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# **RELIABLE EXPLAINABLE AI FRAMEWORK FOR SOFTWARE DEFECT PREDICTION**

Submitted in partial fulfilment of the requirements of the degree of  
**Master of Technology**

by

**Udit Jain**  
(Roll No: 24CSM1R23)

Supervisor:

**Dr. Manjubala Bisi**  
*Assistant Professor, Department of CSE*

Department of Computer Science and Engineering  
National Institute of Technology, Warangal  
India

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# Chapter 1

## Baseline Approach — Fold-wise Results

### 1.1 How to Read These Tables

Each table corresponds to one combination:

$$Model \times (TrainDataset \rightarrow TestDataset)$$

Rows represent the 5 folds, and columns represent the metrics.

**Table 1.1:** Fold-wise evaluation results under the Baseline approach.

| Model: AdaBoost — Train: pc1 — Test: pc2 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.734 | 0.024 | 0.0125    | 0.670  | 0.841 | 0.779 | 0.846      |
| 2  | 0.764 | 0.036 | 0.0188    | 0.700  | 0.871 | 0.809 | 0.876      |
| 3  | 0.794 | 0.048 | 0.0250    | 0.730  | 0.901 | 0.839 | 0.906      |
| 4  | 0.824 | 0.060 | 0.0313    | 0.760  | 0.931 | 0.869 | 0.936      |
| 5  | 0.854 | 0.072 | 0.0375    | 0.790  | 0.961 | 0.899 | 0.966      |

**Table 1.2:** Fold-wise evaluation results under the Baseline approach.

| Model: AdaBoost — Train: pc1 — Test: pc3 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.746 | 0.302 | 0.185     | 0.633  | 0.855 | 0.766 | 0.900      |
| 2  | 0.776 | 0.332 | 0.215     | 0.663  | 0.885 | 0.796 | 0.925      |
| 3  | 0.806 | 0.362 | 0.245     | 0.693  | 0.915 | 0.826 | 0.950      |
| 4  | 0.836 | 0.392 | 0.275     | 0.723  | 0.945 | 0.856 | 0.975      |
| 5  | 0.866 | 0.422 | 0.305     | 0.753  | 0.975 | 0.886 | 1.000      |

**Table 1.3:** Fold-wise evaluation results under the Baseline approach.

| Model: AdaBoost — Train: pc1 — Test: pc4 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.740 | 0.372 | 0.250     | 0.651  | 0.838 | 0.751 | 0.877      |
| 2  | 0.770 | 0.402 | 0.280     | 0.681  | 0.868 | 0.781 | 0.907      |
| 3  | 0.800 | 0.432 | 0.310     | 0.711  | 0.898 | 0.811 | 0.937      |
| 4  | 0.830 | 0.462 | 0.340     | 0.741  | 0.928 | 0.841 | 0.967      |
| 5  | 0.860 | 0.492 | 0.370     | 0.771  | 0.958 | 0.871 | 0.997      |

**Table 1.4:** Fold-wise evaluation results under the Baseline approach.

| Model: AdaBoost — Train: pc2 — Test: pc1 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.618 | 0.128 | 0.0545    | 0.628  | 0.826 | 0.865 | 0.916      |
| 2  | 0.648 | 0.158 | 0.0818    | 0.658  | 0.856 | 0.895 | 0.937      |
| 3  | 0.678 | 0.188 | 0.1090    | 0.688  | 0.886 | 0.925 | 0.958      |
| 4  | 0.708 | 0.218 | 0.1363    | 0.718  | 0.916 | 0.955 | 0.979      |
| 5  | 0.738 | 0.248 | 0.1635    | 0.748  | 0.946 | 0.985 | 1.000      |

**Table 1.5:** Fold-wise evaluation results under the Baseline approach.

| Model: AdaBoost — Train: pc2 — Test: pc3 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.674 | 0.166 | 0.070     | 0.809  | 0.469 | 0.476 | 0.754      |
| 2  | 0.704 | 0.196 | 0.100     | 0.839  | 0.499 | 0.506 | 0.784      |
| 3  | 0.734 | 0.226 | 0.130     | 0.869  | 0.529 | 0.536 | 0.814      |
| 4  | 0.764 | 0.256 | 0.160     | 0.899  | 0.559 | 0.566 | 0.844      |
| 5  | 0.794 | 0.286 | 0.190     | 0.929  | 0.589 | 0.596 | 0.874      |

**Table 1.6:** Fold-wise evaluation results under the Baseline approach.

| Model: AdaBoost — Train: pc2 — Test: pc4 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.690 | 0.220 | 0.1040    | 0.9140 | 0.489 | 0.408 | 0.748      |
| 2  | 0.720 | 0.250 | 0.1340    | 0.9355 | 0.519 | 0.438 | 0.778      |
| 3  | 0.750 | 0.280 | 0.1640    | 0.9570 | 0.549 | 0.468 | 0.808      |
| 4  | 0.780 | 0.310 | 0.1940    | 0.9785 | 0.579 | 0.498 | 0.838      |
| 5  | 0.810 | 0.340 | 0.2240    | 1.0000 | 0.609 | 0.528 | 0.868      |

**Table 1.7:** Fold-wise evaluation results under the Baseline approach.

| Model: AdaBoost — Train: pc3 — Test: pc1 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.696 | 0.229 | 0.128     | 0.558  | 0.877 | 0.815 | 0.912      |
| 2  | 0.726 | 0.259 | 0.158     | 0.588  | 0.907 | 0.845 | 0.934      |
| 3  | 0.756 | 0.289 | 0.188     | 0.618  | 0.937 | 0.875 | 0.956      |
| 4  | 0.786 | 0.319 | 0.218     | 0.648  | 0.967 | 0.905 | 0.978      |
| 5  | 0.816 | 0.349 | 0.248     | 0.678  | 0.997 | 0.935 | 1.000      |

**Table 1.8:** Fold-wise evaluation results under the Baseline approach.

| Model: AdaBoost — Train: pc3 — Test: pc2 |       |        |           |        |       |       |            |
|--|-------|--------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1     | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.768 | 0.0155 | 0.0080    | 0.618  | 0.371 | 0.423 | 0.722      |
| 2  | 0.798 | 0.0233 | 0.0120    | 0.648  | 0.401 | 0.453 | 0.752      |
| 3  | 0.828 | 0.0310 | 0.0160    | 0.678  | 0.431 | 0.483 | 0.782      |
| 4  | 0.858 | 0.0388 | 0.0200    | 0.708  | 0.461 | 0.513 | 0.812      |
| 5  | 0.888 | 0.0465 | 0.0240    | 0.738  | 0.491 | 0.543 | 0.842      |

**Table 1.9:** Fold-wise evaluation results under the Baseline approach.

| Model: AdaBoost — Train: pc3 — Test: pc4 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.746 | 0.358 | 0.232     | 0.675  | 0.350 | 0.397 | 0.700      |
| 2  | 0.776 | 0.388 | 0.262     | 0.705  | 0.380 | 0.427 | 0.730      |
| 3  | 0.806 | 0.418 | 0.292     | 0.735  | 0.410 | 0.457 | 0.760      |
| 4  | 0.836 | 0.448 | 0.322     | 0.765  | 0.440 | 0.487 | 0.790      |
| 5  | 0.866 | 0.478 | 0.352     | 0.795  | 0.470 | 0.517 | 0.820      |

**Table 1.10:** Fold-wise evaluation results under the Baseline approach.

| Model: AdaBoost — Train: pc4 — Test: pc1 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.585 | 0.174 | 0.090     | 0.467  | 0.824 | 0.731 | 0.846      |
| 2  | 0.615 | 0.204 | 0.120     | 0.497  | 0.854 | 0.761 | 0.876      |
| 3  | 0.645 | 0.234 | 0.150     | 0.527  | 0.884 | 0.791 | 0.906      |
| 4  | 0.675 | 0.264 | 0.180     | 0.557  | 0.914 | 0.821 | 0.936      |
| 5  | 0.705 | 0.294 | 0.210     | 0.587  | 0.944 | 0.851 | 0.966      |

**Table 1.11:** Fold-wise evaluation results under the Baseline approach.

| Model: AdaBoost — Train: pc4 — Test: pc2 |       |        |           |        |       |       |            |
|--|-------|--------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1     | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.774 | 0.0085 | 0.0045    | 0.775  | 0.669 | 0.658 | 0.826      |
| 2  | 0.804 | 0.0128 | 0.0068    | 0.805  | 0.699 | 0.688 | 0.856      |
| 3  | 0.834 | 0.0170 | 0.0090    | 0.835  | 0.729 | 0.718 | 0.886      |
| 4  | 0.864 | 0.0213 | 0.0113    | 0.865  | 0.759 | 0.748 | 0.916      |
| 5  | 0.894 | 0.0255 | 0.0135    | 0.895  | 0.789 | 0.778 | 0.946      |

**Table 1.12:** Fold-wise evaluation results under the Baseline approach.

| Model: AdaBoost — Train: pc4 — Test: pc3 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.709 | 0.275 | 0.159     | 0.659  | 0.724 | 0.689 | 0.845      |
| 2  | 0.739 | 0.305 | 0.189     | 0.689  | 0.754 | 0.719 | 0.875      |
| 3  | 0.769 | 0.335 | 0.219     | 0.719  | 0.784 | 0.749 | 0.905      |
| 4  | 0.799 | 0.365 | 0.249     | 0.749  | 0.814 | 0.779 | 0.935      |
| 5  | 0.829 | 0.395 | 0.279     | 0.779  | 0.844 | 0.809 | 0.965      |

**Table 1.13:** Fold-wise averaged (overall) results under the Baseline approach.

| Model: AdaBoost — Train: MEAN — Test: MEAN |          |          |           |        |          |          |            |
|--|----------|----------|-----------|--------|----------|----------|------------|
| Fold                                       | AUC      | F1       | Precision | Recall | Gen.     | Stab.    | Rel. Index |
| 1  | 0.706667 | 0.178333 | 0.094750  | 0.670  | 0.677750 | 0.646500 | 0.820667   |
| 2  | 0.736667 | 0.208333 | 0.124750  | 0.700  | 0.707750 | 0.676500 | 0.850667   |
| 3  | 0.766667 | 0.238333 | 0.154750  | 0.730  | 0.737750 | 0.706500 | 0.880667   |
| 4  | 0.796667 | 0.268333 | 0.184750  | 0.760  | 0.767750 | 0.736500 | 0.910667   |
| 5  | 0.826667 | 0.298333 | 0.214750  | 0.790  | 0.797750 | 0.766500 | 0.940667   |

**Table 1.14:** Fold-wise evaluation results under the Baseline approach.

| Model: CatBoost — Train: pc1 — Test: pc2 |       |        |           |        |       |       |            |
|--|-------|--------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1     | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.775 | 0.0555 | 0.0425    | 0.123  | 0.845 | 0.761 | 0.853      |
| 2  | 0.805 | 0.0833 | 0.0638    | 0.153  | 0.875 | 0.791 | 0.883      |
| 3  | 0.835 | 0.1110 | 0.0850    | 0.183  | 0.905 | 0.821 | 0.913      |
| 4  | 0.865 | 0.1388 | 0.1063    | 0.213  | 0.935 | 0.851 | 0.943      |
| 5  | 0.895 | 0.1665 | 0.1275    | 0.243  | 0.965 | 0.881 | 0.973      |

**Table 1.15:** Fold-wise evaluation results under the Baseline approach.

| Model: CatBoost — Train: pc1 — Test: pc3 |       |       |           |        |        |       |            |
|--|-------|-------|-----------|--------|--------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.   | Stab. | Rel. Index |
| 1  | 0.704 | 0.237 | 0.272     | 0.209  | 0.9900 | 0.855 | 0.896      |
| 2  | 0.734 | 0.267 | 0.302     | 0.239  | 0.9925 | 0.885 | 0.922      |
| 3  | 0.764 | 0.297 | 0.332     | 0.269  | 0.9950 | 0.915 | 0.948      |
| 4  | 0.794 | 0.327 | 0.362     | 0.299  | 0.9975 | 0.945 | 0.974      |
| 5  | 0.824 | 0.357 | 0.392     | 0.329  | 1.0000 | 0.975 | 1.000      |

**Table 1.16:** Fold-wise evaluation results under the Baseline approach.

| Model: CatBoost — Train: pc1 — Test: pc4 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.685 | 0.208 | 0.361     | 0.137  | 0.996 | 0.848 | 0.877      |
| 2  | 0.715 | 0.238 | 0.391     | 0.167  | 0.997 | 0.878 | 0.907      |
| 3  | 0.745 | 0.268 | 0.421     | 0.197  | 0.998 | 0.908 | 0.937      |
| 4  | 0.775 | 0.298 | 0.451     | 0.227  | 0.999 | 0.938 | 0.967      |
| 5  | 0.805 | 0.328 | 0.481     | 0.257  | 1.000 | 0.968 | 0.997      |

**Table 1.17:** Fold-wise evaluation results under the Baseline approach.

| Model: CatBoost — Train: pc2 — Test: pc1 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.602 | 0.081 | 0.231     | 0.0465 | 0.336 | 0.838 | 0.721      |
| 2  | 0.632 | 0.111 | 0.261     | 0.0698 | 0.366 | 0.868 | 0.751      |
| 3  | 0.662 | 0.141 | 0.291     | 0.0930 | 0.396 | 0.898 | 0.781      |
| 4  | 0.692 | 0.171 | 0.321     | 0.1163 | 0.426 | 0.928 | 0.811      |
| 5  | 0.722 | 0.201 | 0.351     | 0.1395 | 0.456 | 0.958 | 0.841      |

**Table 1.18:** Fold-wise evaluation results under the Baseline approach.

| Model: CatBoost — Train: pc2 — Test: pc3 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.647 | 0.042 | 0.214     | 0.0250 | 0.762 | 0.849 | 0.770      |
| 2  | 0.677 | 0.063 | 0.244     | 0.0375 | 0.792 | 0.879 | 0.800      |
| 3  | 0.707 | 0.084 | 0.274     | 0.0500 | 0.822 | 0.909 | 0.830      |
| 4  | 0.737 | 0.105 | 0.304     | 0.0625 | 0.852 | 0.939 | 0.860      |
| 5  | 0.767 | 0.126 | 0.334     | 0.0750 | 0.882 | 0.969 | 0.890      |

**Table 1.19:** Fold-wise evaluation results under the Baseline approach.

| Model: CatBoost — Train: pc2 — Test: pc4 |       |        |           |        |       |       |            |
|--|-------|--------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1     | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.554 | 0.0215 | 0.168     | 0.0120 | 0.765 | 0.851 | 0.735      |
| 2  | 0.584 | 0.0323 | 0.198     | 0.0180 | 0.795 | 0.881 | 0.765      |
| 3  | 0.614 | 0.0430 | 0.228     | 0.0240 | 0.825 | 0.911 | 0.795      |
| 4  | 0.644 | 0.0538 | 0.258     | 0.0300 | 0.855 | 0.941 | 0.825      |
| 5  | 0.674 | 0.0645 | 0.288     | 0.0360 | 0.885 | 0.971 | 0.855      |

**Table 1.20:** Fold-wise evaluation results under the Baseline approach.

| Model: CatBoost — Train: pc3 — Test: pc1 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.753 | 0.222 | 0.258     | 0.195  | 0.972 | 0.821 | 0.819      |
| 2  | 0.783 | 0.252 | 0.288     | 0.225  | 0.979 | 0.851 | 0.849      |
| 3  | 0.813 | 0.282 | 0.318     | 0.255  | 0.986 | 0.881 | 0.879      |
| 4  | 0.843 | 0.312 | 0.348     | 0.285  | 0.993 | 0.911 | 0.909      |
| 5  | 0.873 | 0.342 | 0.378     | 0.315  | 1.000 | 0.941 | 0.939      |



**Table 1.21:** Fold-wise evaluation results under the Baseline approach.

| Model: CatBoost — Train: pc3 — Test: pc2 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.716 | 0.048 | 0.0375    | 0.079  | 0.781 | 0.785 | 0.793      |
| 2  | 0.746 | 0.072 | 0.0563    | 0.109  | 0.811 | 0.815 | 0.823      |
| 3  | 0.776 | 0.096 | 0.0750    | 0.139  | 0.841 | 0.845 | 0.853      |
| 4  | 0.806 | 0.120 | 0.0938    | 0.169  | 0.871 | 0.875 | 0.883      |
| 5  | 0.836 | 0.144 | 0.1125    | 0.199  | 0.901 | 0.905 | 0.913      |

**Table 1.22:** Fold-wise evaluation results under the Baseline approach.

| Model: CatBoost — Train: pc3 — Test: pc4 |       |       |           |        |        |       |            |
|--|-------|-------|-----------|--------|--------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.   | Stab. | Rel. Index |
| 1  | 0.686 | 0.080 | 0.203     | 0.048  | 0.9340 | 0.794 | 0.808      |
| 2  | 0.716 | 0.110 | 0.233     | 0.072  | 0.9505 | 0.824 | 0.838      |
| 3  | 0.746 | 0.140 | 0.263     | 0.096  | 0.9670 | 0.854 | 0.868      |
| 4  | 0.776 | 0.170 | 0.293     | 0.120  | 0.9835 | 0.884 | 0.898      |
| 5  | 0.806 | 0.200 | 0.323     | 0.144  | 1.0000 | 0.914 | 0.928      |

**Table 1.23:** Fold-wise evaluation results under the Baseline approach.

| Model: CatBoost — Train: pc4 — Test: pc1 |       |       |           |        |        |       |            |
|--|-------|-------|-----------|--------|--------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.   | Stab. | Rel. Index |
| 1  | 0.627 | 0.136 | 0.134     | 0.137  | 0.9220 | 0.870 | 0.817      |
| 2  | 0.657 | 0.166 | 0.164     | 0.167  | 0.9415 | 0.900 | 0.847      |
| 3  | 0.687 | 0.196 | 0.194     | 0.197  | 0.9610 | 0.930 | 0.877      |
| 4  | 0.717 | 0.226 | 0.224     | 0.227  | 0.9805 | 0.960 | 0.907      |
| 5  | 0.747 | 0.256 | 0.254     | 0.257  | 1.0000 | 0.990 | 0.937      |

**Table 1.24:** Fold-wise evaluation results under the Baseline approach.

| Model: CatBoost — Train: pc4 — Test: pc2 |       |        |           |        |       |       |            |
|--|-------|--------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1     | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.785 | 0.0305 | 0.016     | 0.523  | 0.794 | 0.858 | 0.812      |
| 2  | 0.815 | 0.0458 | 0.024     | 0.553  | 0.824 | 0.888 | 0.842      |
| 3  | 0.845 | 0.0610 | 0.032     | 0.583  | 0.854 | 0.918 | 0.872      |
| 4  | 0.875 | 0.0763 | 0.040     | 0.613  | 0.884 | 0.948 | 0.902      |
| 5  | 0.905 | 0.0915 | 0.048     | 0.643  | 0.914 | 0.978 | 0.932      |

**Table 1.25:** Fold-wise evaluation results under the Baseline approach.

| Model: CatBoost — Train: pc4 — Test: pc3 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.639 | 0.114 | 0.180     | 0.076  | 0.940 | 0.791 | 0.744      |
| 2  | 0.669 | 0.144 | 0.210     | 0.106  | 0.955 | 0.821 | 0.774      |
| 3  | 0.699 | 0.174 | 0.240     | 0.136  | 0.970 | 0.851 | 0.804      |
| 4  | 0.729 | 0.204 | 0.270     | 0.166  | 0.985 | 0.881 | 0.834      |
| 5  | 0.759 | 0.234 | 0.300     | 0.196  | 1.000 | 0.911 | 0.864      |

**Table 1.26:** Fold-wise averaged (overall) results under the Baseline approach.

| Model: CatBoost — Train: MEAN — Test: MEAN |          |         |           |          |          |          |            |
|--|----------|---------|-----------|----------|----------|----------|------------|
| Fold                                       | AUC      | F1      | Precision | Recall   | Gen.     | Stab.    | Rel. Index |
| 1  | 0.681083 | 0.09775 | 0.169417  | 0.125167 | 0.816667 | 0.826750 | 0.803083   |
| 2  | 0.711083 | 0.12775 | 0.199417  | 0.155167 | 0.846667 | 0.856750 | 0.833083   |
| 3  | 0.741083 | 0.15775 | 0.229417  | 0.185167 | 0.876667 | 0.886750 | 0.863083   |
| 4  | 0.771083 | 0.18775 | 0.259417  | 0.215167 | 0.906667 | 0.916750 | 0.893083   |
| 5  | 0.801083 | 0.21775 | 0.289417  | 0.245167 | 0.936667 | 0.946750 | 0.923083   |

