main-notebook-output

April 15, 2024

1 Data Loading

[ ]:
```
from scipy import stats
import pandas as pd
import numpy as np
from sklearn.preprocessing import LabelEncoder, StandardScaler
from sklearn.model_selection import (
    train_test_split,
    StratifiedShuffleSplit,
)
from sklearn.metrics import confusion_matrix, ConfusionMatrixDisplay,␣
 ↪RocCurveDisplay
from sklearn.ensemble import RandomForestClassifier
from sklearn.svm import SVC
from sklearn.neighbors import KNeighborsClassifier
from utils import custom_calculate_f1_score, get_all_metrics,␣
 ↪TorchKFoldCrossValidation
import torch
from torch import nn
from torch.utils.data import TensorDataset
from torchinfo import summary
```

[ ]:
```
df = pd.read_csv('./dataset/Dry_Bean_Dataset.csv')
df.head()
```

[ ]:

	Area	Perimeter	MajorAxisLength	MinorAxisLength	AspectRation	\
0	28395	610.291	208.178117	173.888747	1.197191	
1	28734	638.018	200.524796	182.734419	1.097356	
2	29380	624.110	212.826130	175.931143	1.209713	
3	30008	645.884	210.557999	182.516516	1.153638	
4	30140	620.134	201.847882	190.279279	1.060798	

	Eccentricity	ConvexArea	EquivDiameter	Extent	Solidity	roundness	\
0	0.549812	28715	190.141097	0.763923	0.988856	0.958027	
1	0.411785	29172	191.272751	0.783968	0.984986	0.887034	
2	0.562727	29690	193.410904	0.778113	0.989559	0.947849	
3	0.498616	30724	195.467062	0.782681	0.976696	0.903936	

```
4      0.333680       30417     195.896503  0.773098  0.990893    0.984877

   Compactness  ShapeFactor1  ShapeFactor2  ShapeFactor3  ShapeFactor4  Class
0     0.913358      0.007332      0.003147      0.834222      0.998724  SEKER
1     0.953861      0.006979      0.003564      0.909851      0.998430  SEKER
2     0.908774      0.007244      0.003048      0.825871      0.999066  SEKER
3     0.928329      0.007017      0.003215      0.861794      0.994199  SEKER
4     0.970516      0.006697      0.003665      0.941900      0.999166  SEKER
```

[ ]:
```
## Dataset is multi-class, but we will convert it to binary
df['Class'] = df['Class'].apply(lambda x: 'DERMASON' if x == 'DERMASON' else␣
 ↪'Non-DERMASON')
```

