7))

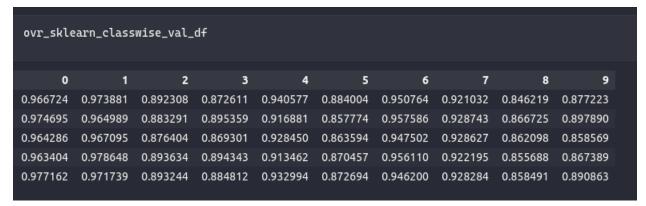
Accuracy table:



Class Wise training accuracies for each fold:



Class Wise validation accuracies for each fold:



Sklearn's OVR implementation outperforms self implementation both in training and validation accuracies indicating better convergence and generalizability. This difference arises due to differences in hyperparameters, convergence algorithms, etc.