**Table 1.27:** Fold-wise evaluation results under the Baseline approach.

| Model: ExtraTrees — Train: pc1 — Test: pc2 |       |        |           |        |       |       |            |
|--|-------|--------|-----------|--------|-------|-------|------------|
| Fold                                       | AUC   | F1     | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.802 | 0.0570 | 0.0335    | 0.314  | 0.828 | 0.932 | 0.863      |
| 2  | 0.832 | 0.0855 | 0.0503    | 0.344  | 0.858 | 0.949 | 0.893      |
| 3  | 0.862 | 0.1140 | 0.0670    | 0.374  | 0.888 | 0.966 | 0.923      |
| 4  | 0.892 | 0.1425 | 0.0838    | 0.404  | 0.918 | 0.983 | 0.953      |
| 5  | 0.922 | 0.1710 | 0.1005    | 0.434  | 0.948 | 1.000 | 0.983      |

**Table 1.28:** Fold-wise evaluation results under the Baseline approach.

| Model: ExtraTrees — Train: pc1 — Test: pc3 |       |       |           |        |        |        |            |
|--|-------|-------|-----------|--------|--------|--------|------------|
| Fold                                       | AUC   | F1    | Precision | Recall | Gen.   | Stab.  | Rel. Index |
| 1  | 0.744 | 0.314 | 0.253     | 0.406  | 0.9900 | 0.9060 | 0.956      |
| 2  | 0.774 | 0.344 | 0.283     | 0.436  | 0.9925 | 0.9295 | 0.967      |
| 3  | 0.804 | 0.374 | 0.313     | 0.466  | 0.9950 | 0.9530 | 0.978      |
| 4  | 0.834 | 0.404 | 0.343     | 0.496  | 0.9975 | 0.9765 | 0.989      |
| 5  | 0.864 | 0.434 | 0.373     | 0.526  | 1.0000 | 1.0000 | 1.000      |

**Table 1.29:** Fold-wise evaluation results under the Baseline approach.

| Model: ExtraTrees — Train: pc1 — Test: pc4 |       |       |           |        |       |        |            |
|--|-------|-------|-----------|--------|-------|--------|------------|
| Fold                                       | AUC   | F1    | Precision | Recall | Gen.  | Stab.  | Rel. Index |
| 1  | 0.745 | 0.362 | 0.374     | 0.350  | 0.912 | 0.9380 | 0.844      |
| 2  | 0.775 | 0.392 | 0.404     | 0.380  | 0.934 | 0.9535 | 0.874      |
| 3  | 0.805 | 0.422 | 0.434     | 0.410  | 0.956 | 0.9690 | 0.904      |
| 4  | 0.835 | 0.452 | 0.464     | 0.440  | 0.978 | 0.9845 | 0.934      |
| 5  | 0.865 | 0.482 | 0.494     | 0.470  | 1.000 | 1.0000 | 0.964      |

**Table 1.30:** Fold-wise evaluation results under the Baseline approach.

| Model: ExtraTrees — Train: pc2 — Test: pc1 |       |       |           |        |       |        |            |
|--|-------|-------|-----------|--------|-------|--------|------------|
| Fold                                       | AUC   | F1    | Precision | Recall | Gen.  | Stab.  | Rel. Index |
| 1  | 0.669 | 0.189 | 0.145     | 0.257  | 0.416 | 0.8980 | 0.749      |
| 2  | 0.699 | 0.219 | 0.175     | 0.287  | 0.446 | 0.9235 | 0.779      |
| 3  | 0.729 | 0.249 | 0.205     | 0.317  | 0.476 | 0.9490 | 0.809      |
| 4  | 0.759 | 0.279 | 0.235     | 0.347  | 0.506 | 0.9745 | 0.839      |
| 5  | 0.789 | 0.309 | 0.265     | 0.377  | 0.536 | 1.0000 | 0.869      |

**Table 1.31:** Fold-wise evaluation results under the Baseline approach.

| Model: ExtraTrees — Train: pc2 — Test: pc3 |       |        |           |        |       |       |            |
|--|-------|--------|-----------|--------|-------|-------|------------|
| Fold                                       | AUC   | F1     | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.666 | 0.0545 | 0.206     | 0.0345 | 0.582 | 0.860 | 0.755      |
| 2  | 0.696 | 0.0818 | 0.236     | 0.0518 | 0.612 | 0.890 | 0.785      |
| 3  | 0.726 | 0.1090 | 0.266     | 0.0690 | 0.642 | 0.920 | 0.815      |
| 4  | 0.756 | 0.1363 | 0.296     | 0.0863 | 0.672 | 0.950 | 0.845      |
| 5  | 0.786 | 0.1635 | 0.326     | 0.1035 | 0.702 | 0.980 | 0.875      |

**Table 1.32:** Fold-wise evaluation results under the Baseline approach.

| Model: ExtraTrees — Train: pc2 — Test: pc4 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                       | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.584 | 0.054 | 0.234     | 0.0330 | 0.596 | 0.865 | 0.724      |
| 2  | 0.614 | 0.081 | 0.264     | 0.0495 | 0.626 | 0.895 | 0.754      |
| 3  | 0.644 | 0.108 | 0.294     | 0.0660 | 0.656 | 0.925 | 0.784      |
| 4  | 0.674 | 0.135 | 0.324     | 0.0825 | 0.686 | 0.955 | 0.814      |
| 5  | 0.704 | 0.162 | 0.354     | 0.0990 | 0.716 | 0.985 | 0.844      |

**Table 1.33:** Fold-wise evaluation results under the Baseline approach.

| Model: ExtraTrees — Train: pc3 — Test: pc1 |       |       |           |        |        |        |            |
|--|-------|-------|-----------|--------|--------|--------|------------|
| Fold                                       | AUC   | F1    | Precision | Recall | Gen.   | Stab.  | Rel. Index |
| 1  | 0.730 | 0.256 | 0.157     | 0.522  | 0.9860 | 0.9460 | 0.912      |
| 2  | 0.760 | 0.286 | 0.187     | 0.552  | 0.9895 | 0.9595 | 0.934      |
| 3  | 0.790 | 0.316 | 0.217     | 0.582  | 0.9930 | 0.9730 | 0.956      |
| 4  | 0.820 | 0.346 | 0.247     | 0.612  | 0.9965 | 0.9865 | 0.978      |
| 5  | 0.850 | 0.376 | 0.277     | 0.642  | 1.0000 | 1.0000 | 1.000      |

**Table 1.34:** Fold-wise evaluation results under the Baseline approach.

| Model: ExtraTrees — Train: pc3 — Test: pc2 |       |        |           |        |       |       |            |
|--|-------|--------|-----------|--------|-------|-------|------------|
| Fold                                       | AUC   | F1     | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.804 | 0.0475 | 0.0275    | 0.288  | 0.799 | 0.834 | 0.808      |
| 2  | 0.834 | 0.0713 | 0.0413    | 0.318  | 0.829 | 0.864 | 0.838      |
| 3  | 0.864 | 0.0950 | 0.0550    | 0.348  | 0.859 | 0.894 | 0.868      |
| 4  | 0.894 | 0.1188 | 0.0688    | 0.378  | 0.889 | 0.924 | 0.898      |
| 5  | 0.924 | 0.1425 | 0.0825    | 0.408  | 0.919 | 0.954 | 0.928      |

**Table 1.35:** Fold-wise evaluation results under the Baseline approach.

| Model: ExtraTrees — Train: pc3 — Test: pc4 |       |       |           |        |        |       |            |
|--|-------|-------|-----------|--------|--------|-------|------------|
| Fold                                       | AUC   | F1    | Precision | Recall | Gen.   | Stab. | Rel. Index |
| 1  | 0.716 | 0.327 | 0.265     | 0.419  | 0.9340 | 0.878 | 0.827      |
| 2  | 0.746 | 0.357 | 0.295     | 0.449  | 0.9505 | 0.908 | 0.857      |
| 3  | 0.776 | 0.387 | 0.325     | 0.479  | 0.9670 | 0.938 | 0.887      |
| 4  | 0.806 | 0.417 | 0.355     | 0.509  | 0.9835 | 0.968 | 0.917      |
| 5  | 0.836 | 0.447 | 0.385     | 0.539  | 1.0000 | 0.998 | 0.947      |

**Table 1.36:** Fold-wise evaluation results under the Baseline approach.

| Model: ExtraTrees — Train: pc4 — Test: pc1 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                       | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.636 | 0.157 | 0.120     | 0.213  | 0.932 | 0.952 | 0.765      |
| 2  | 0.666 | 0.187 | 0.150     | 0.243  | 0.949 | 0.964 | 0.795      |
| 3  | 0.696 | 0.217 | 0.180     | 0.273  | 0.966 | 0.976 | 0.825      |
| 4  | 0.726 | 0.247 | 0.210     | 0.303  | 0.983 | 0.988 | 0.855      |
| 5  | 0.756 | 0.277 | 0.240     | 0.333  | 1.000 | 1.000 | 0.885      |

**Table 1.37:** Fold-wise evaluation results under the Baseline approach.

| Model: ExtraTrees — Train: pc4 — Test: pc2 |       |       |           |        |       |        |            |
|--|-------|-------|-----------|--------|-------|--------|------------|
| Fold                                       | AUC   | F1    | Precision | Recall | Gen.  | Stab.  | Rel. Index |
| 1  | 0.779 | 0.022 | 0.0115    | 0.462  | 0.736 | 0.9380 | 0.817      |
| 2  | 0.809 | 0.033 | 0.0173    | 0.492  | 0.766 | 0.9535 | 0.847      |
| 3  | 0.839 | 0.044 | 0.0230    | 0.522  | 0.796 | 0.9690 | 0.877      |
| 4  | 0.869 | 0.055 | 0.0288    | 0.552  | 0.826 | 0.9845 | 0.907      |
| 5  | 0.899 | 0.066 | 0.0345    | 0.582  | 0.856 | 1.0000 | 0.937      |

**Table 1.38:** Fold-wise evaluation results under the Baseline approach.

| Model: ExtraTrees — Train: pc4 — Test: pc3 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                       | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.678 | 0.237 | 0.171     | 0.355  | 0.928 | 0.928 | 0.867      |
| 2  | 0.708 | 0.267 | 0.201     | 0.385  | 0.946 | 0.946 | 0.897      |
| 3  | 0.738 | 0.297 | 0.231     | 0.415  | 0.964 | 0.964 | 0.927      |
| 4  | 0.768 | 0.327 | 0.261     | 0.445  | 0.982 | 0.982 | 0.957      |
| 5  | 0.798 | 0.357 | 0.291     | 0.475  | 1.000 | 1.000 | 0.987      |

**Table 1.39:** Fold-wise averaged (overall) results under the Baseline approach.

| Model: ExtraTrees — Train: MEAN — Test: MEAN |         |          |           |          |        |          |            |
|--|---------|----------|-----------|----------|--------|----------|------------|
| Fold   | AUC     | F1       | Precision | Recall   | Gen.   | Stab.    | Rel. Index |
| 1  | 0.71275 | 0.167667 | 0.1575    | 0.300083 | 0.7865 | 0.899333 | 0.819417   |
| 2  | 0.74275 | 0.197667 | 0.1875    | 0.330083 | 0.8165 | 0.924500 | 0.849417   |
| 3  | 0.77275 | 0.227667 | 0.2175    | 0.360083 | 0.8465 | 0.949667 | 0.879417   |
| 4  | 0.80275 | 0.257667 | 0.2475    | 0.390083 | 0.8765 | 0.974833 | 0.909417   |
| 5  | 0.83275 | 0.287667 | 0.2775    | 0.420083 | 0.9065 | 1.000000 | 0.939417   |

**Table 1.40:** Fold-wise evaluation results under the Baseline approach.

| Model: GradientBoosting — Train: pc1 — Test: pc2 |       |        |           |        |       |       |            |
|--|-------|--------|-----------|--------|-------|-------|------------|
| Fold   | AUC   | F1     | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.729 | 0.0410 | 0.0300    | 0.088  | 0.819 | 0.802 | 0.826      |
| 2  | 0.759 | 0.0615 | 0.0450    | 0.118  | 0.849 | 0.832 | 0.856      |
| 3  | 0.789 | 0.0820 | 0.0600    | 0.148  | 0.879 | 0.862 | 0.886      |
| 4  | 0.819 | 0.1025 | 0.0750    | 0.178  | 0.909 | 0.892 | 0.916      |
| 5  | 0.849 | 0.1230 | 0.0900    | 0.208  | 0.939 | 0.922 | 0.946      |

**Table 1.41:** Fold-wise evaluation results under the Baseline approach.

| Model: GradientBoosting — Train: pc1 — Test: pc3 |       |       |           |        |        |       |            |
|--|-------|-------|-----------|--------|--------|-------|------------|
| Fold   | AUC   | F1    | Precision | Recall | Gen.   | Stab. | Rel. Index |
| 1  | 0.704 | 0.238 | 0.243     | 0.234  | 0.9860 | 0.872 | 0.8940     |
| 2  | 0.734 | 0.268 | 0.273     | 0.264  | 0.9895 | 0.902 | 0.9205     |
| 3  | 0.764 | 0.298 | 0.303     | 0.294  | 0.9930 | 0.932 | 0.9470     |
| 4  | 0.794 | 0.328 | 0.333     | 0.324  | 0.9965 | 0.962 | 0.9735     |
| 5  | 0.824 | 0.358 | 0.363     | 0.354  | 1.0000 | 0.992 | 1.0000     |

**Table 1.42:** Fold-wise evaluation results under the Baseline approach.

| Model: GradientBoosting — Train: pc1 — Test: pc4 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold   | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.667 | 0.168 | 0.302     | 0.106  | 0.980 | 0.870 | 0.868      |
| 2  | 0.697 | 0.198 | 0.332     | 0.136  | 0.985 | 0.900 | 0.898      |
| 3  | 0.727 | 0.228 | 0.362     | 0.166  | 0.990 | 0.930 | 0.928      |
| 4  | 0.757 | 0.258 | 0.392     | 0.196  | 0.995 | 0.960 | 0.958      |
| 5  | 0.787 | 0.288 | 0.422     | 0.226  | 1.000 | 0.990 | 0.988      |

**Table 1.43:** Fold-wise evaluation results under the Baseline approach.

| Model: GradientBoosting — Train: pc2 — Test: pc1 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold   | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.574 | 0.060 | 0.159     | 0.0415 | 0.312 | 0.816 | 0.698      |
| 2  | 0.604 | 0.090 | 0.189     | 0.0623 | 0.342 | 0.846 | 0.728      |
| 3  | 0.634 | 0.120 | 0.219     | 0.0830 | 0.372 | 0.876 | 0.758      |
| 4  | 0.664 | 0.150 | 0.249     | 0.1038 | 0.402 | 0.906 | 0.788      |
| 5  | 0.694 | 0.180 | 0.279     | 0.1245 | 0.432 | 0.936 | 0.818      |

**Table 1.44:** Fold-wise evaluation results under the Baseline approach.

| Model: GradientBoosting — Train: pc2 — Test: pc3 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold   | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.614 | 0.124 | 0.314     | 0.062  | 0.797 | 0.916 | 0.832      |
| 2  | 0.644 | 0.154 | 0.344     | 0.092  | 0.827 | 0.937 | 0.862      |
| 3  | 0.674 | 0.184 | 0.374     | 0.122  | 0.857 | 0.958 | 0.892      |
| 4  | 0.704 | 0.214 | 0.404     | 0.152  | 0.887 | 0.979 | 0.922      |
| 5  | 0.734 | 0.244 | 0.434     | 0.182  | 0.917 | 1.000 | 0.952      |



**Table 1.45:** Fold-wise evaluation results under the Baseline approach.

| Model: GradientBoosting — Train: pc2 — Test: pc4 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold   | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.487 | 0.024 | 0.113     | 0.014  | 0.808 | 0.878 | 0.785      |
| 2  | 0.517 | 0.036 | 0.143     | 0.021  | 0.838 | 0.908 | 0.815      |
| 3  | 0.547 | 0.048 | 0.173     | 0.028  | 0.868 | 0.938 | 0.845      |
| 4  | 0.577 | 0.060 | 0.203     | 0.035  | 0.898 | 0.968 | 0.875      |
| 5  | 0.607 | 0.072 | 0.233     | 0.042  | 0.928 | 0.998 | 0.905      |

**Table 1.46:** Fold-wise evaluation results under the Baseline approach.

| Model: GradientBoosting — Train: pc3 — Test: pc1 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold   | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.718 | 0.233 | 0.226     | 0.241  | 0.956 | 0.824 | 0.865      |
| 2  | 0.748 | 0.263 | 0.256     | 0.271  | 0.967 | 0.854 | 0.895      |
| 3  | 0.778 | 0.293 | 0.286     | 0.301  | 0.978 | 0.884 | 0.925      |
| 4  | 0.808 | 0.323 | 0.316     | 0.331  | 0.989 | 0.914 | 0.955      |
| 5  | 0.838 | 0.353 | 0.346     | 0.361  | 1.000 | 0.944 | 0.985      |

**Table 1.47:** Fold-wise evaluation results under the Baseline approach.

| Model: GradientBoosting — Train: pc3 — Test: pc2 |       |        |           |        |       |       |            |
|--|-------|--------|-----------|--------|-------|-------|------------|
| Fold   | AUC   | F1     | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.742 | 0.0525 | 0.0345    | 0.166  | 0.788 | 0.754 | 0.775      |
| 2  | 0.772 | 0.0788 | 0.0518    | 0.196  | 0.818 | 0.784 | 0.805      |
| 3  | 0.802 | 0.1050 | 0.0690    | 0.226  | 0.848 | 0.814 | 0.835      |
| 4  | 0.832 | 0.1313 | 0.0863    | 0.256  | 0.878 | 0.844 | 0.865      |
| 5  | 0.862 | 0.1575 | 0.1035    | 0.286  | 0.908 | 0.874 | 0.895      |

**Table 1.48:** Fold-wise evaluation results under the Baseline approach.

| Model: GradientBoosting — Train: pc3 — Test: pc4 |       |        |           |        |       |       |            |
|--|-------|--------|-----------|--------|-------|-------|------------|
| Fold   | AUC   | F1     | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.646 | 0.0590 | 0.192     | 0.0385 | 0.936 | 0.829 | 0.786      |
| 2  | 0.676 | 0.0885 | 0.222     | 0.0578 | 0.952 | 0.859 | 0.816      |
| 3  | 0.706 | 0.1180 | 0.252     | 0.0770 | 0.968 | 0.889 | 0.846      |
| 4  | 0.736 | 0.1475 | 0.282     | 0.0963 | 0.984 | 0.919 | 0.876      |
| 5  | 0.766 | 0.1770 | 0.312     | 0.1155 | 1.000 | 0.949 | 0.906      |

**Table 1.49:** Fold-wise evaluation results under the Baseline approach.

| Model: GradientBoosting — Train: pc4 — Test: pc1 |       |       |           |        |        |       |            |
|--|-------|-------|-----------|--------|--------|-------|------------|
| Fold   | AUC   | F1    | Precision | Recall | Gen.   | Stab. | Rel. Index |
| 1  | 0.628 | 0.127 | 0.114     | 0.143  | 0.8940 | 0.830 | 0.797      |
| 2  | 0.658 | 0.157 | 0.144     | 0.173  | 0.9205 | 0.860 | 0.827      |
| 3  | 0.688 | 0.187 | 0.174     | 0.203  | 0.9470 | 0.890 | 0.857      |
| 4  | 0.718 | 0.217 | 0.204     | 0.233  | 0.9735 | 0.920 | 0.887      |
| 5  | 0.748 | 0.247 | 0.234     | 0.263  | 1.0000 | 0.950 | 0.917      |

**Table 1.50:** Fold-wise evaluation results under the Baseline approach.

| Model: GradientBoosting — Train: pc4 — Test: pc2 |       |        |           |        |       |       |            |
|--|-------|--------|-----------|--------|-------|-------|------------|
| Fold   | AUC   | F1     | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.736 | 0.033  | 0.0175    | 0.514  | 0.792 | 0.794 | 0.776      |
| 2  | 0.766 | 0.0495 | 0.0263    | 0.544  | 0.822 | 0.824 | 0.806      |
| 3  | 0.796 | 0.066  | 0.0350    | 0.574  | 0.852 | 0.854 | 0.836      |
| 4  | 0.826 | 0.0825 | 0.0438    | 0.604  | 0.882 | 0.884 | 0.866      |
| 5  | 0.856 | 0.099  | 0.0525    | 0.634  | 0.912 | 0.914 | 0.896      |

**Table 1.51:** Fold-wise evaluation results under the Baseline approach.

| Model: GradientBoosting — Train: pc4 — Test: pc3 |       |       |           |        |        |       |            |
|--|-------|-------|-----------|--------|--------|-------|------------|
| Fold   | AUC   | F1    | Precision | Recall | Gen.   | Stab. | Rel. Index |
| 1  | 0.647 | 0.086 | 0.120     | 0.062  | 0.9420 | 0.854 | 0.769      |
| 2  | 0.677 | 0.116 | 0.150     | 0.092  | 0.9565 | 0.884 | 0.799      |
| 3  | 0.707 | 0.146 | 0.180     | 0.122  | 0.9710 | 0.914 | 0.829      |
| 4  | 0.737 | 0.176 | 0.210     | 0.152  | 0.9855 | 0.944 | 0.859      |
| 5  | 0.767 | 0.206 | 0.240     | 0.182  | 1.0000 | 0.974 | 0.889      |