2 Data analysis

2.0.1 Check for nullish values

The isna function checks if there are any nullish values in the dataframe or not

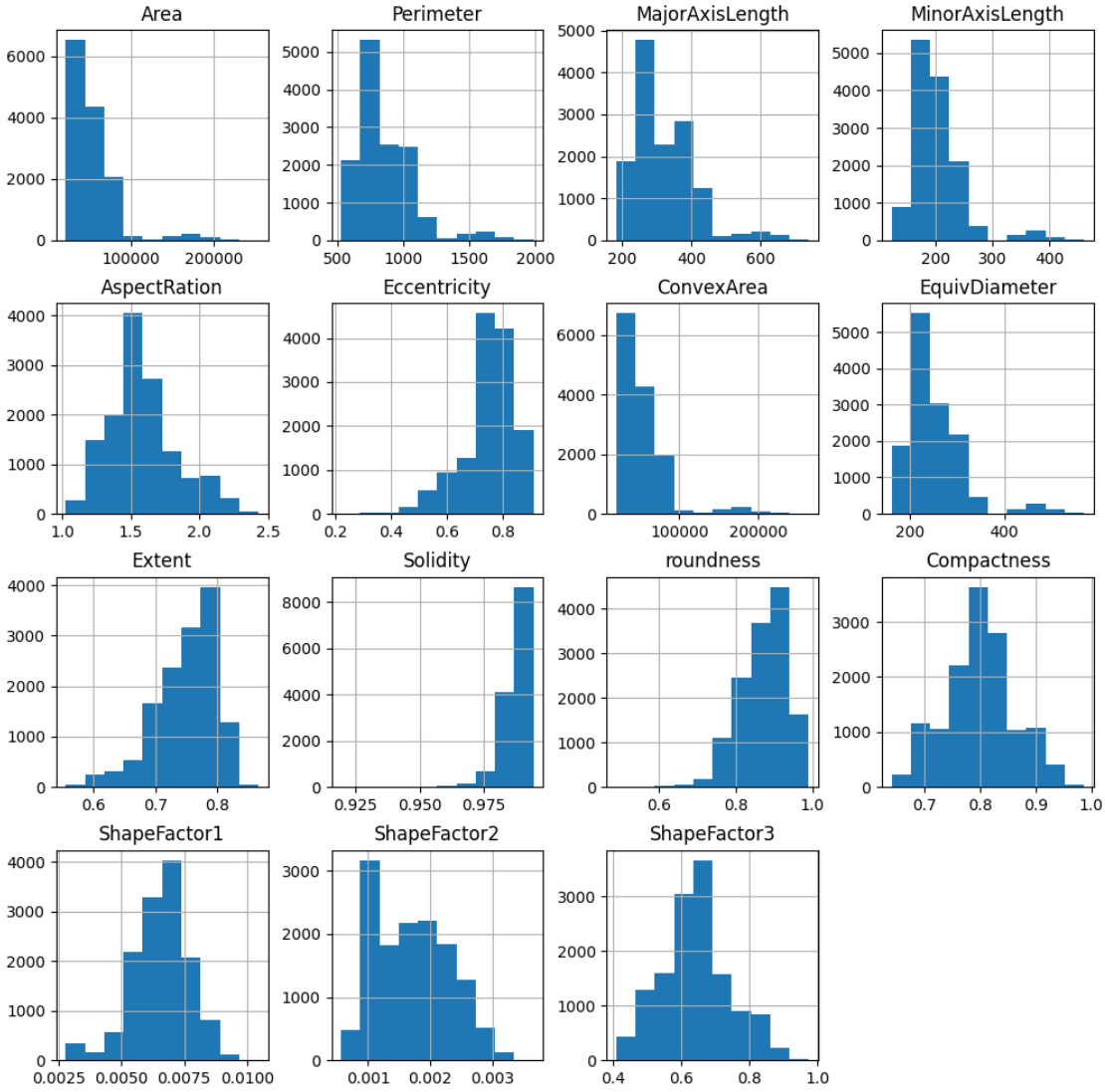
[ ]:
```
df.isna().any()
```

[ ]:
```
Area               False
Perimeter          False
MajorAxisLength    False
MinorAxisLength    False
AspectRation       False
Eccentricity       False
ConvexArea         False
EquivDiameter      False
Extent             False
Solidity           False
roundness          False
Compactness        False
ShapeFactor1       False
ShapeFactor2       False
ShapeFactor3       False
ShapeFactor4       False
Class              False
dtype: bool
```

2.0.2 Data distribution

From the histograms below, it can be observed that the value range of the attributes are high and needs to be standardized for ML models to converge faster

[ ]:
```
_ = df.iloc[:, :-2].hist(figsize=(12, 12))
```



2.0.3 Correlations

From the correlations heatmap below, it can be observed: 1. Some features have very high correlation with other variables (so they are not independent) 2. Some attributes like Area, Perimeter, MajorAxisLength, MinorAxisLength, etc have direct correlation to some extent with labels

[ ]:
```
class_factorized_df = pd.concat([df.iloc[:, :-1], pd.Series(df['Class'].
  ↪factorize()[0], name='Class')], axis=1)
class_factorized_df.corr().style.background_gradient(cmap='coolwarm')
```

