Appendix A

Data Validation Techniques

This section gives insight into various validation techniques that are used in the study. Validation techniques help in generalising the model's performance without any bias. All the validation techniques work by splitting the data into train and test sets. This helps in estimating the model's performance on new data i.e unseen data. Three kinds of validation techniques namely leave one out, percentage split and k fold cross validation are discussed herewith:

1. Percentage split: It is most common validation technique in which $p\%$ of data is used for training and remaining $q\%(= 1 - p)$ of the data is used for testing. Commonly, 80-20 and 70-30 splits are employed. The advantage of the approach is that it helps in evaluating the performance on previously unseen data. However, that may lead to sampling bias in case of uneven distribution of samples in the set.

2. k-Fold cross validation: In this technique, the entire dataset is split into k parts or folds. (k - 1) parts are used for training and remaining one part is used for testing the model. The entire process is iterated a number of times

and averages are henceforth employed. This way all the samples get to be part of train and test sets.

3. Leave one out: It is a variant of k-Fold cross validation in which k is equal to number of samples in the dataset implying all the samples except one is used for training and remaining single sample is used for testing.

These are some of commonly employed validation techniques used for evaluating model's performance. In case of feature selection, training data is employed to find the compact set of most meaningful features and the testing set is thereby evaluated using only those features.

Appendix B

Performance Evaluation Metrics

The prediction performances of the machine learning algorithms are evaluated using threshold-dependent and threshold-independent parameters. These parameters are determined using true positive (TP), true negative (TN), false positive (FP) and false negative (FN). TP is number of correctly classified positive instances; TN is number of correctly classified negative instances. FN is number of incorrectly classified positive instances while FP is number of incorrectly classified negative instances.

Sensitivity: It gives the percentage of correctly classified positive instances and is calculated by given formula:

$$Sensitivity = \frac{TP}{(TP + FN)} \times 100 \tag{B.1}$$

Specificity: It gives the percentage of correctly classified negative instances and is calculated as follows:

$$Specificity = \frac{TN}{(TN + FP)} \times 100 \tag{B.2}$$

Accuracy: It is the percentage of correctly classified instances (both positive and negative), and is given as follows:

$$Accuracy = \frac{(TP + TN)}{(TP + FP + TN + FN)} \times 100 \tag{B.3}$$

MCC (Mathew's correlation coefficient): Ideal value of MCC is taken as 1. It is generally used for binary data and is calculated by using the formula as below:

$$MCC = \frac{(TP \times TN - FP \times FN)}{\sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}} \tag{B.4}$$

AUC: Area under curve (AUC) of a receiver operating characteristics curve (ROC) [95]. Best value of AUC is considered as 1, while 0 is taken as the worst case. Its value lies between 0 and 1. Its value is not affected by the imbalanced nature of the datasets.

g-means: It is defined as the geometric mean of sensitivity and specificity [83] and is defined as follows:

$$g - means = \sqrt{Sensitivity \times Specificity} \tag{B.5}$$

All these performance parameters are evaluated using open source Java based machine learning platform WEKA [56].

Appendix C

Statistical Testing

The significance of the approaches is illustrated using statistical test. Two tests namely t test and Freidman test and Bonferoni Dunn test are employed in the thesis to demonstrate statistical significance.

1. **t test**: Two tailed student's t test is employed for calculating difference between average accuracy of two models statistically. The value of t statistic for $2(N-1)$ degree of freedom (where $N = 10$ for 10 fold cross validation) is calculated using the following formula:

$$t = \frac{\bar{x}_1 - \bar{x}_2}{\frac{s_1^2+s_2^2}{N}}$$

where $\bar{x}_1$ and $\bar{x}_2$ are the average classification accuracies obtained by two models and s_1^2, s_2^2 are the corresponding standard deviations. The level of significance is set to 0.05 for the experiments conducted during the research. The probability p-val associated with t test is found out using t table. The small p-val values (less than 0.05) illustrates the significant differences amongst the algorithms. Various signs like +, -, o are used to show corresponding statistical win, loss and tie respectively of the respective approach at 5% level of significance.

2. **Freidman test [50, 51] and Bonferoni Dunn test [39]**: Freidman test is used for multiple hypothesis testing employing F statistics, which is defined as:
$$F = \frac{(M-1)\chi^2}{M(N-1)-\chi^2}$$
and
$$\chi^2 = \frac{12M}{N(N+1)}\sum_{j=1}^{N}(R_j - \frac{(N+1)}{2})^2$$
where M is the number of dataset, N is the number of employed algorithms and R_j is the average rank of algorithm j calculated from all the datasets. If the F statistics that follows Freidman distribution is greater than critical value of F (F_{crit}) at $N-1$ and $(N-1)(M-1)$ degrees of freedom, the null hypothesis that all algorithm are equivalent in terms of classification accuracy is rejected. In such case, Bonferroni Dunn is used to find which algorithm is significantly different from proposed approach. Two approaches are significantly different at α% level of significance if distance between their R_j is greater than critical distance Cd_α given as:
$$Cd_\alpha = q_\alpha\sqrt{\frac{N(N+1)}{6M}}$$
where q_α is tabulated value at α% level of significance.[32]. All the statistical tests are conducted at 5% level of significance during the research.

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