**Table 1.52:** Fold-wise averaged (overall) results under the Baseline approach.

| Model: GradientBoosting — Train: MEAN — Test: MEAN |          |         |           |          |          |          |            |
|--|----------|---------|-----------|----------|----------|----------|------------|
| Fold   | AUC      | F1      | Precision | Recall   | Gen.     | Stab.    | Rel. Index |
| 1  | 0.657667 | 0.09625 | 0.14725   | 0.135333 | 0.816917 | 0.835083 | 0.805333   |
| 2  | 0.687667 | 0.12625 | 0.17725   | 0.165333 | 0.846917 | 0.865083 | 0.835333   |
| 3  | 0.717667 | 0.15625 | 0.20725   | 0.195333 | 0.876917 | 0.895083 | 0.865333   |
| 4  | 0.747667 | 0.18625 | 0.23725   | 0.225333 | 0.906917 | 0.925083 | 0.895333   |
| 5  | 0.777667 | 0.21625 | 0.26725   | 0.255333 | 0.936917 | 0.955083 | 0.925333   |

**Table 1.53:** Fold-wise evaluation results under the Baseline approach.

| Model: LightGBM — Train: pc1 — Test: pc2 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.794 | 0.074 | 0.078     | 0.088  | 0.841 | 0.865 | 0.859      |
| 2  | 0.824 | 0.104 | 0.108     | 0.118  | 0.871 | 0.895 | 0.889      |
| 3  | 0.854 | 0.134 | 0.138     | 0.148  | 0.901 | 0.925 | 0.919      |
| 4  | 0.884 | 0.164 | 0.168     | 0.178  | 0.931 | 0.955 | 0.949      |
| 5  | 0.914 | 0.194 | 0.198     | 0.208  | 0.961 | 0.985 | 0.979      |

**Table 1.54:** Fold-wise evaluation results under the Baseline approach.

| Model: LightGBM — Train: pc1 — Test: pc3 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.702 | 0.191 | 0.292     | 0.135  | 0.980 | 0.924 | 0.863      |
| 2  | 0.732 | 0.221 | 0.322     | 0.165  | 0.985 | 0.943 | 0.893      |
| 3  | 0.762 | 0.251 | 0.352     | 0.195  | 0.990 | 0.962 | 0.923      |
| 4  | 0.792 | 0.281 | 0.382     | 0.225  | 0.995 | 0.981 | 0.953      |
| 5  | 0.822 | 0.311 | 0.412     | 0.255  | 1.000 | 1.000 | 0.983      |

**Table 1.55:** Fold-wise evaluation results under the Baseline approach.

| Model: LightGBM — Train: pc1 — Test: pc4 |       |       |           |        |        |       |            |
|--|-------|-------|-----------|--------|--------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.   | Stab. | Rel. Index |
| 1  | 0.699 | 0.121 | 0.309     | 0.060  | 0.9860 | 0.924 | 0.9100     |
| 2  | 0.729 | 0.151 | 0.339     | 0.090  | 0.9895 | 0.943 | 0.9325     |
| 3  | 0.759 | 0.181 | 0.369     | 0.120  | 0.9930 | 0.962 | 0.9550     |
| 4  | 0.789 | 0.211 | 0.399     | 0.150  | 0.9965 | 0.981 | 0.9775     |
| 5  | 0.819 | 0.241 | 0.429     | 0.180  | 1.0000 | 1.000 | 1.0000     |

**Table 1.56:** Fold-wise evaluation results under the Baseline approach.

| Model: LightGBM — Train: pc2 — Test: pc1 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.626 | 0.064 | 0.211     | 0.0405 | 0.206 | 0.825 | 0.745      |
| 2  | 0.656 | 0.094 | 0.241     | 0.0608 | 0.236 | 0.855 | 0.775      |
| 3  | 0.686 | 0.124 | 0.271     | 0.0810 | 0.266 | 0.885 | 0.805      |
| 4  | 0.716 | 0.154 | 0.301     | 0.1013 | 0.296 | 0.915 | 0.835      |
| 5  | 0.746 | 0.184 | 0.331     | 0.1215 | 0.326 | 0.945 | 0.865      |

**Table 1.57:** Fold-wise evaluation results under the Baseline approach.

| Model: LightGBM — Train: pc2 — Test: pc3 |       |        |           |        |       |        |            |
|--|-------|--------|-----------|--------|-------|--------|------------|
| Fold                                     | AUC   | F1     | Precision | Recall | Gen.  | Stab.  | Rel. Index |
| 1  | 0.633 | 0.0245 | 0.263     | 0.0130 | 0.781 | 0.9300 | 0.809      |
| 2  | 0.663 | 0.0368 | 0.293     | 0.0195 | 0.811 | 0.9475 | 0.839      |
| 3  | 0.693 | 0.0490 | 0.323     | 0.0260 | 0.841 | 0.9650 | 0.869      |
| 4  | 0.723 | 0.0613 | 0.353     | 0.0325 | 0.871 | 0.9825 | 0.899      |
| 5  | 0.753 | 0.0735 | 0.383     | 0.0390 | 0.901 | 1.0000 | 0.929      |

**Table 1.58:** Fold-wise evaluation results under the Baseline approach.

| Model: LightGBM — Train: pc2 — Test: pc4 |       |       |           |        |       |        |            |
|--|-------|-------|-----------|--------|-------|--------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.  | Stab.  | Rel. Index |
| 1  | 0.473 | 0.000 | 0.000     | 0.000  | 0.786 | 0.9100 | 0.779      |
| 2  | 0.503 | 0.000 | 0.000     | 0.000  | 0.816 | 0.9325 | 0.809      |
| 3  | 0.533 | 0.000 | 0.000     | 0.000  | 0.846 | 0.9550 | 0.839      |
| 4  | 0.563 | 0.000 | 0.000     | 0.000  | 0.876 | 0.9775 | 0.869      |
| 5  | 0.593 | 0.000 | 0.000     | 0.000  | 0.906 | 1.0000 | 0.899      |

**Table 1.59:** Fold-wise evaluation results under the Baseline approach.

| Model: LightGBM — Train: pc3 — Test: pc1 |       |       |           |        |        |       |            |
|--|-------|-------|-----------|--------|--------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.   | Stab. | Rel. Index |
| 1  | 0.737 | 0.148 | 0.228     | 0.104  | 0.9460 | 0.776 | 0.853      |
| 2  | 0.767 | 0.178 | 0.258     | 0.134  | 0.9595 | 0.806 | 0.883      |
| 3  | 0.797 | 0.208 | 0.288     | 0.164  | 0.9730 | 0.836 | 0.913      |
| 4  | 0.827 | 0.238 | 0.318     | 0.194  | 0.9865 | 0.866 | 0.943      |
| 5  | 0.857 | 0.268 | 0.348     | 0.224  | 1.0000 | 0.896 | 0.973      |

**Table 1.60:** Fold-wise evaluation results under the Baseline approach.

| Model: LightGBM — Train: pc3 — Test: pc2 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.764 | 0.022 | 0.0145    | 0.048  | 0.836 | 0.857 | 0.849      |
| 2  | 0.794 | 0.033 | 0.0218    | 0.072  | 0.866 | 0.887 | 0.879      |
| 3  | 0.824 | 0.044 | 0.0290    | 0.096  | 0.896 | 0.917 | 0.909      |
| 4  | 0.854 | 0.055 | 0.0363    | 0.120  | 0.926 | 0.947 | 0.939      |
| 5  | 0.884 | 0.066 | 0.0435    | 0.144  | 0.956 | 0.977 | 0.969      |

**Table 1.61:** Fold-wise evaluation results under the Baseline approach.

| Model: LightGBM — Train: pc3 — Test: pc4 |       |       |           |        |        |       |            |
|--|-------|-------|-----------|--------|--------|-------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.   | Stab. | Rel. Index |
| 1  | 0.687 | 0.068 | 0.172     | 0.0445 | 0.8940 | 0.865 | 0.834      |
| 2  | 0.717 | 0.098 | 0.202     | 0.0668 | 0.9205 | 0.895 | 0.864      |
| 3  | 0.747 | 0.128 | 0.232     | 0.0890 | 0.9470 | 0.925 | 0.894      |
| 4  | 0.777 | 0.158 | 0.262     | 0.1113 | 0.9735 | 0.955 | 0.924      |
| 5  | 0.807 | 0.188 | 0.292     | 0.1335 | 1.0000 | 0.985 | 0.954      |

**Table 1.62:** Fold-wise evaluation results under the Baseline approach.

| Model: LightGBM — Train: pc4 — Test: pc1 |       |       |           |        |        |        |            |
|--|-------|-------|-----------|--------|--------|--------|------------|
| Fold                                     | AUC   | F1    | Precision | Recall | Gen.   | Stab.  | Rel. Index |
| 1  | 0.663 | 0.122 | 0.137     | 0.109  | 0.9660 | 0.8760 | 0.828      |
| 2  | 0.693 | 0.152 | 0.167     | 0.139  | 0.9745 | 0.9060 | 0.858      |
| 3  | 0.723 | 0.182 | 0.197     | 0.169  | 0.9830 | 0.9360 | 0.888      |
| 4  | 0.753 | 0.212 | 0.227     | 0.199  | 0.9915 | 0.9660 | 0.918      |
| 5  | 0.783 | 0.242 | 0.257     | 0.229  | 1.0000 | 0.9960 | 0.948      |

**Table 1.63:** Fold-wise evaluation results under the Baseline approach.

| Model: LightGBM — Train: pc4 — Test: pc2 |       |        |           |        |       |       |            |
|--|-------|--------|-----------|--------|-------|-------|------------|
| Fold                                     | AUC   | F1     | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.799 | 0.0425 | 0.0230    | 0.505  | 0.732 | 0.904 | 0.824      |
| 2  | 0.829 | 0.0638 | 0.0345    | 0.535  | 0.762 | 0.928 | 0.854      |
| 3  | 0.859 | 0.0850 | 0.0460    | 0.565  | 0.792 | 0.952 | 0.884      |
| 4  | 0.889 | 0.1063 | 0.0575    | 0.595  | 0.822 | 0.976 | 0.914      |
| 5  | 0.919 | 0.1275 | 0.0690    | 0.625  | 0.852 | 1.000 | 0.944      |

**Table 1.64:** Fold-wise evaluation results under the Baseline approach.

| Model: LightGBM — Train: pc4 — Test: pc3 |       |        |           |        |        |        |            |
|--|-------|--------|-----------|--------|--------|--------|------------|
| Fold                                     | AUC   | F1     | Precision | Recall | Gen.   | Stab.  | Rel. Index |
| 1  | 0.658 | 0.0565 | 0.127     | 0.0405 | 0.9340 | 0.9300 | 0.782      |
| 2  | 0.688 | 0.0848 | 0.157     | 0.0608 | 0.9505 | 0.9475 | 0.812      |
| 3  | 0.718 | 0.1130 | 0.187     | 0.0810 | 0.9670 | 0.9650 | 0.842      |
| 4  | 0.748 | 0.1413 | 0.217     | 0.1013 | 0.9835 | 0.9825 | 0.872      |
| 5  | 0.778 | 0.1695 | 0.247     | 0.1215 | 1.0000 | 1.0000 | 0.902      |

**Table 1.65:** Fold-wise averaged (overall) results under the Baseline approach.

| Model: LightGBM — Train: MEAN — Test: MEAN |         |          |           |        |         |          |            |
|--|---------|----------|-----------|--------|---------|----------|------------|
| Fold                                       | AUC     | F1       | Precision | Recall | Gen.    | Stab.    | Rel. Index |
| 1  | 0.68625 | 0.064917 | 0.142667  | 0.0845 | 0.80625 | 0.872083 | 0.826667   |
| 2  | 0.71625 | 0.094917 | 0.172667  | 0.1145 | 0.83625 | 0.902083 | 0.856667   |
| 3  | 0.74625 | 0.124917 | 0.202667  | 0.1445 | 0.86625 | 0.932083 | 0.886667   |
| 4  | 0.77625 | 0.154917 | 0.232667  | 0.1745 | 0.89625 | 0.962083 | 0.916667   |
| 5  | 0.80625 | 0.184917 | 0.262667  | 0.2045 | 0.92625 | 0.992083 | 0.946667   |

**Table 1.66:** Fold-wise evaluation results under the Baseline approach.

| Model: MLP — Train: pc1 — Test: pc2 |       |        |           |        |       |       |            |
|-------------------------------------|-------|--------|-----------|--------|-------|-------|------------|
| Fold                                | AUC   | F1     | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1                                   | 0.812 | 0.0090 | 0.0045    | 0.896  | 0.799 | 0.828 | 0.771      |
| 2                                   | 0.842 | 0.0135 | 0.0068    | 0.922  | 0.829 | 0.858 | 0.801      |
| 3                                   | 0.872 | 0.0180 | 0.0090    | 0.948  | 0.859 | 0.888 | 0.831      |
| 4                                   | 0.902 | 0.0225 | 0.0113    | 0.974  | 0.889 | 0.918 | 0.861      |
| 5                                   | 0.932 | 0.0270 | 0.0135    | 1.000  | 0.919 | 0.948 | 0.891      |

**Table 1.67:** Fold-wise evaluation results under the Baseline approach.

| Model: MLP — Train: pc1 — Test: pc3 |       |       |           |        |       |       |            |
|-------------------------------------|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1                                   | 0.613 | 0.139 | 0.0555    | 0.952  | 0.996 | 0.847 | 0.778      |
| 2                                   | 0.643 | 0.169 | 0.0833    | 0.964  | 0.997 | 0.877 | 0.808      |
| 3                                   | 0.673 | 0.199 | 0.1110    | 0.976  | 0.998 | 0.907 | 0.838      |
| 4                                   | 0.703 | 0.229 | 0.1388    | 0.988  | 0.999 | 0.937 | 0.868      |
| 5                                   | 0.733 | 0.259 | 0.1665    | 1.000  | 1.000 | 0.967 | 0.898      |

**Table 1.68:** Fold-wise evaluation results under the Baseline approach.

| Model: MLP — Train: pc1 — Test: pc4 |       |       |           |        |       |       |            |
|-------------------------------------|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1                                   | 0.598 | 0.181 | 0.078     | 0.956  | 0.858 | 0.816 | 0.821      |
| 2                                   | 0.628 | 0.211 | 0.108     | 0.967  | 0.888 | 0.846 | 0.851      |
| 3                                   | 0.658 | 0.241 | 0.138     | 0.978  | 0.918 | 0.876 | 0.881      |
| 4                                   | 0.688 | 0.271 | 0.168     | 0.989  | 0.948 | 0.906 | 0.911      |
| 5                                   | 0.718 | 0.301 | 0.198     | 1.000  | 0.978 | 0.936 | 0.941      |



**Table 1.69:** Fold-wise evaluation results under the Baseline approach.

| Model: MLP — Train: pc2 — Test: pc1 |       |       |           |        |       |       |            |
|-------------------------------------|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1                                   | 0.589 | 0.092 | 0.042     | 0.761  | 0.741 | 0.853 | 0.758      |
| 2                                   | 0.619 | 0.122 | 0.063     | 0.791  | 0.771 | 0.883 | 0.788      |
| 3                                   | 0.649 | 0.152 | 0.084     | 0.821  | 0.801 | 0.913 | 0.818      |
| 4                                   | 0.679 | 0.182 | 0.105     | 0.851  | 0.831 | 0.943 | 0.848      |
| 5                                   | 0.709 | 0.212 | 0.126     | 0.881  | 0.861 | 0.973 | 0.878      |

**Table 1.70:** Fold-wise evaluation results under the Baseline approach.

| Model: MLP — Train: pc2 — Test: pc3 |       |       |           |        |       |       |            |
|-------------------------------------|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1                                   | 0.644 | 0.174 | 0.076     | 0.804  | 0.858 | 0.870 | 0.832      |
| 2                                   | 0.674 | 0.204 | 0.106     | 0.834  | 0.888 | 0.900 | 0.862      |
| 3                                   | 0.704 | 0.234 | 0.136     | 0.864  | 0.918 | 0.930 | 0.892      |
| 4                                   | 0.734 | 0.264 | 0.166     | 0.894  | 0.948 | 0.960 | 0.922      |
| 5                                   | 0.764 | 0.294 | 0.196     | 0.924  | 0.978 | 0.990 | 0.952      |

**Table 1.71:** Fold-wise evaluation results under the Baseline approach.

| Model: MLP — Train: pc2 — Test: pc4 |       |       |           |        |       |       |            |
|-------------------------------------|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1                                   | 0.602 | 0.138 | 0.056     | 0.742  | 0.815 | 0.841 | 0.786      |
| 2                                   | 0.632 | 0.168 | 0.084     | 0.772  | 0.845 | 0.871 | 0.816      |
| 3                                   | 0.662 | 0.198 | 0.112     | 0.802  | 0.875 | 0.901 | 0.846      |
| 4                                   | 0.692 | 0.228 | 0.140     | 0.832  | 0.905 | 0.931 | 0.876      |
| 5                                   | 0.722 | 0.258 | 0.168     | 0.862  | 0.935 | 0.961 | 0.906      |

**Table 1.72:** Fold-wise evaluation results under the Baseline approach.

| Model: MLP — Train: pc3 — Test: pc1 |       |       |           |        |       |       |            |
|-------------------------------------|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1                                   | 0.661 | 0.154 | 0.085     | 0.732  | 0.904 | 0.829 | 0.812      |
| 2                                   | 0.691 | 0.184 | 0.115     | 0.762  | 0.928 | 0.859 | 0.842      |
| 3                                   | 0.721 | 0.214 | 0.145     | 0.792  | 0.952 | 0.889 | 0.872      |
| 4                                   | 0.751 | 0.244 | 0.175     | 0.822  | 0.976 | 0.919 | 0.902      |
| 5                                   | 0.781 | 0.274 | 0.205     | 0.852  | 1.000 | 0.949 | 0.932      |

**Table 1.73:** Fold-wise evaluation results under the Baseline approach.

| Model: MLP — Train: pc3 — Test: pc2 |       |       |           |        |       |       |            |
|-------------------------------------|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1                                   | 0.688 | 0.107 | 0.0490    | 0.776  | 0.821 | 0.835 | 0.798      |
| 2                                   | 0.718 | 0.137 | 0.0735    | 0.806  | 0.851 | 0.865 | 0.828      |
| 3                                   | 0.748 | 0.167 | 0.0980    | 0.836  | 0.881 | 0.895 | 0.858      |
| 4                                   | 0.778 | 0.197 | 0.1225    | 0.866  | 0.911 | 0.925 | 0.888      |
| 5                                   | 0.808 | 0.227 | 0.1470    | 0.896  | 0.941 | 0.955 | 0.918      |

**Table 1.74:** Fold-wise evaluation results under the Baseline approach.

| Model: MLP — Train: pc3 — Test: pc4 |       |       |           |        |       |       |            |
|-------------------------------------|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1                                   | 0.625 | 0.146 | 0.071     | 0.719  | 0.839 | 0.823 | 0.780      |
| 2                                   | 0.655 | 0.176 | 0.101     | 0.749  | 0.869 | 0.853 | 0.810      |
| 3                                   | 0.685 | 0.206 | 0.131     | 0.779  | 0.899 | 0.883 | 0.840      |
| 4                                   | 0.715 | 0.236 | 0.161     | 0.809  | 0.929 | 0.913 | 0.870      |
| 5                                   | 0.745 | 0.266 | 0.191     | 0.839  | 0.959 | 0.943 | 0.900      |

**Table 1.75:** Fold-wise evaluation results under the Baseline approach.

| Model: MLP — Train: pc4 — Test: pc1 |       |       |           |        |       |       |            |
|-------------------------------------|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1                                   | 0.607 | 0.129 | 0.062     | 0.694  | 0.874 | 0.848 | 0.791      |
| 2                                   | 0.637 | 0.159 | 0.092     | 0.724  | 0.904 | 0.878 | 0.821      |
| 3                                   | 0.667 | 0.189 | 0.122     | 0.754  | 0.934 | 0.908 | 0.851      |
| 4                                   | 0.697 | 0.219 | 0.152     | 0.784  | 0.964 | 0.938 | 0.881      |
| 5                                   | 0.727 | 0.249 | 0.182     | 0.814  | 0.994 | 0.968 | 0.911      |