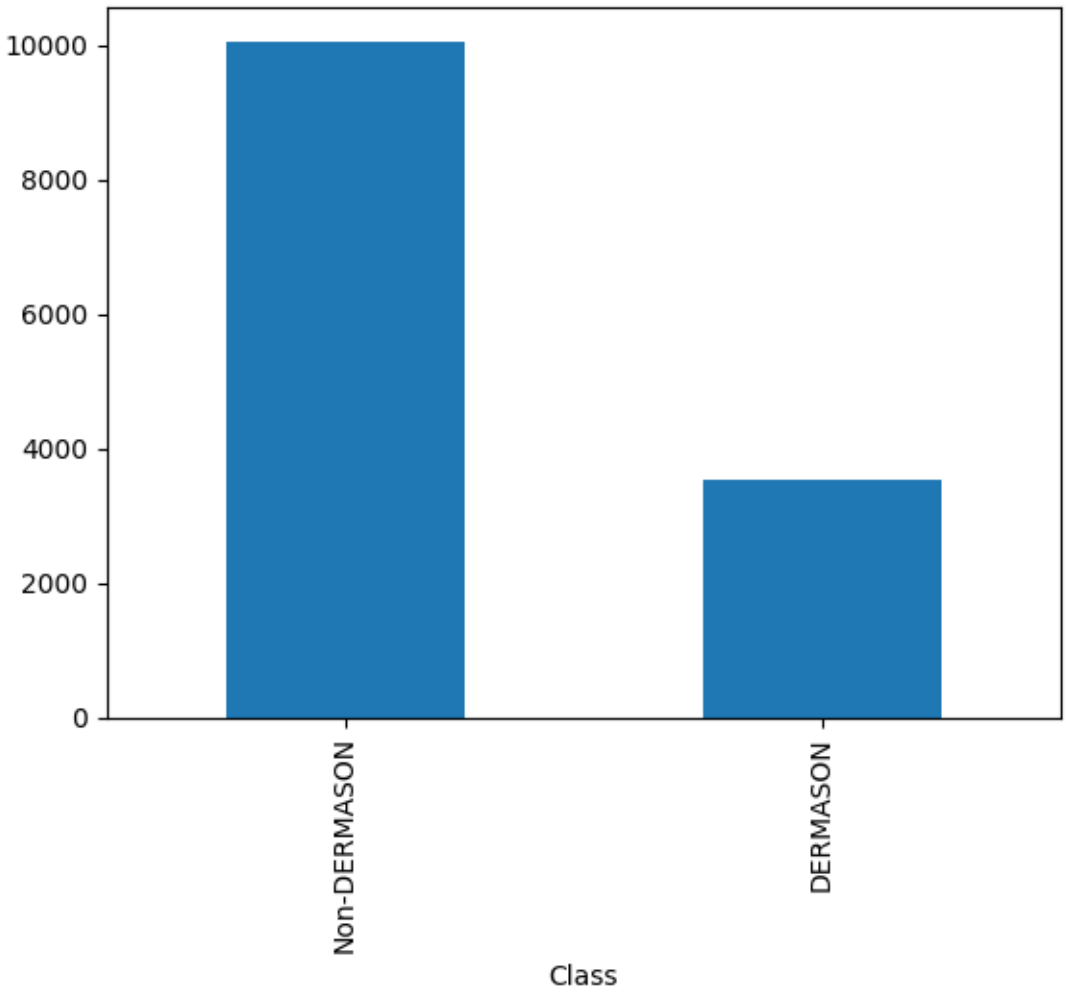
[ ]: <pandas.io.formats.style.Styler at 0x30cde2190>

2.0.4 Label distribution

From the below bar graph, we can infer following points: 1. There aren't any out-of-place/nullish class values 2. We need to convert the string values of class to numerical representation 3. The class distribution is unbalanced, so the training data needs to be split with stratification.

[ ]:
```
df['Class'].value_counts().plot(kind='bar')
```

[ ]:
```
<Axes: xlabel='Class'>
```



3 Data Preprocessing

3.0.1 Converting string to numerical representation

[ ]:
```
encoder = LabelEncoder()
df['Class_numerical'] = encoder.fit_transform(df['Class'])
```

[ ]:
```
encoder.inverse_transform([0, 1])
```

[ ]:
```
array(['DERMASON', 'Non-DERMASON'], dtype=object)
```

3.0.2 Normalizing dataset

[ ]:
```
X_train, X_test, y_train, y_test = train_test_split(
    df.iloc[:, :-2],
    df["Class_numerical"],
    test_size=0.2,
    random_state=42,
    shuffle=True,
    stratify=df["Class_numerical"],
)
```

[ ]:
```
scaler = StandardScaler()
scaled_features = scaler.fit_transform(X_train)
X_train = pd.DataFrame(scaled_features, columns=df.columns[:-2])
X_test = pd.DataFrame(scaler.transform(X_test), columns=df.columns[:-2])
X_train.head()
```

[ ]:

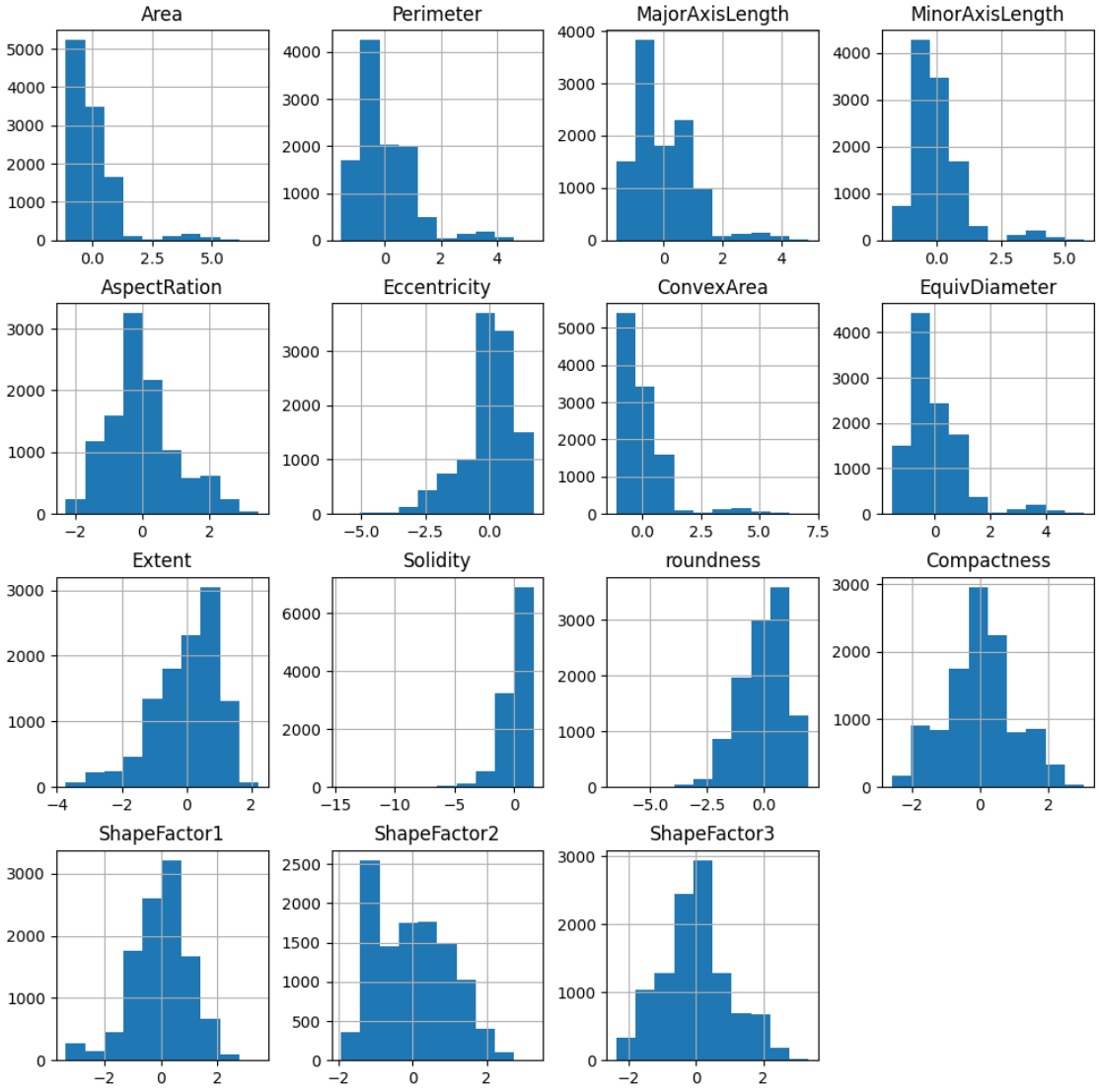
	Area	Perimeter	MajorAxisLength	MinorAxisLength	AspectRation	\
0	-0.094682	0.123942	0.534241	-0.594340	2.031821	
1	0.878664	1.006483	1.163613	0.850757	0.655072	
2	-0.692833	-0.941668	-1.172820	-0.268002	-1.735064	
3	-0.224897	-0.212262	-0.184148	-0.158521	-0.095074	
4	-0.211924	-0.156527	-0.107921	-0.217161	0.129117	