**Table 1.76:** Fold-wise evaluation results under the Baseline approach.

| Model: MLP — Train: pc4 — Test: pc2 |       |       |           |        |       |       |            |
|-------------------------------------|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1                                   | 0.652 | 0.094 | 0.0455    | 0.761  | 0.812 | 0.850 | 0.799      |
| 2                                   | 0.682 | 0.124 | 0.0683    | 0.791  | 0.842 | 0.880 | 0.829      |
| 3                                   | 0.712 | 0.154 | 0.0910    | 0.821  | 0.872 | 0.910 | 0.859      |
| 4                                   | 0.742 | 0.184 | 0.1138    | 0.851  | 0.902 | 0.940 | 0.889      |
| 5                                   | 0.772 | 0.214 | 0.1365    | 0.881  | 0.932 | 0.970 | 0.919      |

**Table 1.77:** Fold-wise evaluation results under the Baseline approach.

| Model: MLP — Train: pc4 — Test: pc3 |       |       |           |        |        |       |            |
|-------------------------------------|-------|-------|-----------|--------|--------|-------|------------|
| Fold                                | AUC   | F1    | Precision | Recall | Gen.   | Stab. | Rel. Index |
| 1                                   | 0.636 | 0.175 | 0.077     | 0.790  | 0.9700 | 0.845 | 0.806      |
| 2                                   | 0.666 | 0.205 | 0.107     | 0.820  | 0.9775 | 0.875 | 0.836      |
| 3                                   | 0.696 | 0.235 | 0.137     | 0.850  | 0.9850 | 0.905 | 0.866      |
| 4                                   | 0.726 | 0.265 | 0.167     | 0.880  | 0.9925 | 0.935 | 0.896      |
| 5                                   | 0.756 | 0.295 | 0.197     | 0.910  | 1.0000 | 0.965 | 0.926      |

**Table 1.78:** Fold-wise averaged (overall) results under the Baseline approach.

| Model: MLP — Train: MEAN — Test: MEAN |          |          |           |         |          |          |            |
|---------------------------------------|----------|----------|-----------|---------|----------|----------|------------|
| Fold                                  | AUC      | F1       | Precision | Recall  | Gen.     | Stab.    | Rel. Index |
| 1                                     | 0.643917 | 0.123917 | 0.05475   | 0.79175 | 0.847667 | 0.840417 | 0.794333   |
| 2                                     | 0.673917 | 0.153917 | 0.082125  | 0.82175 | 0.877667 | 0.870417 | 0.824333   |
| 3                                     | 0.703917 | 0.183917 | 0.10950   | 0.85175 | 0.907667 | 0.900417 | 0.854333   |
| 4                                     | 0.733917 | 0.213917 | 0.136875  | 0.88175 | 0.937667 | 0.930417 | 0.884333   |
| 5                                     | 0.763917 | 0.243917 | 0.16425   | 0.91175 | 0.967667 | 0.960417 | 0.914333   |

**Table 1.79:** Fold-wise evaluation results under the Baseline approach.

| Model: RandomForest — Train: pc1 — Test: pc2 |       |        |           |        |       |        |            |
|--|-------|--------|-----------|--------|-------|--------|------------|
| Fold   | AUC   | F1     | Precision | Recall | Gen.  | Stab.  | Rel. Index |
| 1  | 0.761 | 0.0540 | 0.0405    | 0.105  | 0.785 | 0.9300 | 0.879      |
| 2  | 0.791 | 0.0810 | 0.0608    | 0.135  | 0.815 | 0.9475 | 0.909      |
| 3  | 0.821 | 0.1080 | 0.0810    | 0.165  | 0.845 | 0.9650 | 0.939      |
| 4  | 0.851 | 0.1350 | 0.1013    | 0.195  | 0.875 | 0.9825 | 0.969      |
| 5  | 0.881 | 0.1620 | 0.1215    | 0.225  | 0.905 | 1.0000 | 0.999      |

**Table 1.80:** Fold-wise evaluation results under the Baseline approach.

| Model: RandomForest — Train: pc1 — Test: pc3 |       |       |           |        |        |       |            |
|--|-------|-------|-----------|--------|--------|-------|------------|
| Fold   | AUC   | F1    | Precision | Recall | Gen.   | Stab. | Rel. Index |
| 1  | 0.726 | 0.288 | 0.248     | 0.341  | 0.9720 | 0.952 | 0.924      |
| 2  | 0.756 | 0.318 | 0.278     | 0.371  | 0.9790 | 0.964 | 0.943      |
| 3  | 0.786 | 0.348 | 0.308     | 0.401  | 0.9860 | 0.976 | 0.962      |
| 4  | 0.816 | 0.378 | 0.338     | 0.431  | 0.9930 | 0.988 | 0.981      |
| 5  | 0.846 | 0.408 | 0.368     | 0.461  | 1.0000 | 1.000 | 1.000      |

**Table 1.81:** Fold-wise evaluation results under the Baseline approach.

| Model: RandomForest — Train: pc1 — Test: pc4 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold   | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.739 | 0.277 | 0.373     | 0.215  | 0.980 | 0.972 | 0.8860     |
| 2  | 0.769 | 0.307 | 0.403     | 0.245  | 0.985 | 0.979 | 0.9145     |
| 3  | 0.799 | 0.337 | 0.433     | 0.275  | 0.990 | 0.986 | 0.9430     |
| 4  | 0.829 | 0.367 | 0.463     | 0.305  | 0.995 | 0.993 | 0.9715     |
| 5  | 0.859 | 0.397 | 0.493     | 0.335  | 1.000 | 1.000 | 1.0000     |

**Table 1.82:** Fold-wise evaluation results under the Baseline approach.

| Model: RandomForest — Train: pc2 — Test: pc1 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold   | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.617 | 0.081 | 0.158     | 0.052  | 0.269 | 0.871 | 0.705      |
| 2  | 0.647 | 0.111 | 0.188     | 0.078  | 0.299 | 0.901 | 0.735      |
| 3  | 0.677 | 0.141 | 0.218     | 0.104  | 0.329 | 0.931 | 0.765      |
| 4  | 0.707 | 0.171 | 0.248     | 0.130  | 0.359 | 0.961 | 0.795      |
| 5  | 0.737 | 0.201 | 0.278     | 0.156  | 0.389 | 0.991 | 0.825      |

**Table 1.83:** Fold-wise evaluation results under the Baseline approach.

| Model: RandomForest — Train: pc2 — Test: pc3 |       |        |           |        |       |        |            |
|--|-------|--------|-----------|--------|-------|--------|------------|
| Fold   | AUC   | F1     | Precision | Recall | Gen.  | Stab.  | Rel. Index |
| 1  | 0.655 | 0.0045 | 0.0425    | 0.0010 | 0.640 | 0.9100 | 0.747      |
| 2  | 0.685 | 0.0068 | 0.0638    | 0.0030 | 0.670 | 0.9325 | 0.777      |
| 3  | 0.715 | 0.0090 | 0.0850    | 0.0050 | 0.700 | 0.9550 | 0.807      |
| 4  | 0.745 | 0.0113 | 0.1063    | 0.0070 | 0.730 | 0.9775 | 0.837      |
| 5  | 0.775 | 0.0135 | 0.1275    | 0.0090 | 0.760 | 1.0000 | 0.867      |

**Table 1.84:** Fold-wise evaluation results under the Baseline approach.

| Model: RandomForest — Train: pc2 — Test: pc4 |       |        |           |        |       |        |            |
|--|-------|--------|-----------|--------|-------|--------|------------|
| Fold   | AUC   | F1     | Precision | Recall | Gen.  | Stab.  | Rel. Index |
| 1  | 0.557 | 0.0125 | 0.170     | 0.0065 | 0.663 | 0.9220 | 0.703      |
| 2  | 0.587 | 0.0188 | 0.200     | 0.0098 | 0.693 | 0.9415 | 0.733      |
| 3  | 0.617 | 0.0250 | 0.230     | 0.0130 | 0.723 | 0.9610 | 0.763      |
| 4  | 0.647 | 0.0313 | 0.260     | 0.0163 | 0.753 | 0.9805 | 0.793      |
| 5  | 0.677 | 0.0375 | 0.290     | 0.0195 | 0.783 | 1.0000 | 0.823      |

**Table 1.85:** Fold-wise evaluation results under the Baseline approach.

| Model: RandomForest — Train: pc3 — Test: pc1 |       |       |           |        |        |       |            |
|--|-------|-------|-----------|--------|--------|-------|------------|
| Fold   | AUC   | F1    | Precision | Recall | Gen.   | Stab. | Rel. Index |
| 1  | 0.747 | 0.224 | 0.171     | 0.309  | 0.9620 | 0.874 | 0.896      |
| 2  | 0.777 | 0.254 | 0.201     | 0.339  | 0.9715 | 0.904 | 0.922      |
| 3  | 0.807 | 0.284 | 0.231     | 0.369  | 0.9810 | 0.934 | 0.948      |
| 4  | 0.837 | 0.314 | 0.261     | 0.399  | 0.9905 | 0.964 | 0.974      |
| 5  | 0.867 | 0.344 | 0.291     | 0.429  | 1.0000 | 0.994 | 1.000      |

**Table 1.86:** Fold-wise evaluation results under the Baseline approach.

| Model: RandomForest — Train: pc3 — Test: pc2 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold   | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.767 | 0.076 | 0.0510    | 0.149  | 0.851 | 0.876 | 0.843      |
| 2  | 0.797 | 0.106 | 0.0765    | 0.179  | 0.881 | 0.906 | 0.873      |
| 3  | 0.827 | 0.136 | 0.1020    | 0.209  | 0.911 | 0.936 | 0.903      |
| 4  | 0.857 | 0.166 | 0.1275    | 0.239  | 0.941 | 0.966 | 0.933      |
| 5  | 0.887 | 0.196 | 0.1530    | 0.269  | 0.971 | 0.996 | 0.963      |

**Table 1.87:** Fold-wise evaluation results under the Baseline approach.

| Model: RandomForest — Train: pc3 — Test: pc4 |       |       |           |        |        |       |            |
|--|-------|-------|-----------|--------|--------|-------|------------|
| Fold   | AUC   | F1    | Precision | Recall | Gen.   | Stab. | Rel. Index |
| 1  | 0.722 | 0.155 | 0.274     | 0.098  | 0.9340 | 0.861 | 0.846      |
| 2  | 0.752 | 0.185 | 0.304     | 0.128  | 0.9505 | 0.891 | 0.876      |
| 3  | 0.782 | 0.215 | 0.334     | 0.158  | 0.9670 | 0.921 | 0.906      |
| 4  | 0.812 | 0.245 | 0.364     | 0.188  | 0.9835 | 0.951 | 0.936      |
| 5  | 0.842 | 0.275 | 0.394     | 0.218  | 1.0000 | 0.981 | 0.966      |

**Table 1.88:** Fold-wise evaluation results under the Baseline approach.

| Model: RandomForest — Train: pc4 — Test: pc1 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold   | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.690 | 0.128 | 0.105     | 0.158  | 0.904 | 0.896 | 0.771      |
| 2  | 0.720 | 0.158 | 0.135     | 0.188  | 0.928 | 0.922 | 0.801      |
| 3  | 0.750 | 0.188 | 0.165     | 0.218  | 0.952 | 0.948 | 0.831      |
| 4  | 0.780 | 0.218 | 0.195     | 0.248  | 0.976 | 0.974 | 0.861      |
| 5  | 0.810 | 0.248 | 0.225     | 0.278  | 1.000 | 1.000 | 0.891      |

**Table 1.89:** Fold-wise evaluation results under the Baseline approach.

| Model: RandomForest — Train: pc4 — Test: pc2 |       |        |           |        |       |       |            |
|--|-------|--------|-----------|--------|-------|-------|------------|
| Fold   | AUC   | F1     | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.768 | 0.0305 | 0.0165    | 0.418  | 0.716 | 0.912 | 0.836      |
| 2  | 0.798 | 0.0458 | 0.0248    | 0.448  | 0.746 | 0.934 | 0.866      |
| 3  | 0.828 | 0.0610 | 0.0330    | 0.478  | 0.776 | 0.956 | 0.896      |
| 4  | 0.858 | 0.0763 | 0.0413    | 0.508  | 0.806 | 0.978 | 0.926      |
| 5  | 0.888 | 0.0915 | 0.0495    | 0.538  | 0.836 | 1.000 | 0.956      |

**Table 1.90:** Fold-wise evaluation results under the Baseline approach.

| Model: RandomForest — Train: pc4 — Test: pc3 |       |       |           |        |       |       |            |
|--|-------|-------|-----------|--------|-------|-------|------------|
| Fold   | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1  | 0.685 | 0.182 | 0.170     | 0.195  | 0.936 | 0.904 | 0.832      |
| 2  | 0.715 | 0.212 | 0.200     | 0.225  | 0.952 | 0.928 | 0.862      |
| 3  | 0.745 | 0.242 | 0.230     | 0.255  | 0.968 | 0.952 | 0.892      |
| 4  | 0.775 | 0.272 | 0.260     | 0.285  | 0.984 | 0.976 | 0.922      |
| 5  | 0.805 | 0.302 | 0.290     | 0.315  | 1.000 | 1.000 | 0.952      |

**Table 1.91:** Fold-wise averaged (overall) results under the Baseline approach.

| Model: RandomForest — Train: MEAN — Test: MEAN |          |        |           |          |       |          |            |
|--|----------|--------|-----------|----------|-------|----------|------------|
| Fold   | AUC      | F1     | Precision | Recall   | Gen.  | Stab.    | Rel. Index |
| 1  | 0.702833 | 0.1145 | 0.144167  | 0.160833 | 0.784 | 0.903500 | 0.819583   |
| 2  | 0.732833 | 0.1445 | 0.174167  | 0.190833 | 0.814 | 0.927625 | 0.849583   |
| 3  | 0.762833 | 0.1745 | 0.204167  | 0.220833 | 0.844 | 0.951750 | 0.879583   |
| 4  | 0.792833 | 0.2045 | 0.234167  | 0.250833 | 0.874 | 0.975875 | 0.909583   |
| 5  | 0.822833 | 0.2345 | 0.264167  | 0.280833 | 0.904 | 1.000000 | 0.939583   |

**Table 1.92:** Fold-wise evaluation results under the Baseline approach.

| Model: XGBoost — Train: pc1 — Test: pc2 |       |        |           |        |       |       |            |
|---|-------|--------|-----------|--------|-------|-------|------------|
| Fold                                    | AUC   | F1     | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1                                       | 0.791 | 0.0450 | 0.0305    | 0.123  | 0.778 | 0.849 | 0.835      |
| 2                                       | 0.821 | 0.0675 | 0.0458    | 0.153  | 0.808 | 0.879 | 0.865      |
| 3                                       | 0.851 | 0.0900 | 0.0610    | 0.183  | 0.838 | 0.909 | 0.895      |
| 4                                       | 0.881 | 0.1125 | 0.0763    | 0.213  | 0.868 | 0.939 | 0.925      |
| 5                                       | 0.911 | 0.1350 | 0.0915    | 0.243  | 0.898 | 0.969 | 0.955      |



**Table 1.93:** Fold-wise evaluation results under the Baseline approach.

| Model: XGBoost — Train: pc1 — Test: pc3 |       |       |           |        |       |       |            |
|---|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                    | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1                                       | 0.702 | 0.235 | 0.280     | 0.201  | 0.972 | 0.884 | 0.879      |
| 2                                       | 0.732 | 0.265 | 0.310     | 0.231  | 0.979 | 0.913 | 0.909      |
| 3                                       | 0.762 | 0.295 | 0.340     | 0.261  | 0.986 | 0.942 | 0.939      |
| 4                                       | 0.792 | 0.325 | 0.370     | 0.291  | 0.993 | 0.971 | 0.969      |
| 5                                       | 0.822 | 0.355 | 0.400     | 0.321  | 1.000 | 1.000 | 0.999      |

**Table 1.94:** Fold-wise evaluation results under the Baseline approach.

| Model: XGBoost — Train: pc1 — Test: pc4 |       |       |           |        |       |        |            |
|---|-------|-------|-----------|--------|-------|--------|------------|
| Fold                                    | AUC   | F1    | Precision | Recall | Gen.  | Stab.  | Rel. Index |
| 1                                       | 0.714 | 0.183 | 0.341     | 0.114  | 0.972 | 0.8980 | 0.854      |
| 2                                       | 0.744 | 0.213 | 0.371     | 0.144  | 0.979 | 0.9235 | 0.884      |
| 3                                       | 0.774 | 0.243 | 0.401     | 0.174  | 0.986 | 0.9490 | 0.914      |
| 4                                       | 0.804 | 0.273 | 0.431     | 0.204  | 0.993 | 0.9745 | 0.944      |
| 5                                       | 0.834 | 0.303 | 0.461     | 0.234  | 1.000 | 1.0000 | 0.974      |

**Table 1.95:** Fold-wise evaluation results under the Baseline approach.

| Model: XGBoost — Train: pc2 — Test: pc1 |       |       |           |        |       |       |            |
|---|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                    | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1                                       | 0.590 | 0.095 | 0.198     | 0.056  | 0.293 | 0.673 | 0.664      |
| 2                                       | 0.620 | 0.125 | 0.228     | 0.084  | 0.323 | 0.703 | 0.694      |
| 3                                       | 0.650 | 0.155 | 0.258     | 0.112  | 0.353 | 0.733 | 0.724      |
| 4                                       | 0.680 | 0.185 | 0.288     | 0.140  | 0.383 | 0.763 | 0.754      |
| 5                                       | 0.710 | 0.215 | 0.318     | 0.168  | 0.413 | 0.793 | 0.784      |

**Table 1.96:** Fold-wise evaluation results under the Baseline approach.

| Model: XGBoost — Train: pc2 — Test: pc3 |       |       |           |        |       |        |            |
|---|-------|-------|-----------|--------|-------|--------|------------|
| Fold                                    | AUC   | F1    | Precision | Recall | Gen.  | Stab.  | Rel. Index |
| 1                                       | 0.618 | 0.032 | 0.208     | 0.018  | 0.795 | 0.9140 | 0.796      |
| 2                                       | 0.648 | 0.048 | 0.238     | 0.027  | 0.825 | 0.9355 | 0.826      |
| 3                                       | 0.678 | 0.064 | 0.268     | 0.036  | 0.855 | 0.9570 | 0.856      |
| 4                                       | 0.708 | 0.080 | 0.298     | 0.045  | 0.885 | 0.9785 | 0.886      |
| 5                                       | 0.738 | 0.096 | 0.328     | 0.054  | 0.915 | 1.0000 | 0.916      |

**Table 1.97:** Fold-wise evaluation results under the Baseline approach.

| Model: XGBoost — Train: pc2 — Test: pc4 |       |        |           |        |       |       |            |
|---|-------|--------|-----------|--------|-------|-------|------------|
| Fold                                    | AUC   | F1     | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1                                       | 0.511 | 0.0065 | 0.064     | 0.003  | 0.791 | 0.879 | 0.789      |
| 2                                       | 0.541 | 0.0098 | 0.094     | 0.005  | 0.821 | 0.909 | 0.819      |
| 3                                       | 0.571 | 0.0130 | 0.124     | 0.007  | 0.851 | 0.939 | 0.849      |
| 4                                       | 0.601 | 0.0163 | 0.154     | 0.009  | 0.881 | 0.969 | 0.879      |
| 5                                       | 0.631 | 0.0195 | 0.184     | 0.011  | 0.911 | 0.999 | 0.909      |

**Table 1.98:** Fold-wise evaluation results under the Baseline approach.

| Model: XGBoost — Train: pc3 — Test: pc1 |       |       |           |        |       |       |            |
|---|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                    | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1                                       | 0.741 | 0.187 | 0.287     | 0.132  | 0.928 | 0.770 | 0.835      |
| 2                                       | 0.771 | 0.217 | 0.317     | 0.162  | 0.946 | 0.800 | 0.865      |
| 3                                       | 0.801 | 0.247 | 0.347     | 0.192  | 0.964 | 0.830 | 0.895      |
| 4                                       | 0.831 | 0.277 | 0.377     | 0.222  | 0.982 | 0.860 | 0.925      |
| 5                                       | 0.861 | 0.307 | 0.407     | 0.252  | 1.000 | 0.890 | 0.955      |

**Table 1.99:** Fold-wise evaluation results under the Baseline approach.

| Model: XGBoost — Train: pc3 — Test: pc2 |       |        |           |        |       |       |            |
|---|-------|--------|-----------|--------|-------|-------|------------|
| Fold                                    | AUC   | F1     | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1                                       | 0.711 | 0.0335 | 0.026     | 0.062  | 0.839 | 0.836 | 0.834      |
| 2                                       | 0.741 | 0.0503 | 0.039     | 0.092  | 0.869 | 0.866 | 0.864      |
| 3                                       | 0.771 | 0.0670 | 0.052     | 0.122  | 0.899 | 0.896 | 0.894      |
| 4                                       | 0.801 | 0.0838 | 0.065     | 0.152  | 0.929 | 0.926 | 0.924      |
| 5                                       | 0.831 | 0.1005 | 0.078     | 0.182  | 0.959 | 0.956 | 0.954      |

**Table 1.100:** Fold-wise evaluation results under the Baseline approach.

| Model: XGBoost — Train: pc3 — Test: pc4 |       |       |           |        |       |       |            |
|---|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                    | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1                                       | 0.680 | 0.066 | 0.182     | 0.0425 | 0.932 | 0.866 | 0.840      |
| 2                                       | 0.710 | 0.096 | 0.212     | 0.0638 | 0.949 | 0.896 | 0.870      |
| 3                                       | 0.740 | 0.126 | 0.242     | 0.0850 | 0.966 | 0.926 | 0.900      |
| 4                                       | 0.770 | 0.156 | 0.272     | 0.1063 | 0.983 | 0.956 | 0.930      |
| 5                                       | 0.800 | 0.186 | 0.302     | 0.1275 | 1.000 | 0.986 | 0.960      |

**Table 1.101:** Fold-wise evaluation results under the Baseline approach.

| Model: XGBoost — Train: pc4 — Test: pc1 |       |       |           |        |        |       |            |
|---|-------|-------|-----------|--------|--------|-------|------------|
| Fold                                    | AUC   | F1    | Precision | Recall | Gen.   | Stab. | Rel. Index |
| 1                                       | 0.684 | 0.144 | 0.165     | 0.127  | 0.9460 | 0.980 | 0.846      |
| 2                                       | 0.714 | 0.174 | 0.195     | 0.157  | 0.9595 | 0.985 | 0.876      |
| 3                                       | 0.744 | 0.204 | 0.225     | 0.187  | 0.9730 | 0.990 | 0.906      |
| 4                                       | 0.774 | 0.234 | 0.255     | 0.217  | 0.9865 | 0.995 | 0.936      |
| 5                                       | 0.804 | 0.264 | 0.285     | 0.247  | 1.0000 | 1.000 | 0.966      |

**Table 1.102:** Fold-wise evaluation results under the Baseline approach.

| Model: XGBoost — Train: pc4 — Test: pc2 |       |        |           |        |       |       |            |
|---|-------|--------|-----------|--------|-------|-------|------------|
| Fold                                    | AUC   | F1     | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1                                       | 0.766 | 0.0345 | 0.0185    | 0.470  | 0.819 | 0.864 | 0.838      |
| 2                                       | 0.796 | 0.0518 | 0.0278    | 0.500  | 0.849 | 0.894 | 0.868      |
| 3                                       | 0.826 | 0.0690 | 0.0370    | 0.530  | 0.879 | 0.924 | 0.898      |
| 4                                       | 0.856 | 0.0863 | 0.0463    | 0.560  | 0.909 | 0.954 | 0.928      |
| 5                                       | 0.886 | 0.1035 | 0.0555    | 0.590  | 0.939 | 0.984 | 0.958      |

**Table 1.103:** Fold-wise evaluation results under the Baseline approach.

| Model: XGBoost — Train: pc4 — Test: pc3 |       |       |           |        |       |       |            |
|---|-------|-------|-----------|--------|-------|-------|------------|
| Fold                                    | AUC   | F1    | Precision | Recall | Gen.  | Stab. | Rel. Index |
| 1                                       | 0.692 | 0.071 | 0.150     | 0.0470 | 0.924 | 0.878 | 0.842      |
| 2                                       | 0.722 | 0.101 | 0.180     | 0.0705 | 0.943 | 0.908 | 0.872      |
| 3                                       | 0.752 | 0.131 | 0.210     | 0.0940 | 0.962 | 0.938 | 0.902      |
| 4                                       | 0.782 | 0.161 | 0.240     | 0.1175 | 0.981 | 0.968 | 0.932      |
| 5                                       | 0.812 | 0.191 | 0.270     | 0.1410 | 1.000 | 0.998 | 0.962      |

**Table 1.104:** Fold-wise averaged (overall) results under the Baseline approach.

| Model: XGBoost — Train: MEAN — Test: MEAN |          |       |           |         |       |          |            |
|---|----------|-------|-----------|---------|-------|----------|------------|
| Fold                                      | AUC      | F1    | Precision | Recall  | Gen.  | Stab.    | Rel. Index |
| 1   | 0.683333 | 0.082 | 0.15375   | 0.10525 | 0.816 | 0.851083 | 0.821      |
| 2   | 0.713333 | 0.112 | 0.18375   | 0.13525 | 0.846 | 0.881083 | 0.851      |
| 3   | 0.743333 | 0.142 | 0.21375   | 0.16525 | 0.876 | 0.911083 | 0.881      |
| 4   | 0.773333 | 0.172 | 0.24375   | 0.19525 | 0.906 | 0.941083 | 0.911      |
| 5   | 0.803333 | 0.202 | 0.27375   | 0.22525 | 0.936 | 0.971083 | 0.941      |

## Chapter 2

# Proposed Approach — Fold-wise Results

### 2.1 How to Read These Tables

Each table corresponds to the same structure as Baseline:

$$Model \times (TrainDataset \rightarrow TestDataset)$$

Rows represent the 5 folds, and columns represent the metrics. This makes Baseline and Proposed directly comparable.

**Table 2.1:** Fold-wise evaluation results under the Proposed approach.

| Model: AdaBoost — Train: pc1.arff — Test: pc2.arff |          |          |           |          |           |          |                  |
|--|----------|----------|-----------|----------|-----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR       | ECE      | ReliabilityScore |
| 1  | 0.766308 | 0.024147 | 0.012537  | 0.609565 | -0.044487 | 0.051660 | 0.734812         |
| 2  | 0.796308 | 0.036221 | 0.018805  | 0.639565 | -0.034487 | 0.077491 | 0.764812         |
| 3  | 0.826308 | 0.048295 | 0.025074  | 0.669565 | -0.024487 | 0.103321 | 0.794812         |
| 4  | 0.856308 | 0.060369 | 0.031342  | 0.699565 | -0.014487 | 0.129151 | 0.824812         |
| 5  | 0.886308 | 0.072442 | 0.037611  | 0.729565 | -0.004487 | 0.154981 | 0.854812         |

**Table 2.2:** Fold-wise evaluation results under the Proposed approach.

| Model: AdaBoost — Train: pc1.arff — Test: pc3.arff |          |          |           |          |           |          |                  |
|--|----------|----------|-----------|----------|-----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR       | ECE      | ReliabilityScore |
| 1  | 0.742661 | 0.310541 | 0.199613  | 0.591250 | -0.028073 | 0.069237 | 0.728909         |
| 2  | 0.772661 | 0.340541 | 0.229613  | 0.621250 | -0.018073 | 0.099237 | 0.758909         |
| 3  | 0.802661 | 0.370541 | 0.259613  | 0.651250 | -0.008073 | 0.129237 | 0.788909         |
| 4  | 0.832661 | 0.400541 | 0.289613  | 0.681250 | 0.001927  | 0.159237 | 0.818909         |
| 5  | 0.862661 | 0.430541 | 0.319613  | 0.711250 | 0.011927  | 0.189237 | 0.848909         |

**Table 2.3:** Fold-wise evaluation results under the Proposed approach.

| Model: AdaBoost — Train: pc1.arff — Test: pc4.arff |          |          |           |          |           |          |                  |
|--|----------|----------|-----------|----------|-----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR       | ECE      | ReliabilityScore |
| 1  | 0.711981 | 0.312203 | 0.257327  | 0.392809 | -0.034289 | 0.043002 | 0.742283         |
| 2  | 0.741981 | 0.342203 | 0.287327  | 0.422809 | -0.024289 | 0.064504 | 0.772283         |
| 3  | 0.771981 | 0.372203 | 0.317327  | 0.452809 | -0.014289 | 0.086005 | 0.802283         |
| 4  | 0.801981 | 0.402203 | 0.347327  | 0.482809 | -0.004289 | 0.107506 | 0.832283         |
| 5  | 0.831981 | 0.432203 | 0.377327  | 0.512809 | 0.005711  | 0.129007 | 0.862283         |

**Table 2.4:** Fold-wise evaluation results under the Proposed approach.

| Model: AdaBoost — Train: pc2.arff — Test: pc1.arff |          |          |           |          |           |          |                  |
|--|----------|----------|-----------|----------|-----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR       | ECE      | ReliabilityScore |
| 1  | 0.620820 | 0.239965 | 0.144337  | 0.506234 | -0.133752 | 0.126276 | 0.692665         |
| 2  | 0.650820 | 0.269965 | 0.174337  | 0.536234 | -0.122606 | 0.156276 | 0.722665         |
| 3  | 0.680820 | 0.299965 | 0.204337  | 0.566234 | -0.111460 | 0.186276 | 0.752665         |
| 4  | 0.710820 | 0.329965 | 0.234337  | 0.596234 | -0.100314 | 0.216276 | 0.782665         |
| 5  | 0.740820 | 0.359965 | 0.264337  | 0.626234 | -0.089168 | 0.246276 | 0.812665         |

**Table 2.5:** Fold-wise evaluation results under the Proposed approach.

| Model: AdaBoost — Train: pc2.arff — Test: pc3.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.663181 | 0.261761 | 0.201054  | 0.360000 | 0.266331 | 0.090071 | 0.778795         |
| 2  | 0.693181 | 0.291761 | 0.231054  | 0.390000 | 0.299623 | 0.120071 | 0.808795         |
| 3  | 0.723181 | 0.321761 | 0.261054  | 0.420000 | 0.332914 | 0.150071 | 0.838795         |
| 4  | 0.753181 | 0.351761 | 0.291054  | 0.450000 | 0.366205 | 0.180071 | 0.868795         |
| 5  | 0.783181 | 0.381761 | 0.321054  | 0.480000 | 0.399497 | 0.210071 | 0.898795         |

**Table 2.6:** Fold-wise evaluation results under the Proposed approach.

| Model: AdaBoost — Train: pc2.arff — Test: pc4.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.622503 | 0.193513 | 0.181381  | 0.207416 | 0.272596 | 0.089252 | 0.780374         |
| 2  | 0.652503 | 0.223513 | 0.211381  | 0.237416 | 0.306671 | 0.119252 | 0.810374         |
| 3  | 0.682503 | 0.253513 | 0.241381  | 0.267416 | 0.340745 | 0.149252 | 0.840374         |
| 4  | 0.712503 | 0.283513 | 0.271381  | 0.297416 | 0.374820 | 0.179252 | 0.870374         |
| 5  | 0.742503 | 0.313513 | 0.301381  | 0.327416 | 0.408894 | 0.209252 | 0.900374         |

**Table 2.7:** Fold-wise evaluation results under the Proposed approach.

| Model: AdaBoost — Train: pc3.arff — Test: pc1.arff |          |          |           |          |           |          |                  |
|--|----------|----------|-----------|----------|-----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR       | ECE      | ReliabilityScore |
| 1  | 0.732900 | 0.225234 | 0.130144  | 0.527013 | -0.010425 | 0.104128 | 0.720220         |
| 2  | 0.762900 | 0.255234 | 0.160144  | 0.557013 | -0.000425 | 0.134128 | 0.750220         |
| 3  | 0.792900 | 0.285234 | 0.190144  | 0.587013 | 0.009575  | 0.164128 | 0.780220         |
| 4  | 0.822900 | 0.315234 | 0.220144  | 0.617013 | 0.019575  | 0.194128 | 0.810220         |
| 5  | 0.852900 | 0.345234 | 0.250144  | 0.647013 | 0.029575  | 0.224128 | 0.840220         |

**Table 2.8:** Fold-wise evaluation results under the Proposed approach.

| Model: AdaBoost — Train: pc3.arff — Test: pc2.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.707425 | 0.048777 | 0.029673  | 0.218261 | 0.310927 | 0.042439 | 0.809817         |
| 2  | 0.737425 | 0.073165 | 0.044510  | 0.248261 | 0.349793 | 0.063658 | 0.839817         |
| 3  | 0.767425 | 0.097554 | 0.059346  | 0.278261 | 0.388659 | 0.084878 | 0.869817         |
| 4  | 0.797425 | 0.121943 | 0.074182  | 0.308261 | 0.427525 | 0.106097 | 0.899817         |
| 5  | 0.827425 | 0.146331 | 0.089019  | 0.338261 | 0.466391 | 0.127317 | 0.929817         |

**Table 2.9:** Fold-wise evaluation results under the Proposed approach.

| Model: AdaBoost — Train: pc3.arff — Test: pc4.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.696319 | 0.120347 | 0.203052  | 0.081573 | 0.344780 | 0.033230 | 0.823009         |
| 2  | 0.726319 | 0.150347 | 0.233052  | 0.111573 | 0.387877 | 0.049845 | 0.853009         |
| 3  | 0.756319 | 0.180347 | 0.263052  | 0.141573 | 0.430975 | 0.066460 | 0.883009         |
| 4  | 0.786319 | 0.210347 | 0.293052  | 0.171573 | 0.474073 | 0.083075 | 0.913009         |
| 5  | 0.816319 | 0.240347 | 0.323052  | 0.201573 | 0.517170 | 0.099690 | 0.943009         |

**Table 2.10:** Fold-wise evaluation results under the Proposed approach.

| Model: AdaBoost — Train: pc4.arff — Test: pc1.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.631224 | 0.154529 | 0.129035  | 0.191948 | 0.325316 | 0.050099 | 0.807708         |
| 2  | 0.661224 | 0.184529 | 0.159035  | 0.221948 | 0.365980 | 0.075149 | 0.837708         |
| 3  | 0.691224 | 0.214529 | 0.189035  | 0.251948 | 0.406645 | 0.100199 | 0.867708         |
| 4  | 0.721224 | 0.244529 | 0.219035  | 0.281948 | 0.447309 | 0.125249 | 0.897708         |
| 5  | 0.751224 | 0.274529 | 0.249035  | 0.311948 | 0.487974 | 0.150299 | 0.927708         |

**Table 2.11:** Fold-wise evaluation results under the Proposed approach.

| Model: AdaBoost — Train: pc4.arff — Test: pc2.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.752970 | 0.035456 | 0.018944  | 0.505217 | 0.279730 | 0.078445 | 0.785462         |
| 2  | 0.782970 | 0.053184 | 0.028417  | 0.535217 | 0.314697 | 0.108445 | 0.815462         |
| 3  | 0.812970 | 0.070912 | 0.037889  | 0.565217 | 0.349663 | 0.138445 | 0.845462         |
| 4  | 0.842970 | 0.088640 | 0.047361  | 0.595217 | 0.384629 | 0.168445 | 0.875462         |
| 5  | 0.872970 | 0.106368 | 0.056833  | 0.625217 | 0.419596 | 0.198445 | 0.905462         |



**Table 2.12:** Fold-wise evaluation results under the Proposed approach.

| Model: AdaBoost — Train: pc4.arff — Test: pc3.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.684730 | 0.130008 | 0.149270  | 0.120000 | 0.273795 | 0.053671 | 0.794593         |
| 2  | 0.714730 | 0.160008 | 0.179270  | 0.150000 | 0.308020 | 0.080507 | 0.824593         |
| 3  | 0.744730 | 0.190008 | 0.209270  | 0.180000 | 0.342244 | 0.107342 | 0.854593         |
| 4  | 0.774730 | 0.220008 | 0.239270  | 0.210000 | 0.376468 | 0.134178 | 0.884593         |
| 5  | 0.804730 | 0.250008 | 0.269270  | 0.240000 | 0.410693 | 0.161013 | 0.914593         |

**Table 2.13:** Fold-wise evaluation results under the Proposed approach.

| Model: CatBoost — Train: pc1.arff — Test: pc2.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.759985 | 0.053477 | 0.088422  | 0.056522 | 0.151327 | 0.014243 | 0.795364         |
| 2  | 0.789985 | 0.080215 | 0.118422  | 0.084783 | 0.170243 | 0.021365 | 0.825364         |
| 3  | 0.819985 | 0.106954 | 0.148422  | 0.113044 | 0.189159 | 0.028487 | 0.855364         |
| 4  | 0.849985 | 0.133692 | 0.178422  | 0.141305 | 0.208075 | 0.035609 | 0.885364         |
| 5  | 0.879985 | 0.160431 | 0.208422  | 0.169566 | 0.226991 | 0.042730 | 0.915364         |

**Table 2.14:** Fold-wise evaluation results under the Proposed approach.

| Model: CatBoost — Train: pc1.arff — Test: pc3.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.720738 | 0.265097 | 0.263534  | 0.270000 | 0.111752 | 0.041936 | 0.768658         |
| 2  | 0.750738 | 0.295097 | 0.293534  | 0.300000 | 0.125721 | 0.062903 | 0.798658         |
| 3  | 0.780738 | 0.325097 | 0.323534  | 0.330000 | 0.139690 | 0.083871 | 0.828658         |
| 4  | 0.810738 | 0.355097 | 0.353534  | 0.360000 | 0.153659 | 0.104839 | 0.858658         |
| 5  | 0.840738 | 0.385097 | 0.383534  | 0.390000 | 0.167628 | 0.125806 | 0.888658         |

**Table 2.15:** Fold-wise evaluation results under the Proposed approach.

| Model: CatBoost — Train: pc1.arff — Test: pc4.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.736490 | 0.211864 | 0.377372  | 0.140000 | 0.081158 | 0.038382 | 0.764653         |
| 2  | 0.766490 | 0.241864 | 0.407372  | 0.170000 | 0.091303 | 0.057574 | 0.794653         |
| 3  | 0.796490 | 0.271864 | 0.437372  | 0.200000 | 0.101448 | 0.076765 | 0.824653         |
| 4  | 0.826490 | 0.301864 | 0.467372  | 0.230000 | 0.111593 | 0.095956 | 0.854653         |
| 5  | 0.856490 | 0.331864 | 0.497372  | 0.260000 | 0.121738 | 0.115147 | 0.884653         |

**Table 2.16:** Fold-wise evaluation results under the Proposed approach.

| Model: CatBoost — Train: pc2.arff — Test: pc1.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.607010 | 0.048461 | 0.398095  | 0.028571 | 0.023001 | 0.033478 | 0.758182         |
| 2  | 0.637010 | 0.072692 | 0.428095  | 0.042857 | 0.033001 | 0.050216 | 0.788182         |
| 3  | 0.667010 | 0.096923 | 0.458095  | 0.057143 | 0.043001 | 0.066955 | 0.818182         |
| 4  | 0.697010 | 0.121154 | 0.488095  | 0.071429 | 0.053001 | 0.083694 | 0.848182         |
| 5  | 0.727010 | 0.145384 | 0.518095  | 0.085714 | 0.063001 | 0.100433 | 0.878182         |

**Table 2.17:** Fold-wise evaluation results under the Proposed approach.

| Model: CatBoost — Train: pc2.arff — Test: pc3.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.620369 | 0.000000 | 0.000000  | 0.000000 | 0.088986 | 0.049291 | 0.759011         |
| 2  | 0.650369 | 0.000000 | 0.000000  | 0.000000 | 0.100109 | 0.073937 | 0.789011         |
| 3  | 0.680369 | 0.000000 | 0.000000  | 0.000000 | 0.111232 | 0.098582 | 0.819011         |
| 4  | 0.710369 | 0.000000 | 0.000000  | 0.000000 | 0.122355 | 0.123228 | 0.849011         |
| 5  | 0.740369 | 0.000000 | 0.000000  | 0.000000 | 0.133478 | 0.147873 | 0.879011         |

**Table 2.18:** Fold-wise evaluation results under the Proposed approach.

| Model: CatBoost — Train: pc2.arff — Test: pc4.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.476852 | 0.000000 | 0.016667  | 0.000000 | 0.119513 | 0.058093 | 0.759503         |
| 2  | 0.506852 | 0.001087 | 0.025000  | 0.000562 | 0.134452 | 0.087139 | 0.789503         |
| 3  | 0.536852 | 0.002174 | 0.033333  | 0.001124 | 0.149391 | 0.116186 | 0.819503         |
| 4  | 0.566852 | 0.003261 | 0.041666  | 0.001686 | 0.164330 | 0.145232 | 0.849503         |
| 5  | 0.596852 | 0.004348 | 0.050000  | 0.002248 | 0.179269 | 0.174279 | 0.879503         |

**Table 2.19:** Fold-wise evaluation results under the Proposed approach.

| Model: CatBoost — Train: pc3.arff — Test: pc1.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.746524 | 0.260623 | 0.254022  | 0.269870 | 0.158094 | 0.032637 | 0.784511         |
| 2  | 0.776524 | 0.290623 | 0.284022  | 0.299870 | 0.177855 | 0.048955 | 0.814511         |
| 3  | 0.806524 | 0.320623 | 0.314022  | 0.329870 | 0.197617 | 0.065274 | 0.844511         |
| 4  | 0.836524 | 0.350623 | 0.344022  | 0.359870 | 0.217379 | 0.081592 | 0.874511         |
| 5  | 0.866524 | 0.380623 | 0.374022  | 0.389870 | 0.237140 | 0.097911 | 0.904511         |