	Eccentricity	ConvexArea	EquivDiameter	Extent	Solidity	roundness	\
0	1.374019	-0.099211	-0.001218	-0.114303	0.462137	-1.022080	
1	0.743798	0.868142	1.074000	0.643785	0.584813	-0.178636	
2	-2.703900	-0.696906	-0.823466	-0.069434	0.889031	1.534785	
3	0.178891	-0.229717	-0.166248	-0.094418	0.579471	0.286425	
4	0.372271	-0.210366	-0.149512	-0.200857	-0.266950	-0.025981	

	Compactness	ShapeFactor1	ShapeFactor2	ShapeFactor3	ShapeFactor4
0	-1.756226	0.630856	-1.156022	-1.671171	0.369200
1	-0.738280	-1.089141	-1.092138	-0.753530	-0.541939
2	2.103855	0.121343	2.297855	2.228919	0.873688
3	-0.011595	-0.011651	-0.113542	-0.049872	0.228672
4	-0.231699	0.064534	-0.262659	-0.267274	0.350360

As you can see in below histograms, the range of features are normalized

[ ]:
```
_ = X_train.iloc[:, :-1].hist(figsize=(12, 12))
```



4 Model Training

[ ]:
```
results_comparison = pd.DataFrame({'RandomForest': {}, 'SVM': {}, 'KNN': {},␣
↪'Conv1D-NN': {}})
```

4.1 Random Forest

[ ]:
```
# params = {
#     "n_estimators": [100, 200, 300, 400],
#     "max_depth": [8, 10, 12],
#     "ccp_alpha": [5e-4, 1e-3],
# }
stratified_split = StratifiedShuffleSplit(n_splits=10, test_size=0.1,␣
 ↪random_state=42)
# gridsearch_rf = GridSearchCV(
#     RandomForestClassifier(n_jobs=-1),
#     params,
#     cv=stratified_split,
#     n_jobs=-1,
#     verbose=3,
#     scoring=custom_calculate_f1_score
# )
# gridsearch_rf.fit(X_train, y_train)
# gridsearch_rf.best_params_

# If you uncomment the commented code above, you will get the following output
# Output - {'ccp_alpha': 0.0005, 'max_depth': 12, 'n_estimators': 300}
```

[ ]:
```
random_forest_cv = {}
random_forest_cv_models = []

for i, (train_index, test_index) in enumerate(stratified_split.split(X_train,␣
 ↪y_train)):
    X_train_fold, X_val_fold = X_train.iloc[train_index], X_train.
 ↪iloc[test_index]
    y_train_fold, y_val_fold = y_train.iloc[train_index], y_train.
 ↪iloc[test_index]

    random_forest = RandomForestClassifier(n_estimators=300, max_depth=12,␣
 ↪ccp_alpha=5e-4, n_jobs=-1)
    random_forest.fit(X_train_fold, y_train_fold)

    y_pred = random_forest.predict(X_val_fold)
    y_pred_proba = random_forest.predict_proba(X_val_fold)[:, 1]
    random_forest_cv[i+1] = get_all_metrics(y_val_fold, y_pred)
    random_forest_cv[i+1]['Brier Score'] = np.mean((y_pred_proba -␣
 ↪y_val_fold)**2)
    random_forest_cv[i+1]['Brier Skill Score'] = random_forest_cv[i+1]['Brier␣
 ↪Score'] / (np.mean((y_val_fold - np.mean(y_pred_proba))**2))
    random_forest_cv_models.append(random_forest)

random_forest_cv['mean'] = pd.DataFrame(random_forest_cv).mean(axis=1)
```

```
pd.DataFrame(random_forest_cv).round(4)
```

[ ]:

	1	2	3	4	5
TP	260.0000	263.0000	257.0000	258.0000	261.0000
TN	777.0000	777.0000	785.0000	783.0000	784.0000
FP	28.0000	28.0000	20.0000	22.0000	21.0000
FN	24.0000	21.0000	27.0000	26.0000	23.0000
P	284.0000	284.0000	284.0000	284.0000	284.0000
N	805.0000	805.0000	805.0000	805.0000	805.0000
TPR	0.9155	0.9261	0.9049	0.9085	0.9190
TNR	0.9652	0.9652	0.9752	0.9727	0.9739
FPR	0.0348	0.0348	0.0248	0.0273	0.0261
FNR	0.0845	0.0739	0.0951	0.0915	0.0810
Recall	0.9155	0.9261	0.9049	0.9085	0.9190
Precision	0.9028	0.9038	0.9278	0.9214	0.9255
F1 Score	0.9091	0.9148	0.9162	0.9149	0.9223
Accuracy	0.9522	0.9550	0.9568	0.9559	0.9596
Error Rate	0.0478	0.0450	0.0432	0.0441	0.0404
Balanced Accuracy	0.9404	0.9456	0.9400	0.9406	0.9465
True Skill Statistics	0.8807	0.8913	0.8801	0.8811	0.8929
Heidke Skill Score	0.8807	0.8913	0.8801	0.8811	0.8929
Brier Score	0.0337	0.0315	0.0292	0.0312	0.0278
Brier Skill Score	0.1750	0.1631	0.1513	0.1620	0.1440

	6	7	8	9	10
TP	262.0000	258.0000	253.0000	256.0000	266.0000
TN	786.0000	779.0000	780.0000	784.0000	784.0000
FP	19.0000	26.0000	25.0000	21.0000	21.0000
FN	22.0000	26.0000	31.0000	28.0000	18.0000
P	284.0000	284.0000	284.0000	284.0000	284.0000
N	805.0000	805.0000	805.0000	805.0000	805.0000
TPR	0.9225	0.9085	0.8908	0.9014	0.9366
TNR	0.9764	0.9677	0.9689	0.9739	0.9739
FPR	0.0236	0.0323	0.0311	0.0261	0.0261
FNR	0.0775	0.0915	0.1092	0.0986	0.0634
Recall	0.9225	0.9085	0.8908	0.9014	0.9366
Precision	0.9324	0.9085	0.9101	0.9242	0.9268
F1 Score	0.9274	0.9085	0.9004	0.9127	0.9317
Accuracy	0.9624	0.9522	0.9486	0.9550	0.9642
Error Rate	0.0376	0.0478	0.0514	0.0450	0.0358
Balanced Accuracy	0.9495	0.9381	0.9299	0.9377	0.9553
True Skill Statistics	0.8989	0.8762	0.8598	0.8753	0.9105
Heidke Skill Score	0.8989	0.8762	0.8598	0.8753	0.9105
Brier Score	0.0271	0.0316	0.0336	0.0331	0.0262
Brier Skill Score	0.1405	0.1641	0.1741	0.1716	0.1361