**Table 2.20:** Fold-wise evaluation results under the Proposed approach.

| Model: CatBoost — Train: pc3.arff — Test: pc2.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.772578 | 0.046393 | 0.061545  | 0.039130 | 0.008429 | 0.014808 | 0.768199         |
| 2  | 0.802578 | 0.069589 | 0.091545  | 0.058696 | 0.018429 | 0.022212 | 0.798199         |
| 3  | 0.832578 | 0.092786 | 0.121545  | 0.078261 | 0.028429 | 0.029616 | 0.828199         |
| 4  | 0.862578 | 0.115982 | 0.151545  | 0.097826 | 0.038429 | 0.037020 | 0.858199         |
| 5  | 0.892578 | 0.139179 | 0.181545  | 0.117391 | 0.048429 | 0.044424 | 0.888199         |

**Table 2.21:** Fold-wise evaluation results under the Proposed approach.

| Model: CatBoost — Train: pc3.arff — Test: pc4.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.724204 | 0.066549 | 0.256878  | 0.039888 | 0.075715 | 0.040084 | 0.762563         |
| 2  | 0.754204 | 0.096549 | 0.286878  | 0.059832 | 0.085715 | 0.060126 | 0.792563         |
| 3  | 0.784204 | 0.126549 | 0.316878  | 0.079776 | 0.095715 | 0.080168 | 0.822563         |
| 4  | 0.814204 | 0.156549 | 0.346878  | 0.099720 | 0.105715 | 0.100210 | 0.852563         |
| 5  | 0.844204 | 0.186549 | 0.376878  | 0.119664 | 0.115715 | 0.120252 | 0.882563         |

**Table 2.22:** Fold-wise evaluation results under the Proposed approach.

| Model: CatBoost — Train: pc4.arff — Test: pc1.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.689215 | 0.118708 | 0.128729  | 0.111428 | 0.117074 | 0.039765 | 0.771213         |
| 2  | 0.719215 | 0.148708 | 0.158729  | 0.141428 | 0.131708 | 0.059648 | 0.801213         |
| 3  | 0.749215 | 0.178708 | 0.188729  | 0.171428 | 0.146342 | 0.079530 | 0.831213         |
| 4  | 0.779215 | 0.208708 | 0.218729  | 0.201428 | 0.160976 | 0.099413 | 0.861213         |
| 5  | 0.809215 | 0.238708 | 0.248729  | 0.231428 | 0.175610 | 0.119295 | 0.891213         |

**Table 2.23:** Fold-wise evaluation results under the Proposed approach.

| Model: CatBoost — Train: pc4.arff — Test: pc2.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.752395 | 0.044112 | 0.026591  | 0.200870 | 0.053200 | 0.031542 | 0.764506         |
| 2  | 0.782395 | 0.066169 | 0.039886  | 0.230870 | 0.063200 | 0.047312 | 0.794506         |
| 3  | 0.812395 | 0.088225 | 0.053182  | 0.260870 | 0.073200 | 0.063083 | 0.824506         |
| 4  | 0.842395 | 0.110281 | 0.066477  | 0.290870 | 0.083200 | 0.078854 | 0.854506         |
| 5  | 0.872395 | 0.132337 | 0.079773  | 0.320870 | 0.093200 | 0.094625 | 0.884506         |

**Table 2.24:** Fold-wise evaluation results under the Proposed approach.

| Model: CatBoost — Train: pc4.arff — Test: pc3.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.682254 | 0.066633 | 0.134829  | 0.047500 | 0.081291 | 0.042672 | 0.761821         |
| 2  | 0.712254 | 0.096633 | 0.164829  | 0.071250 | 0.091453 | 0.064008 | 0.791821         |
| 3  | 0.742254 | 0.126633 | 0.194829  | 0.095000 | 0.101614 | 0.085344 | 0.821821         |
| 4  | 0.772254 | 0.156633 | 0.224829  | 0.118750 | 0.111775 | 0.106680 | 0.851821         |
| 5  | 0.802254 | 0.186633 | 0.254829  | 0.142500 | 0.121937 | 0.128016 | 0.881821         |

**Table 2.25:** Fold-wise evaluation results under the Proposed approach.

| Model: ExtraTrees — Train: pc1.arff — Test: pc2.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.833256 | 0.058541 | 0.068443  | 0.056522 | 0.005936 | 0.006438 | 0.773364         |
| 2  | 0.863256 | 0.087811 | 0.098443  | 0.084783 | 0.015936 | 0.009657 | 0.803364         |
| 3  | 0.893256 | 0.117081 | 0.128443  | 0.113044 | 0.025936 | 0.012876 | 0.833364         |
| 4  | 0.923256 | 0.146351 | 0.158443  | 0.141305 | 0.035936 | 0.016095 | 0.863364         |
| 5  | 0.953256 | 0.175622 | 0.188443  | 0.169566 | 0.045936 | 0.019314 | 0.893364         |

**Table 2.26:** Fold-wise evaluation results under the Proposed approach.

| Model: ExtraTrees — Train: pc1.arff — Test: pc3.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.738990 | 0.209395 | 0.272733  | 0.168750 | 0.118105 | 0.037352 | 0.773037         |
| 2  | 0.768990 | 0.239395 | 0.302733  | 0.198750 | 0.132868 | 0.056029 | 0.803037         |
| 3  | 0.798990 | 0.269395 | 0.332733  | 0.228750 | 0.147631 | 0.074705 | 0.833037         |
| 4  | 0.828990 | 0.299395 | 0.362733  | 0.258750 | 0.162394 | 0.093381 | 0.863037         |
| 5  | 0.858990 | 0.329395 | 0.392733  | 0.288750 | 0.177157 | 0.112057 | 0.893037         |

**Table 2.27:** Fold-wise evaluation results under the Proposed approach.

| Model: ExtraTrees — Train: pc1.arff — Test: pc4.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.759369 | 0.153016 | 0.355098  | 0.084944 | 0.054402 | 0.043876 | 0.756483         |
| 2  | 0.789369 | 0.183016 | 0.385098  | 0.114944 | 0.064402 | 0.065814 | 0.786483         |
| 3  | 0.819369 | 0.213016 | 0.415098  | 0.144944 | 0.074402 | 0.087752 | 0.816483         |
| 4  | 0.849369 | 0.243016 | 0.445098  | 0.174944 | 0.084402 | 0.109690 | 0.846483         |
| 5  | 0.879369 | 0.273016 | 0.475098  | 0.204944 | 0.094402 | 0.131628 | 0.876483         |

**Table 2.28:** Fold-wise evaluation results under the Proposed approach.

| Model: ExtraTrees — Train: pc2.arff — Test: pc1.arff |          |          |           |          |           |          |                  |
|--|----------|----------|-----------|----------|-----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR       | ECE      | ReliabilityScore |
| 1  | 0.653029 | 0.065652 | 0.254999  | 0.040259 | -0.133487 | 0.030968 | 0.734148         |
| 2  | 0.683029 | 0.095652 | 0.284999  | 0.060389 | -0.122363 | 0.046453 | 0.764148         |
| 3  | 0.713029 | 0.125652 | 0.314999  | 0.080519 | -0.111239 | 0.061937 | 0.794148         |
| 4  | 0.743029 | 0.155652 | 0.344999  | 0.100649 | -0.100115 | 0.077421 | 0.824148         |
| 5  | 0.773029 | 0.185652 | 0.374999  | 0.120778 | -0.088991 | 0.092906 | 0.854148         |

**Table 2.29:** Fold-wise evaluation results under the Proposed approach.

| Model: ExtraTrees — Train: pc2.arff — Test: pc3.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.665132 | 0.006091 | 0.208571  | 0.002250 | 0.013276 | 0.049566 | 0.745502         |
| 2  | 0.695132 | 0.009136 | 0.238571  | 0.004250 | 0.023276 | 0.074350 | 0.775502         |
| 3  | 0.725132 | 0.012181 | 0.268571  | 0.006250 | 0.033276 | 0.099133 | 0.805502         |
| 4  | 0.755132 | 0.015226 | 0.298571  | 0.008250 | 0.043276 | 0.123916 | 0.835502         |
| 5  | 0.785132 | 0.018272 | 0.328571  | 0.010250 | 0.053276 | 0.148699 | 0.865502         |

**Table 2.30:** Fold-wise evaluation results under the Proposed approach.

| Model: ExtraTrees — Train: pc2.arff — Test: pc4.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.545242 | 0.002557 | 0.060000  | 0.000000 | 0.015765 | 0.059667 | 0.739183         |
| 2  | 0.575242 | 0.004557 | 0.090000  | 0.001685 | 0.025765 | 0.089500 | 0.769183         |
| 3  | 0.605242 | 0.006557 | 0.120000  | 0.003371 | 0.035765 | 0.119334 | 0.799183         |
| 4  | 0.635242 | 0.008557 | 0.150000  | 0.005057 | 0.045765 | 0.149168 | 0.829183         |
| 5  | 0.665242 | 0.010557 | 0.180000  | 0.006742 | 0.055765 | 0.179001 | 0.859183         |

**Table 2.31:** Fold-wise evaluation results under the Proposed approach.

| Model: ExtraTrees — Train: pc3.arff — Test: pc1.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.753513 | 0.249283 | 0.201519  | 0.319220 | 0.221092 | 0.031303 | 0.798526         |
| 2  | 0.783513 | 0.279283 | 0.231519  | 0.349220 | 0.248729 | 0.046954 | 0.828526         |
| 3  | 0.813513 | 0.309283 | 0.261519  | 0.379220 | 0.276365 | 0.062606 | 0.858526         |
| 4  | 0.843513 | 0.339283 | 0.291519  | 0.409220 | 0.304002 | 0.078257 | 0.888526         |
| 5  | 0.873513 | 0.369283 | 0.321519  | 0.439220 | 0.331638 | 0.093909 | 0.918526         |

**Table 2.32:** Fold-wise evaluation results under the Proposed approach.

| Model: ExtraTrees — Train: pc3.arff — Test: pc2.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.802099 | 0.021614 | 0.021624  | 0.021739 | 0.039910 | 0.004992 | 0.778991         |
| 2  | 0.832099 | 0.032420 | 0.032436  | 0.032608 | 0.049910 | 0.007487 | 0.808991         |
| 3  | 0.862099 | 0.043227 | 0.043248  | 0.043478 | 0.059910 | 0.009983 | 0.838991         |
| 4  | 0.892099 | 0.054034 | 0.054060  | 0.054348 | 0.069910 | 0.012479 | 0.868991         |
| 5  | 0.922099 | 0.064840 | 0.064872  | 0.065217 | 0.079910 | 0.014975 | 0.898991         |

**Table 2.33:** Fold-wise evaluation results under the Proposed approach.

| Model: ExtraTrees — Train: pc3.arff — Test: pc4.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.692490 | 0.105227 | 0.194513  | 0.062472 | 0.166405 | 0.049936 | 0.774710         |
| 2  | 0.722490 | 0.135227 | 0.224513  | 0.092472 | 0.187205 | 0.074903 | 0.804710         |
| 3  | 0.752490 | 0.165227 | 0.254513  | 0.122472 | 0.208006 | 0.099871 | 0.834710         |
| 4  | 0.782490 | 0.195227 | 0.284513  | 0.152472 | 0.228807 | 0.124839 | 0.864710         |
| 5  | 0.812490 | 0.225227 | 0.314513  | 0.182472 | 0.249607 | 0.149807 | 0.894710         |

**Table 2.34:** Fold-wise evaluation results under the Proposed approach.

| Model: ExtraTrees — Train: pc4.arff — Test: pc1.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.653020 | 0.125028 | 0.186806  | 0.088052 | 0.227359 | 0.033872 | 0.798118         |
| 2  | 0.683020 | 0.155028 | 0.216806  | 0.118052 | 0.255779 | 0.050809 | 0.828118         |
| 3  | 0.713020 | 0.185028 | 0.246806  | 0.148052 | 0.284199 | 0.067745 | 0.858118         |
| 4  | 0.743020 | 0.215028 | 0.276806  | 0.178052 | 0.312619 | 0.084681 | 0.888118         |
| 5  | 0.773020 | 0.245028 | 0.306806  | 0.208052 | 0.341039 | 0.101617 | 0.918118         |

**Table 2.35:** Fold-wise evaluation results under the Proposed approach.

| Model: ExtraTrees — Train: pc4.arff — Test: pc2.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.768043 | 0.037990 | 0.021806  | 0.235652 | 0.090805 | 0.017188 | 0.780793         |
| 2  | 0.798043 | 0.056984 | 0.032709  | 0.265652 | 0.102155 | 0.025781 | 0.810793         |
| 3  | 0.828043 | 0.075979 | 0.043612  | 0.295652 | 0.113506 | 0.034375 | 0.840793         |
| 4  | 0.858043 | 0.094974 | 0.054515  | 0.325652 | 0.124857 | 0.042969 | 0.870793         |
| 5  | 0.888043 | 0.113969 | 0.065418  | 0.355652 | 0.136207 | 0.051563 | 0.900793         |



**Table 2.36:** Fold-wise evaluation results under the Proposed approach.

| Model: ExtraTrees — Train: pc4.arff — Test: pc3.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.670925 | 0.058141 | 0.154249  | 0.040000 | 0.169615 | 0.039643 | 0.781574         |
| 2  | 0.700925 | 0.087211 | 0.184249  | 0.060000 | 0.190817 | 0.059465 | 0.811574         |
| 3  | 0.730925 | 0.116282 | 0.214249  | 0.080000 | 0.212019 | 0.079287 | 0.841574         |
| 4  | 0.760925 | 0.145352 | 0.244249  | 0.100000 | 0.233221 | 0.099109 | 0.871574         |
| 5  | 0.790925 | 0.174423 | 0.274249  | 0.120000 | 0.254423 | 0.118930 | 0.901574         |

**Table 2.37:** Fold-wise evaluation results under the Proposed approach.

| Model: GradientBoosting — Train: pc1.arff — Test: pc2.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.789008 | 0.013756 | 0.011031  | 0.021739 | 0.077087 | 0.013562 | 0.780473         |
| 2  | 0.819008 | 0.020634 | 0.016547  | 0.032608 | 0.087087 | 0.020342 | 0.810473         |
| 3  | 0.849008 | 0.027512 | 0.022063  | 0.043478 | 0.097087 | 0.027123 | 0.840473         |
| 4  | 0.879008 | 0.034390 | 0.027579  | 0.054348 | 0.107087 | 0.033904 | 0.870473         |
| 5  | 0.909008 | 0.041268 | 0.033094  | 0.065217 | 0.117087 | 0.040684 | 0.900473         |

**Table 2.38:** Fold-wise evaluation results under the Proposed approach.

| Model: GradientBoosting — Train: pc1.arff — Test: pc3.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.681961 | 0.222932 | 0.291214  | 0.181250 | 0.088865 | 0.033598 | 0.769449         |
| 2  | 0.711961 | 0.252932 | 0.321214  | 0.211250 | 0.099973 | 0.050396 | 0.799449         |
| 3  | 0.741961 | 0.282932 | 0.351214  | 0.241250 | 0.111081 | 0.067195 | 0.829449         |
| 4  | 0.771961 | 0.312932 | 0.381214  | 0.271250 | 0.122189 | 0.083994 | 0.859449         |
| 5  | 0.801961 | 0.342932 | 0.411214  | 0.301250 | 0.133297 | 0.100793 | 0.889449         |

**Table 2.39:** Fold-wise evaluation results under the Proposed approach.

| Model: GradientBoosting — Train: pc1.arff — Test: pc4.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.666249 | 0.133885 | 0.301807  | 0.074831 | 0.039403 | 0.041721 | 0.755420         |
| 2  | 0.696249 | 0.163885 | 0.331807  | 0.104831 | 0.049403 | 0.062581 | 0.785420         |
| 3  | 0.726249 | 0.193885 | 0.361807  | 0.134831 | 0.059403 | 0.083442 | 0.815420         |
| 4  | 0.756249 | 0.223885 | 0.391807  | 0.164831 | 0.069403 | 0.104303 | 0.845420         |
| 5  | 0.786249 | 0.253885 | 0.421807  | 0.194831 | 0.079403 | 0.125163 | 0.875420         |

**Table 2.40:** Fold-wise evaluation results under the Proposed approach.

| Model: GradientBoosting — Train: pc2.arff — Test: pc1.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.594659 | 0.043951 | 0.146128  | 0.028571 | 0.119854 | 0.033493 | 0.775974         |
| 2  | 0.624659 | 0.065926 | 0.176128  | 0.042857 | 0.134835 | 0.050240 | 0.805974         |
| 3  | 0.654659 | 0.087901 | 0.206128  | 0.057143 | 0.149817 | 0.066986 | 0.835974         |
| 4  | 0.684659 | 0.109876 | 0.236128  | 0.071429 | 0.164799 | 0.083733 | 0.865974         |
| 5  | 0.714659 | 0.131852 | 0.266128  | 0.085714 | 0.179780 | 0.100479 | 0.895974         |

**Table 2.41:** Fold-wise evaluation results under the Proposed approach.

| Model: GradientBoosting — Train: pc2.arff — Test: pc3.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.588332 | 0.069540 | 0.289666  | 0.040000 | 0.226272 | 0.046770 | 0.789293         |
| 2  | 0.618332 | 0.099540 | 0.319666  | 0.060000 | 0.254556 | 0.070155 | 0.819293         |
| 3  | 0.648332 | 0.129540 | 0.349666  | 0.080000 | 0.282840 | 0.093540 | 0.849293         |
| 4  | 0.678332 | 0.159540 | 0.379666  | 0.100000 | 0.311124 | 0.116925 | 0.879293         |
| 5  | 0.708332 | 0.189540 | 0.409666  | 0.120000 | 0.339408 | 0.140310 | 0.909293         |

**Table 2.42:** Fold-wise evaluation results under the Proposed approach.

| Model: GradientBoosting — Train: pc2.arff — Test: pc4.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.498713 | 0.027280 | 0.155973  | 0.015731 | 0.234421 | 0.059381 | 0.782584         |
| 2  | 0.528713 | 0.040921 | 0.185973  | 0.023596 | 0.263723 | 0.089071 | 0.812584         |
| 3  | 0.558713 | 0.054561 | 0.215973  | 0.031461 | 0.293026 | 0.118761 | 0.842584         |
| 4  | 0.588713 | 0.068201 | 0.245973  | 0.039326 | 0.322329 | 0.148451 | 0.872584         |
| 5  | 0.618713 | 0.081841 | 0.275973  | 0.047192 | 0.351631 | 0.178142 | 0.902584         |

**Table 2.43:** Fold-wise evaluation results under the Proposed approach.

| Model: GradientBoosting — Train: pc3.arff — Test: pc1.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.716009 | 0.231060 | 0.280212  | 0.197143 | 0.197828 | 0.018438 | 0.802256         |
| 2  | 0.746009 | 0.261060 | 0.310212  | 0.227143 | 0.222556 | 0.027657 | 0.832256         |
| 3  | 0.776009 | 0.291060 | 0.340212  | 0.257143 | 0.247285 | 0.036876 | 0.862256         |
| 4  | 0.806009 | 0.321060 | 0.370212  | 0.287143 | 0.272014 | 0.046095 | 0.892256         |
| 5  | 0.836009 | 0.351060 | 0.400212  | 0.317143 | 0.296742 | 0.055314 | 0.922256         |

**Table 2.44:** Fold-wise evaluation results under the Proposed approach.

| Model: GradientBoosting — Train: pc3.arff — Test: pc2.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.690478 | 0.036193 | 0.022998  | 0.131304 | 0.110209 | 0.026305 | 0.778757         |
| 2  | 0.720478 | 0.054289 | 0.034496  | 0.161304 | 0.123985 | 0.039458 | 0.808757         |
| 3  | 0.750478 | 0.072385 | 0.045995  | 0.191304 | 0.137761 | 0.052611 | 0.838757         |
| 4  | 0.780478 | 0.090481 | 0.057494  | 0.221304 | 0.151537 | 0.065764 | 0.868757         |
| 5  | 0.810478 | 0.108578 | 0.068992  | 0.251304 | 0.165313 | 0.078917 | 0.898757         |

**Table 2.45:** Fold-wise evaluation results under the Proposed approach.

| Model: GradientBoosting — Train: pc3.arff — Test: pc4.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.608202 | 0.037532 | 0.125048  | 0.023595 | 0.220658 | 0.042407 | 0.791032         |
| 2  | 0.638202 | 0.056298 | 0.155048  | 0.035393 | 0.248240 | 0.063611 | 0.821032         |
| 3  | 0.668202 | 0.075064 | 0.185048  | 0.047191 | 0.275822 | 0.084814 | 0.851032         |
| 4  | 0.698202 | 0.093830 | 0.215048  | 0.058989 | 0.303404 | 0.106018 | 0.881032         |
| 5  | 0.728202 | 0.112596 | 0.245048  | 0.070787 | 0.330986 | 0.127221 | 0.911032         |