	mean

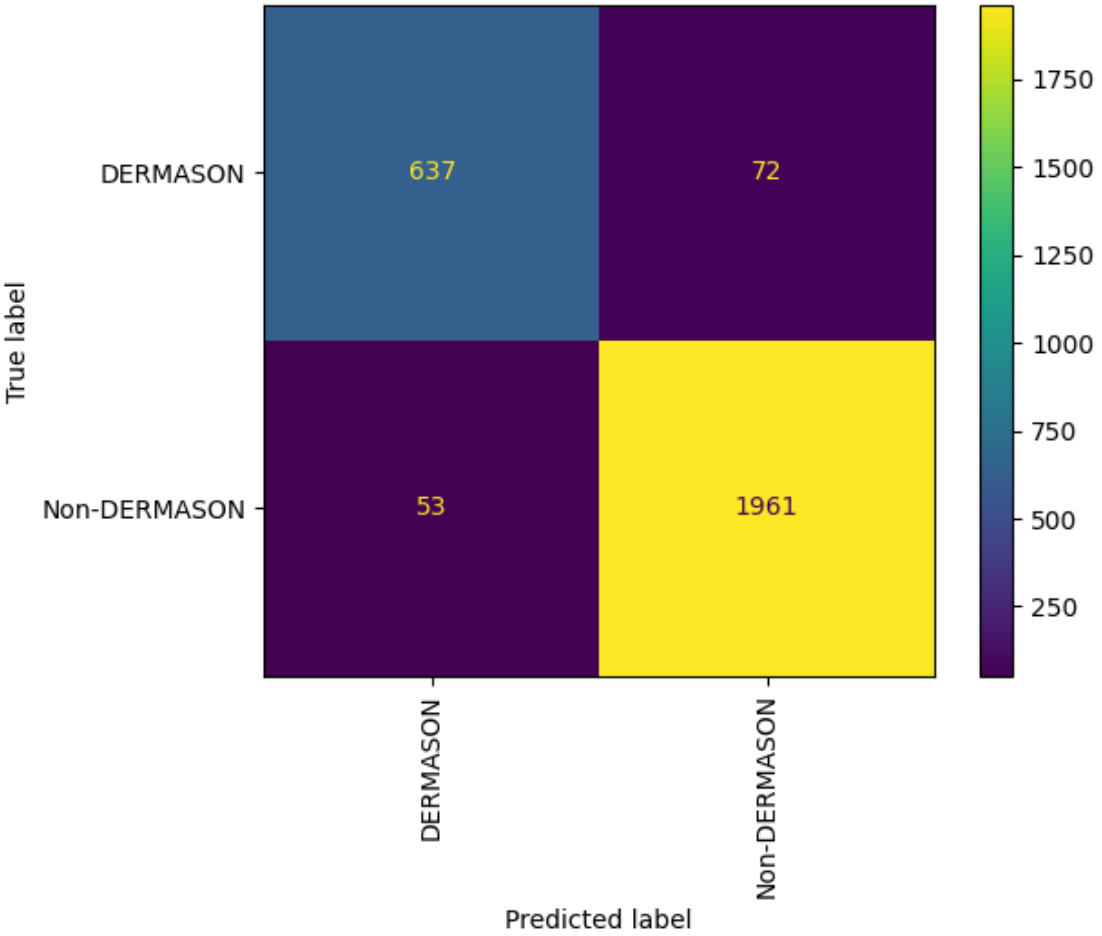
```
TP                     259.4000
TN                     781.9000
FP                      23.1000
FN                      24.6000
P                      284.0000
N                      805.0000
TPR                      0.9134
TNR                      0.9713
FPR                      0.0287
FNR                      0.0866
Recall                   0.9134
Precision                0.9183
F1 Score                 0.9158
Accuracy                 0.9562
Error Rate               0.0438
Balanced Accuracy        0.9423
True Skill Statistics    0.8847
Heidke Skill Score       0.8847
Brier Score              0.0305
Brier Skill Score        0.1582
```