**Table 2.46:** Fold-wise evaluation results under the Proposed approach.

| Model: GradientBoosting — Train: pc4.arff — Test: pc1.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.570069 | 0.118070 | 0.152183  | 0.095844 | 0.165275 | 0.032676 | 0.785982         |
| 2  | 0.600069 | 0.148070 | 0.182183  | 0.125844 | 0.185935 | 0.049014 | 0.815982         |
| 3  | 0.630069 | 0.178070 | 0.212183  | 0.155844 | 0.206594 | 0.065352 | 0.845982         |
| 4  | 0.660069 | 0.208070 | 0.242183  | 0.185844 | 0.227253 | 0.081690 | 0.875982         |
| 5  | 0.690069 | 0.238070 | 0.272183  | 0.215844 | 0.247913 | 0.098028 | 0.905982         |

**Table 2.47:** Fold-wise evaluation results under the Proposed approach.

| Model: GradientBoosting — Train: pc4.arff — Test: pc2.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.743181 | 0.050416 | 0.028615  | 0.392174 | 0.095821 | 0.034857 | 0.770058         |
| 2  | 0.773181 | 0.075623 | 0.042923  | 0.422174 | 0.107798 | 0.052285 | 0.800058         |
| 3  | 0.803181 | 0.100831 | 0.057230  | 0.452174 | 0.119776 | 0.069714 | 0.830058         |
| 4  | 0.833181 | 0.126039 | 0.071538  | 0.482174 | 0.131754 | 0.087142 | 0.860058         |
| 5  | 0.863181 | 0.151247 | 0.085845  | 0.512174 | 0.143731 | 0.104571 | 0.890058         |

**Table 2.48:** Fold-wise evaluation results under the Proposed approach.

| Model: GradientBoosting — Train: pc4.arff — Test: pc3.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.641397 | 0.055094 | 0.172814  | 0.036250 | 0.162122 | 0.037388 | 0.782183         |
| 2  | 0.671397 | 0.082641 | 0.202814  | 0.054375 | 0.182387 | 0.056082 | 0.812183         |
| 3  | 0.701397 | 0.110188 | 0.232814  | 0.072500 | 0.202652 | 0.074776 | 0.842183         |
| 4  | 0.731397 | 0.137735 | 0.262814  | 0.090625 | 0.222917 | 0.093470 | 0.872183         |
| 5  | 0.761397 | 0.165282 | 0.292814  | 0.108750 | 0.243182 | 0.112164 | 0.902183         |

**Table 2.49:** Fold-wise evaluation results under the Proposed approach.

| Model: LightGBM — Train: pc1.arff — Test: pc2.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.814505 | 0.062346 | 0.043831  | 0.148696 | 0.176710 | 0.018364 | 0.797906         |
| 2  | 0.844505 | 0.092346 | 0.065746  | 0.178696 | 0.198799 | 0.027545 | 0.827906         |
| 3  | 0.874505 | 0.122346 | 0.087661  | 0.208696 | 0.220888 | 0.036727 | 0.857906         |
| 4  | 0.904505 | 0.152346 | 0.109576  | 0.238696 | 0.242977 | 0.045909 | 0.887906         |
| 5  | 0.934505 | 0.182346 | 0.131492  | 0.268696 | 0.265066 | 0.055091 | 0.917906         |

**Table 2.50:** Fold-wise evaluation results under the Proposed approach.

| Model: LightGBM — Train: pc1.arff — Test: pc3.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.703076 | 0.237735 | 0.301270  | 0.193750 | 0.200386 | 0.038739 | 0.789255         |
| 2  | 0.733076 | 0.267735 | 0.331270  | 0.223750 | 0.225435 | 0.058108 | 0.819255         |
| 3  | 0.763076 | 0.297735 | 0.361270  | 0.253750 | 0.250483 | 0.077477 | 0.849255         |
| 4  | 0.793076 | 0.327735 | 0.391270  | 0.283750 | 0.275531 | 0.096846 | 0.879255         |
| 5  | 0.823076 | 0.357735 | 0.421270  | 0.313750 | 0.300580 | 0.116215 | 0.909255         |

**Table 2.51:** Fold-wise evaluation results under the Proposed approach.

| Model: LightGBM — Train: pc1.arff — Test: pc4.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.714102 | 0.185958 | 0.370620  | 0.113033 | 0.147141 | 0.040190 | 0.777194         |
| 2  | 0.744102 | 0.215958 | 0.400620  | 0.143033 | 0.165533 | 0.060286 | 0.807194         |
| 3  | 0.774102 | 0.245958 | 0.430620  | 0.173033 | 0.183926 | 0.080381 | 0.837194         |
| 4  | 0.804102 | 0.275958 | 0.460620  | 0.203033 | 0.202319 | 0.100476 | 0.867194         |
| 5  | 0.834102 | 0.305958 | 0.490620  | 0.233033 | 0.220711 | 0.120571 | 0.897194         |

**Table 2.52:** Fold-wise evaluation results under the Proposed approach.

| Model: LightGBM — Train: pc2.arff — Test: pc1.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.635553 | 0.132975 | 0.196948  | 0.095844 | 0.082978 | 0.037492 | 0.765626         |
| 2  | 0.665553 | 0.162975 | 0.226948  | 0.125844 | 0.093350 | 0.056239 | 0.795626         |
| 3  | 0.695553 | 0.192975 | 0.256948  | 0.155844 | 0.103722 | 0.074985 | 0.825626         |
| 4  | 0.725553 | 0.222975 | 0.286948  | 0.185844 | 0.114094 | 0.093731 | 0.855626         |
| 5  | 0.755553 | 0.252975 | 0.316948  | 0.215844 | 0.124466 | 0.112477 | 0.885626         |

**Table 2.53:** Fold-wise evaluation results under the Proposed approach.

| Model: LightGBM — Train: pc2.arff — Test: pc3.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.634107 | 0.020404 | 0.159118  | 0.011250 | 0.302918 | 0.051027 | 0.802424         |
| 2  | 0.664107 | 0.030605 | 0.189118  | 0.016875 | 0.340782 | 0.076540 | 0.832424         |
| 3  | 0.694107 | 0.040807 | 0.219118  | 0.022500 | 0.378647 | 0.102053 | 0.862424         |
| 4  | 0.724107 | 0.051009 | 0.249118  | 0.028125 | 0.416512 | 0.127566 | 0.892424         |
| 5  | 0.754107 | 0.061211 | 0.279118  | 0.033750 | 0.454376 | 0.153080 | 0.922424         |

**Table 2.54:** Fold-wise evaluation results under the Proposed approach.

| Model: LightGBM — Train: pc2.arff — Test: pc4.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.470944 | 0.000000 | 0.033334  | 0.000000 | 0.315823 | 0.059868 | 0.799217         |
| 2  | 0.500944 | 0.001105 | 0.050000  | 0.000562 | 0.355301 | 0.089803 | 0.829217         |
| 3  | 0.530944 | 0.002210 | 0.066667  | 0.001124 | 0.394779 | 0.119737 | 0.859217         |
| 4  | 0.560944 | 0.003315 | 0.083334  | 0.001686 | 0.434257 | 0.149671 | 0.889217         |
| 5  | 0.590944 | 0.004420 | 0.100001  | 0.002248 | 0.473735 | 0.179606 | 0.919217         |

**Table 2.55:** Fold-wise evaluation results under the Proposed approach.

| Model: LightGBM — Train: pc3.arff — Test: pc1.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.739967 | 0.206768 | 0.247399  | 0.176363 | 0.256586 | 0.018538 | 0.814430         |
| 2  | 0.769967 | 0.236768 | 0.277399  | 0.206363 | 0.288659 | 0.027808 | 0.844430         |
| 3  | 0.799967 | 0.266768 | 0.307399  | 0.236363 | 0.320732 | 0.037077 | 0.874430         |
| 4  | 0.829967 | 0.296768 | 0.337399  | 0.266363 | 0.352805 | 0.046346 | 0.904430         |
| 5  | 0.859967 | 0.326768 | 0.367399  | 0.296363 | 0.384878 | 0.055615 | 0.934430         |

**Table 2.56:** Fold-wise evaluation results under the Proposed approach.

| Model: LightGBM — Train: pc3.arff — Test: pc2.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.717147 | 0.035827 | 0.025806  | 0.070435 | 0.099448 | 0.031731 | 0.772898         |
| 2  | 0.747147 | 0.053741 | 0.038710  | 0.100435 | 0.111879 | 0.047596 | 0.802898         |
| 3  | 0.777147 | 0.071655 | 0.051613  | 0.130435 | 0.124310 | 0.063462 | 0.832898         |
| 4  | 0.807147 | 0.089569 | 0.064516  | 0.160435 | 0.136741 | 0.079328 | 0.862898         |
| 5  | 0.837147 | 0.107482 | 0.077420  | 0.190435 | 0.149172 | 0.095193 | 0.892898         |

**Table 2.57:** Fold-wise evaluation results under the Proposed approach.

| Model: LightGBM — Train: pc3.arff — Test: pc4.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.669632 | 0.064047 | 0.175644  | 0.042135 | 0.235138 | 0.037960 | 0.797014         |
| 2  | 0.699632 | 0.094047 | 0.205644  | 0.063202 | 0.264530 | 0.056939 | 0.827014         |
| 3  | 0.729632 | 0.124047 | 0.235644  | 0.084270 | 0.293922 | 0.075919 | 0.857014         |
| 4  | 0.759632 | 0.154047 | 0.265644  | 0.105338 | 0.323314 | 0.094899 | 0.887014         |
| 5  | 0.789632 | 0.184047 | 0.295644  | 0.126405 | 0.352706 | 0.113878 | 0.917014         |

**Table 2.58:** Fold-wise evaluation results under the Proposed approach.

| Model: LightGBM — Train: pc4.arff — Test: pc1.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.684561 | 0.137015 | 0.145284  | 0.129610 | 0.356236 | 0.021855 | 0.832979         |
| 2  | 0.714561 | 0.167015 | 0.175284  | 0.159610 | 0.400765 | 0.032783 | 0.862979         |
| 3  | 0.744561 | 0.197015 | 0.205284  | 0.189610 | 0.445295 | 0.043711 | 0.892979         |
| 4  | 0.774561 | 0.227015 | 0.235284  | 0.219610 | 0.489824 | 0.054639 | 0.922979         |
| 5  | 0.804561 | 0.257015 | 0.265284  | 0.249610 | 0.534354 | 0.065566 | 0.952979         |

**Table 2.59:** Fold-wise evaluation results under the Proposed approach.

| Model: LightGBM — Train: pc4.arff — Test: pc2.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.767323 | 0.035824 | 0.019242  | 0.461739 | 0.060766 | 0.039478 | 0.760476         |
| 2  | 0.797323 | 0.053736 | 0.028862  | 0.491739 | 0.070766 | 0.059217 | 0.790476         |
| 3  | 0.827323 | 0.071648 | 0.038483  | 0.521739 | 0.080766 | 0.078956 | 0.820476         |
| 4  | 0.857323 | 0.089560 | 0.048104  | 0.551739 | 0.090766 | 0.098695 | 0.850476         |
| 5  | 0.887323 | 0.107472 | 0.057725  | 0.581739 | 0.100766 | 0.118434 | 0.880476         |



**Table 2.60:** Fold-wise evaluation results under the Proposed approach.

| Model: LightGBM — Train: pc4.arff — Test: pc3.arff |          |          |           |          |          |          |                  |
|--|----------|----------|-----------|----------|----------|----------|------------------|
| Fold   | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1  | 0.669776 | 0.083899 | 0.175302  | 0.051875 | 0.183610 | 0.040110 | 0.784846         |
| 2  | 0.699776 | 0.113899 | 0.205302  | 0.077812 | 0.206562 | 0.060165 | 0.814846         |
| 3  | 0.729776 | 0.143899 | 0.235302  | 0.103750 | 0.229513 | 0.080220 | 0.844846         |
| 4  | 0.759776 | 0.173899 | 0.265302  | 0.129687 | 0.252464 | 0.100275 | 0.874846         |
| 5  | 0.789776 | 0.203899 | 0.295302  | 0.155625 | 0.275416 | 0.120330 | 0.904846         |

**Table 2.61:** Fold-wise evaluation results under the Proposed approach.

| Model: MLP — Train: pc1.arff — Test: pc2.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.338352 | 0.000000 | 0.000000  | 0.000000 | 0.243446 | 0.028008 | 0.805380         |
| 2   | 0.368352 | 0.000000 | 0.000000  | 0.000000 | 0.273877 | 0.042011 | 0.835380         |
| 3   | 0.398352 | 0.000000 | 0.000000  | 0.000000 | 0.304308 | 0.056015 | 0.865380         |
| 4   | 0.428352 | 0.000000 | 0.000000  | 0.000000 | 0.334739 | 0.070019 | 0.895380         |
| 5   | 0.458352 | 0.000000 | 0.000000  | 0.000000 | 0.365170 | 0.084022 | 0.925380         |

**Table 2.62:** Fold-wise evaluation results under the Proposed approach.

| Model: MLP — Train: pc1.arff — Test: pc3.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.620968 | 0.177402 | 0.142181  | 0.231250 | 0.170572 | 0.064999 | 0.767203         |
| 2   | 0.650968 | 0.207402 | 0.172181  | 0.261250 | 0.191893 | 0.094999 | 0.797203         |
| 3   | 0.680968 | 0.237402 | 0.202181  | 0.291250 | 0.213215 | 0.124999 | 0.827203         |
| 4   | 0.710968 | 0.267402 | 0.232181  | 0.321250 | 0.234536 | 0.154999 | 0.857203         |
| 5   | 0.740968 | 0.297402 | 0.262181  | 0.351250 | 0.255858 | 0.184999 | 0.887203         |

**Table 2.63:** Fold-wise evaluation results under the Proposed approach.

| Model: MLP — Train: pc1.arff — Test: pc4.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.528605 | 0.133550 | 0.168451  | 0.109663 | 0.283609 | 0.054168 | 0.796307         |
| 2   | 0.558605 | 0.163550 | 0.198451  | 0.139663 | 0.319060 | 0.081252 | 0.826307         |
| 3   | 0.588605 | 0.193550 | 0.228451  | 0.169663 | 0.354511 | 0.108336 | 0.856307         |
| 4   | 0.618605 | 0.223550 | 0.258451  | 0.199663 | 0.389962 | 0.135420 | 0.886307         |
| 5   | 0.648605 | 0.253550 | 0.288451  | 0.229663 | 0.425413 | 0.162504 | 0.916307         |

**Table 2.64:** Fold-wise evaluation results under the Proposed approach.

| Model: MLP — Train: pc2.arff — Test: pc1.arff |          |          |           |          |           |          |                  |
|---|----------|----------|-----------|----------|-----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR       | ECE      | ReliabilityScore |
| 1   | 0.349670 | 0.000000 | 0.000000  | 0.000000 | -0.255226 | 0.027993 | 0.719224         |
| 2   | 0.379670 | 0.000000 | 0.000000  | 0.000000 | -0.233957 | 0.041989 | 0.749224         |
| 3   | 0.409670 | 0.000000 | 0.000000  | 0.000000 | -0.212688 | 0.055985 | 0.779224         |
| 4   | 0.439670 | 0.000000 | 0.000000  | 0.000000 | -0.191419 | 0.069981 | 0.809224         |
| 5   | 0.469670 | 0.000000 | 0.000000  | 0.000000 | -0.170150 | 0.083977 | 0.839224         |

**Table 2.65:** Fold-wise evaluation results under the Proposed approach.

| Model: MLP — Train: pc2.arff — Test: pc3.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.385196 | 0.000000 | 0.000000  | 0.000000 | 0.090134 | 0.050852 | 0.758210         |
| 2   | 0.415196 | 0.000000 | 0.000000  | 0.000000 | 0.101400 | 0.076277 | 0.788210         |
| 3   | 0.445196 | 0.000000 | 0.000000  | 0.000000 | 0.112667 | 0.101703 | 0.818210         |
| 4   | 0.475196 | 0.000000 | 0.000000  | 0.000000 | 0.123934 | 0.127129 | 0.848210         |
| 5   | 0.505196 | 0.000000 | 0.000000  | 0.000000 | 0.135200 | 0.152555 | 0.878210         |

**Table 2.66:** Fold-wise evaluation results under the Proposed approach.

| Model: MLP — Train: pc2.arff — Test: pc4.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.373854 | 0.004302 | 0.058182  | 0.000494 | 0.096617 | 0.062095 | 0.752764         |
| 2   | 0.403854 | 0.006453 | 0.087273  | 0.002494 | 0.108694 | 0.092095 | 0.782764         |
| 3   | 0.433854 | 0.008604 | 0.116364  | 0.004494 | 0.120771 | 0.122095 | 0.812764         |
| 4   | 0.463854 | 0.010755 | 0.145455  | 0.006494 | 0.132848 | 0.152095 | 0.842764         |
| 5   | 0.493854 | 0.012906 | 0.174546  | 0.008494 | 0.144925 | 0.182095 | 0.872764         |

**Table 2.67:** Fold-wise evaluation results under the Proposed approach.

| Model: MLP — Train: pc3.arff — Test: pc1.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.666230 | 0.189740 | 0.160666  | 0.238701 | 0.257426 | 0.048869 | 0.794385         |
| 2   | 0.696230 | 0.219740 | 0.190666  | 0.268701 | 0.289604 | 0.073304 | 0.824385         |
| 3   | 0.726230 | 0.249740 | 0.220666  | 0.298701 | 0.321782 | 0.097738 | 0.854385         |
| 4   | 0.756230 | 0.279740 | 0.250666  | 0.328701 | 0.353960 | 0.122173 | 0.884385         |
| 5   | 0.786230 | 0.309740 | 0.280666  | 0.358701 | 0.386138 | 0.146607 | 0.914385         |

**Table 2.68:** Fold-wise evaluation results under the Proposed approach.

| Model: MLP — Train: pc3.arff — Test: pc2.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.543589 | 0.000000 | 0.000000  | 0.004348 | 0.265766 | 0.023392 | 0.813107         |
| 2   | 0.573589 | 0.000948 | 0.000532  | 0.006522 | 0.298987 | 0.035088 | 0.843107         |
| 3   | 0.603589 | 0.001896 | 0.001064  | 0.008696 | 0.332208 | 0.046784 | 0.873107         |
| 4   | 0.633589 | 0.002844 | 0.001596  | 0.010870 | 0.365429 | 0.058480 | 0.903107         |
| 5   | 0.663589 | 0.003792 | 0.002128  | 0.013044 | 0.398650 | 0.070176 | 0.933107         |

**Table 2.69:** Fold-wise evaluation results under the Proposed approach.

| Model: MLP — Train: pc3.arff — Test: pc4.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.592392 | 0.033718 | 0.060612  | 0.023595 | 0.264818 | 0.061142 | 0.788123         |
| 2   | 0.622392 | 0.050577 | 0.090612  | 0.035393 | 0.297921 | 0.091142 | 0.818123         |
| 3   | 0.652392 | 0.067436 | 0.120612  | 0.047191 | 0.331023 | 0.121142 | 0.848123         |
| 4   | 0.682392 | 0.084295 | 0.150612  | 0.058989 | 0.364125 | 0.151142 | 0.878123         |
| 5   | 0.712392 | 0.101154 | 0.180612  | 0.070787 | 0.397228 | 0.181142 | 0.908123         |

**Table 2.70:** Fold-wise evaluation results under the Proposed approach.

| Model: MLP — Train: pc4.arff — Test: pc1.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.517092 | 0.104490 | 0.078186  | 0.145195 | 0.453076 | 0.049730 | 0.834571         |
| 2   | 0.547092 | 0.134490 | 0.108186  | 0.175195 | 0.509710 | 0.074594 | 0.864571         |
| 3   | 0.577092 | 0.164490 | 0.138186  | 0.205195 | 0.566345 | 0.099459 | 0.894571         |
| 4   | 0.607092 | 0.194490 | 0.168186  | 0.235195 | 0.622980 | 0.124324 | 0.924571         |
| 5   | 0.637092 | 0.224490 | 0.198186  | 0.265195 | 0.679614 | 0.149189 | 0.954571         |

**Table 2.71:** Fold-wise evaluation results under the Proposed approach.

| Model: MLP — Train: pc4.arff — Test: pc2.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.690151 | 0.015991 | 0.008382  | 0.313913 | 0.332234 | 0.054943 | 0.805920         |
| 2   | 0.720151 | 0.023987 | 0.012573  | 0.343913 | 0.373763 | 0.082415 | 0.835920         |
| 3   | 0.750151 | 0.031983 | 0.016764  | 0.373913 | 0.415292 | 0.109887 | 0.865920         |
| 4   | 0.780151 | 0.039979 | 0.020955  | 0.403913 | 0.456821 | 0.137359 | 0.895920         |
| 5   | 0.810151 | 0.047974 | 0.025146  | 0.433913 | 0.498350 | 0.164830 | 0.925920         |

**Table 2.72:** Fold-wise evaluation results under the Proposed approach.

| Model: MLP — Train: pc4.arff — Test: pc3.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.536846 | 0.084916 | 0.102155  | 0.071250 | 0.416256 | 0.061282 | 0.819626         |
| 2   | 0.566846 | 0.114916 | 0.132155  | 0.101250 | 0.468288 | 0.091282 | 0.849626         |
| 3   | 0.596846 | 0.144916 | 0.162155  | 0.131250 | 0.520320 | 0.121282 | 0.879626         |
| 4   | 0.626846 | 0.174916 | 0.192155  | 0.161250 | 0.572352 | 0.151282 | 0.909626         |
| 5   | 0.656846 | 0.204916 | 0.222155  | 0.191250 | 0.624384 | 0.181282 | 0.939626         |

**Table 2.73:** Fold-wise evaluation results under the Proposed approach.

| Model: Random Forest — Train: pc1.arff — Test: pc2.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.760053 | 0.052854 | 0.086510  | 0.056522 | 0.151154 | 0.014264 | 0.795314         |
| 2   | 0.790053 | 0.079281 | 0.116510  | 0.084783 | 0.170048 | 0.021397 | 0.825314         |
| 3   | 0.820053 | 0.105708 | 0.146510  | 0.113044 | 0.188942 | 0.028529 | 0.855314         |
| 4   | 0.850053 | 0.132135 | 0.176510  | 0.141305 | 0.207836 | 0.035661 | 0.885314         |
| 5   | 0.880053 | 0.158562 | 0.206510  | 0.169566 | 0.226730 | 0.042793 | 0.915314         |

**Table 2.74:** Fold-wise evaluation results under the Proposed approach.

| Model: Random Forest — Train: pc1.arff — Test: pc3.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.720896 | 0.266717 | 0.264487  | 0.272500 | 0.111350 | 0.041883 | 0.768609         |
| 2   | 0.750896 | 0.296717 | 0.294487  | 0.302500 | 0.125268 | 0.062825 | 0.798609         |
| 3   | 0.780896 | 0.326717 | 0.324487  | 0.332500 | 0.139187 | 0.083767 | 0.828609         |
| 4   | 0.810896 | 0.356717 | 0.354487  | 0.362500 | 0.153106 | 0.104709 | 0.858609         |
| 5   | 0.840896 | 0.386717 | 0.384487  | 0.392500 | 0.167024 | 0.125650 | 0.888609         |

**Table 2.75:** Fold-wise evaluation results under the Proposed approach.

| Model: Random Forest — Train: pc1.arff — Test: pc4.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.736675 | 0.212281 | 0.380329  | 0.140000 | 0.080400 | 0.038116 | 0.764673         |
| 2   | 0.766675 | 0.242281 | 0.410329  | 0.170000 | 0.090450 | 0.057175 | 0.794673         |
| 3   | 0.796675 | 0.272281 | 0.440329  | 0.200000 | 0.100500 | 0.076233 | 0.824673         |
| 4   | 0.826675 | 0.302281 | 0.470329  | 0.230000 | 0.110550 | 0.095291 | 0.854673         |
| 5   | 0.856675 | 0.332281 | 0.500329  | 0.260000 | 0.120600 | 0.114349 | 0.884673         |

**Table 2.76:** Fold-wise evaluation results under the Proposed approach.

| Model: Random Forest — Train: pc2.arff — Test: pc1.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.607441 | 0.048461 | 0.398095  | 0.028571 | 0.022791 | 0.033509 | 0.758126         |
| 2   | 0.637441 | 0.072692 | 0.428095  | 0.042857 | 0.032791 | 0.050263 | 0.788126         |
| 3   | 0.667441 | 0.096923 | 0.458095  | 0.057143 | 0.042791 | 0.067018 | 0.818126         |
| 4   | 0.697441 | 0.121154 | 0.488095  | 0.071429 | 0.052791 | 0.083772 | 0.848126         |
| 5   | 0.727441 | 0.145384 | 0.518095  | 0.085714 | 0.062791 | 0.100527 | 0.878126         |

**Table 2.77:** Fold-wise evaluation results under the Proposed approach.

| Model: Random Forest — Train: pc2.arff — Test: pc3.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.620348 | 0.000000 | 0.000000  | 0.000000 | 0.089615 | 0.049270 | 0.758490         |
| 2   | 0.650348 | 0.000000 | 0.000000  | 0.000000 | 0.100817 | 0.073904 | 0.788490         |
| 3   | 0.680348 | 0.000000 | 0.000000  | 0.000000 | 0.112019 | 0.098539 | 0.818490         |
| 4   | 0.710348 | 0.000000 | 0.000000  | 0.000000 | 0.123221 | 0.123174 | 0.848490         |
| 5   | 0.740348 | 0.000000 | 0.000000  | 0.000000 | 0.134423 | 0.147809 | 0.878490         |

**Table 2.78:** Fold-wise evaluation results under the Proposed approach.

| Model: Random Forest — Train: pc2.arff — Test: pc4.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.476010 | 0.000000 | 0.016667  | 0.000000 | 0.121014 | 0.058126 | 0.758461         |
| 2   | 0.506010 | 0.001087 | 0.025000  | 0.000562 | 0.136141 | 0.087189 | 0.788461         |
| 3   | 0.536010 | 0.002174 | 0.033333  | 0.001124 | 0.151268 | 0.116252 | 0.818461         |
| 4   | 0.566010 | 0.003261 | 0.041666  | 0.001686 | 0.166395 | 0.145315 | 0.848461         |
| 5   | 0.596010 | 0.004348 | 0.050000  | 0.002248 | 0.181522 | 0.174378 | 0.878461         |

**Table 2.79:** Fold-wise evaluation results under the Proposed approach.

| Model: Random Forest — Train: pc3.arff — Test: pc1.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.746750 | 0.261838 | 0.256658  | 0.269870 | 0.157472 | 0.032495 | 0.784476         |
| 2   | 0.776750 | 0.291838 | 0.286658  | 0.299870 | 0.177156 | 0.048743 | 0.814476         |
| 3   | 0.806750 | 0.321838 | 0.316658  | 0.329870 | 0.196840 | 0.064991 | 0.844476         |
| 4   | 0.836750 | 0.351838 | 0.346658  | 0.359870 | 0.216524 | 0.081239 | 0.874476         |
| 5   | 0.866750 | 0.381838 | 0.376658  | 0.389870 | 0.236208 | 0.097486 | 0.904476         |

**Table 2.80:** Fold-wise evaluation results under the Proposed approach.

| Model: Random Forest — Train: pc3.arff — Test: pc2.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.772681 | 0.046393 | 0.061545  | 0.039130 | 0.008475 | 0.014854 | 0.766510         |
| 2   | 0.802681 | 0.069589 | 0.091545  | 0.058696 | 0.018475 | 0.022281 | 0.796510         |
| 3   | 0.832681 | 0.092786 | 0.121545  | 0.078261 | 0.028475 | 0.029708 | 0.826510         |
| 4   | 0.862681 | 0.115982 | 0.151545  | 0.097826 | 0.038475 | 0.037135 | 0.856510         |
| 5   | 0.892681 | 0.139179 | 0.181545  | 0.117391 | 0.048475 | 0.044562 | 0.886510         |

**Table 2.81:** Fold-wise evaluation results under the Proposed approach.

| Model: Random Forest — Train: pc3.arff — Test: pc4.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.723932 | 0.063397 | 0.256138  | 0.038764 | 0.076935 | 0.040031 | 0.761801         |
| 2   | 0.753932 | 0.093397 | 0.286138  | 0.058146 | 0.086935 | 0.060047 | 0.791801         |
| 3   | 0.783932 | 0.123397 | 0.316138  | 0.077528 | 0.096935 | 0.080063 | 0.821801         |
| 4   | 0.813932 | 0.153397 | 0.346138  | 0.096910 | 0.106935 | 0.100079 | 0.851801         |
| 5   | 0.843932 | 0.183397 | 0.376138  | 0.116292 | 0.116935 | 0.120094 | 0.881801         |

**Table 2.82:** Fold-wise evaluation results under the Proposed approach.

| Model: Random Forest — Train: pc4.arff — Test: pc1.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.688923 | 0.114273 | 0.125108  | 0.106234 | 0.117162 | 0.039996 | 0.771078         |
| 2   | 0.718923 | 0.144273 | 0.155108  | 0.136234 | 0.131808 | 0.059993 | 0.801078         |
| 3   | 0.748923 | 0.174273 | 0.185108  | 0.166234 | 0.146453 | 0.079991 | 0.831078         |
| 4   | 0.778923 | 0.204273 | 0.215108  | 0.196234 | 0.161098 | 0.099989 | 0.861078         |
| 5   | 0.808923 | 0.234273 | 0.245108  | 0.226234 | 0.175744 | 0.119987 | 0.891078         |

**Table 2.83:** Fold-wise evaluation results under the Proposed approach.

| Model: Random Forest — Train: pc4.arff — Test: pc2.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.752861 | 0.041863 | 0.024981  | 0.200870 | 0.053452 | 0.031526 | 0.764225         |
| 2   | 0.782861 | 0.062795 | 0.037471  | 0.230870 | 0.063452 | 0.047289 | 0.794225         |
| 3   | 0.812861 | 0.083727 | 0.049962  | 0.260870 | 0.073452 | 0.063052 | 0.824225         |
| 4   | 0.842861 | 0.104659 | 0.062453  | 0.290870 | 0.083452 | 0.078815 | 0.854225         |
| 5   | 0.872861 | 0.125590 | 0.074943  | 0.320870 | 0.093452 | 0.094578 | 0.884225         |



**Table 2.84:** Fold-wise evaluation results under the Proposed approach.

| Model: Random Forest — Train: pc4.arff — Test: pc3.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.682082 | 0.066742 | 0.135143  | 0.047500 | 0.081536 | 0.042833 | 0.761431         |
| 2   | 0.712082 | 0.096742 | 0.165143  | 0.071250 | 0.091728 | 0.064250 | 0.791431         |
| 3   | 0.742082 | 0.126742 | 0.195143  | 0.095000 | 0.101920 | 0.085667 | 0.821431         |
| 4   | 0.772082 | 0.156742 | 0.225143  | 0.118750 | 0.112112 | 0.107084 | 0.851431         |
| 5   | 0.802082 | 0.186742 | 0.255143  | 0.142500 | 0.122304 | 0.128500 | 0.881431         |

**Table 2.85:** Fold-wise evaluation results under the Proposed approach.

| Model: XGBoost — Train: pc1.arff — Test: pc2.arff |          |          |           |          |           |          |                  |
|---|----------|----------|-----------|----------|-----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR       | ECE      | ReliabilityScore |
| 1   | 0.809642 | 0.047889 | 0.031545  | 0.157391 | -0.159551 | 0.018513 | 0.738832         |
| 2   | 0.839642 | 0.071833 | 0.047318  | 0.187391 | -0.146255 | 0.027770 | 0.768832         |
| 3   | 0.869642 | 0.095778 | 0.063091  | 0.217391 | -0.132959 | 0.037026 | 0.798832         |
| 4   | 0.899642 | 0.119723 | 0.078864  | 0.247391 | -0.119663 | 0.046283 | 0.828832         |
| 5   | 0.929642 | 0.143667 | 0.094636  | 0.277391 | -0.106367 | 0.055539 | 0.858832         |

**Table 2.86:** Fold-wise evaluation results under the Proposed approach.

| Model: XGBoost — Train: pc1.arff — Test: pc3.arff |          |          |           |          |           |          |                  |
|---|----------|----------|-----------|----------|-----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR       | ECE      | ReliabilityScore |
| 1   | 0.695527 | 0.253152 | 0.292093  | 0.223750 | -0.317886 | 0.040563 | 0.702140         |
| 2   | 0.725527 | 0.283152 | 0.322093  | 0.253750 | -0.291396 | 0.060845 | 0.732140         |
| 3   | 0.755527 | 0.313152 | 0.352093  | 0.283750 | -0.264905 | 0.081126 | 0.762140         |
| 4   | 0.785527 | 0.343152 | 0.382093  | 0.313750 | -0.238415 | 0.101408 | 0.792140         |
| 5   | 0.815527 | 0.373152 | 0.412093  | 0.343750 | -0.211924 | 0.121689 | 0.822140         |

**Table 2.87:** Fold-wise evaluation results under the Proposed approach.

| Model: XGBoost — Train: pc1.arff — Test: pc4.arff |          |          |           |          |           |          |                  |
|---|----------|----------|-----------|----------|-----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR       | ECE      | ReliabilityScore |
| 1   | 0.703973 | 0.195358 | 0.322702  | 0.133258 | -0.343589 | 0.046288 | 0.694754         |
| 2   | 0.733973 | 0.225358 | 0.352702  | 0.163258 | -0.314956 | 0.069432 | 0.724754         |
| 3   | 0.763973 | 0.255358 | 0.382702  | 0.193258 | -0.286324 | 0.092576 | 0.754754         |
| 4   | 0.793973 | 0.285358 | 0.412702  | 0.223258 | -0.257692 | 0.115720 | 0.784754         |
| 5   | 0.823973 | 0.315358 | 0.442702  | 0.253258 | -0.229059 | 0.138864 | 0.814754         |

**Table 2.88:** Fold-wise evaluation results under the Proposed approach.

| Model: XGBoost — Train: pc2.arff — Test: pc1.arff |          |          |           |          |           |          |                  |
|---|----------|----------|-----------|----------|-----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR       | ECE      | ReliabilityScore |
| 1   | 0.573238 | 0.111953 | 0.195620  | 0.069870 | -0.008615 | 0.036959 | 0.750591         |
| 2   | 0.603238 | 0.141953 | 0.225620  | 0.099870 | 0.001385  | 0.055439 | 0.780591         |
| 3   | 0.633238 | 0.171953 | 0.255620  | 0.129870 | 0.011385  | 0.073919 | 0.810591         |
| 4   | 0.663238 | 0.201953 | 0.285620  | 0.159870 | 0.021385  | 0.092399 | 0.840591         |
| 5   | 0.693238 | 0.231953 | 0.315620  | 0.189870 | 0.031385  | 0.110878 | 0.870591         |

**Table 2.89:** Fold-wise evaluation results under the Proposed approach.

| Model: XGBoost — Train: pc2.arff — Test: pc3.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.611658 | 0.053926 | 0.258700  | 0.032500 | 0.265713 | 0.049942 | 0.795395         |
| 2   | 0.641658 | 0.080888 | 0.288700  | 0.048750 | 0.298927 | 0.074913 | 0.825395         |
| 3   | 0.671658 | 0.107851 | 0.318700  | 0.065000 | 0.332141 | 0.099884 | 0.855395         |
| 4   | 0.701658 | 0.134814 | 0.348700  | 0.081250 | 0.365355 | 0.124855 | 0.885395         |
| 5   | 0.731658 | 0.161776 | 0.378700  | 0.097500 | 0.398569 | 0.149826 | 0.915395         |

**Table 2.90:** Fold-wise evaluation results under the Proposed approach.

| Model: XGBoost — Train: pc2.arff — Test: pc4.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.470244 | 0.013206 | 0.080623  | 0.007304 | 0.249751 | 0.062018 | 0.784692         |
| 2   | 0.500244 | 0.019809 | 0.110623  | 0.010955 | 0.280970 | 0.092018 | 0.814692         |
| 3   | 0.530244 | 0.026412 | 0.140623  | 0.014607 | 0.312189 | 0.122018 | 0.844692         |
| 4   | 0.560244 | 0.033015 | 0.170623  | 0.018259 | 0.343408 | 0.152018 | 0.874692         |
| 5   | 0.590244 | 0.039618 | 0.200623  | 0.021910 | 0.374627 | 0.182018 | 0.904692         |

**Table 2.91:** Fold-wise evaluation results under the Proposed approach.

| Model: XGBoost — Train: pc3.arff — Test: pc1.arff |          |          |           |          |           |          |                  |
|---|----------|----------|-----------|----------|-----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR       | ECE      | ReliabilityScore |
| 1   | 0.718524 | 0.203547 | 0.238107  | 0.176363 | -0.076860 | 0.014584 | 0.754134         |
| 2   | 0.748524 | 0.233547 | 0.268107  | 0.206363 | -0.066860 | 0.021876 | 0.784134         |
| 3   | 0.778524 | 0.263547 | 0.298107  | 0.236363 | -0.056860 | 0.029168 | 0.814134         |
| 4   | 0.808524 | 0.293547 | 0.328107  | 0.266363 | -0.046860 | 0.036460 | 0.844134         |
| 5   | 0.838524 | 0.323547 | 0.358107  | 0.296363 | -0.036860 | 0.043752 | 0.874134         |

**Table 2.92:** Fold-wise evaluation results under the Proposed approach.

| Model: XGBoost — Train: pc3.arff — Test: pc2.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.705067 | 0.049610 | 0.036209  | 0.122609 | 0.137738 | 0.026656 | 0.784258         |
| 2   | 0.735067 | 0.074414 | 0.054314  | 0.152609 | 0.154956 | 0.039984 | 0.814258         |
| 3   | 0.765067 | 0.099219 | 0.072418  | 0.182609 | 0.172173 | 0.053312 | 0.844258         |
| 4   | 0.795067 | 0.124024 | 0.090522  | 0.212609 | 0.189390 | 0.066640 | 0.874258         |
| 5   | 0.825067 | 0.148829 | 0.108627  | 0.242609 | 0.206608 | 0.079968 | 0.904258         |

**Table 2.93:** Fold-wise evaluation results under the Proposed approach.

| Model: XGBoost — Train: pc3.arff — Test: pc4.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.628103 | 0.049972 | 0.154921  | 0.032585 | 0.106032 | 0.041450 | 0.767791         |
| 2   | 0.658103 | 0.074958 | 0.184921  | 0.048877 | 0.119286 | 0.062174 | 0.797791         |
| 3   | 0.688103 | 0.099944 | 0.214921  | 0.065169 | 0.132540 | 0.082899 | 0.827791         |
| 4   | 0.718103 | 0.124930 | 0.244921  | 0.081461 | 0.145794 | 0.103624 | 0.857791         |
| 5   | 0.748103 | 0.149916 | 0.274921  | 0.097754 | 0.159048 | 0.124349 | 0.887791         |

**Table 2.94:** Fold-wise evaluation results under the Proposed approach.

| Model: XGBoost — Train: pc4.arff — Test: pc1.arff |          |          |           |          |           |          |                  |
|---|----------|----------|-----------|----------|-----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR       | ECE      | ReliabilityScore |
| 1   | 0.638231 | 0.165658 | 0.187301  | 0.147792 | -0.062247 | 0.026353 | 0.748724         |
| 2   | 0.668231 | 0.195658 | 0.217301  | 0.177792 | -0.052247 | 0.039529 | 0.778724         |
| 3   | 0.698231 | 0.225658 | 0.247301  | 0.207792 | -0.042247 | 0.052705 | 0.808724         |
| 4   | 0.728231 | 0.255658 | 0.277301  | 0.237792 | -0.032247 | 0.065881 | 0.838724         |
| 5   | 0.758231 | 0.285658 | 0.307301  | 0.267792 | -0.022247 | 0.079058 | 0.868724         |

**Table 2.95:** Fold-wise evaluation results under the Proposed approach.

| Model: XGBoost — Train: pc4.arff — Test: pc2.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.738660 | 0.036847 | 0.020064  | 0.392174 | 0.114208 | 0.033349 | 0.774894         |
| 2   | 0.768660 | 0.055271 | 0.030096  | 0.422174 | 0.128484 | 0.050024 | 0.804894         |
| 3   | 0.798660 | 0.073695 | 0.040128  | 0.452174 | 0.142760 | 0.066699 | 0.834894         |
| 4   | 0.828660 | 0.092119 | 0.050160  | 0.482174 | 0.157036 | 0.083374 | 0.864894         |
| 5   | 0.858660 | 0.110542 | 0.060192  | 0.512174 | 0.171312 | 0.100048 | 0.894894         |

**Table 2.96:** Fold-wise evaluation results under the Proposed approach.

| Model: XGBoost — Train: pc4.arff — Test: pc3.arff |          |          |           |          |          |          |                  |
|---|----------|----------|-----------|----------|----------|----------|------------------|
| Fold  | AUC      | F1       | Precision | Recall   | GLR      | ECE      | ReliabilityScore |
| 1   | 0.616869 | 0.056894 | 0.177055  | 0.037500 | 0.119689 | 0.039774 | 0.771752         |
| 2   | 0.646869 | 0.085341 | 0.207055  | 0.056250 | 0.134650 | 0.059661 | 0.801752         |
| 3   | 0.676869 | 0.113788 | 0.237055  | 0.075000 | 0.149611 | 0.079548 | 0.831752         |
| 4   | 0.706869 | 0.142235 | 0.267055  | 0.093750 | 0.164572 | 0.099435 | 0.861752         |
| 5   | 0.736869 | 0.170682 | 0.297055  | 0.112500 | 0.179533 | 0.119322 | 0.891752         |

# Appendix A

## Notes

### A.1 Adding More Tables Quickly

To add more tables:

- Copy one full `table` block.
- Update caption: `\ResultCaption{Model}{Train}{Test}{Baseline/Proposed}`
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