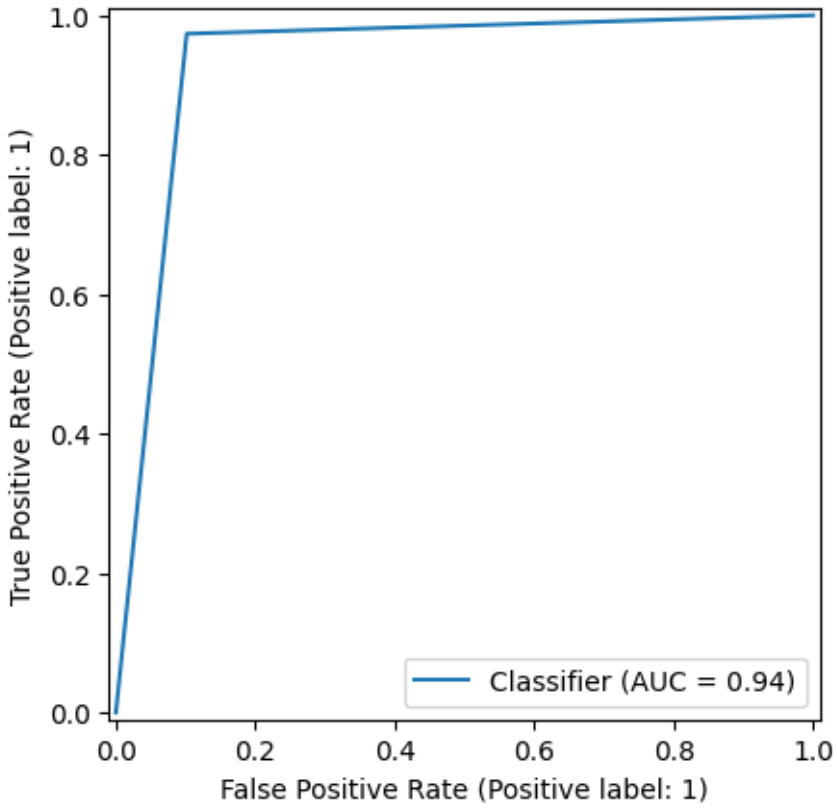
[ ]:
```python
# Mode function returns the values that appear most frequently in the array
y_pred = stats.mode([model.predict(X_test) for model in␣
 ↪random_forest_cv_models]).mode

ConfusionMatrixDisplay.from_predictions(
    y_test,
    y_pred,
    display_labels=encoder.inverse_transform([0, 1]),
    xticks_rotation="vertical",
)

RocCurveDisplay.from_predictions(y_test, y_pred)

results_comparison['RandomForest'] = get_all_metrics(y_test, y_pred)
results_comparison.loc["Brier Score", "RandomForest"] = np.mean((y_pred -␣
 ↪y_test) ** 2)
results_comparison.loc["Brier Skill Score", "RandomForest"] =␣
 ↪results_comparison["RandomForest"][
    "Brier Score"
] / (np.mean((y_test - np.mean(y_pred)) ** 2))
```


DERMASON
Non-DERMASON
True label
637
72
53
1961
DERMASON
Non-DERMASON
Predicted label
1750
1500
1250
1000
750
500
250



4.2 Additional Algorithm - SVM

[ ]:
```
# params = {
#     "C": [10, 100, 1000],
#     "kernel": ["linear", "rbf", "sigmoid", "poly"],
#     'degree': [2, 4, 6]
# }
stratified_split = StratifiedShuffleSplit(n_splits=10, test_size=0.1,␣
↪random_state=42)
# gridsearch_svc = GridSearchCV(
#     SVC(random_state=42),
#     params,
#     cv=stratified_split,
#     n_jobs=-1,
#     verbose=3,
#     scoring=custom_calculate_f1_score
# )
# gridsearch_svc.fit(X_train, y_train)
# gridsearch_svc.best_params_
```

```
# If you uncomment the commented code above, you will get the following output
# Output - {'C': 100, 'degree': 2, 'kernel': 'rbf'}
```

[ ]:
```
svc_cv = {}
svc_cv_models = []

for i, (train_index, test_index) in enumerate(stratified_split.split(X_train,␣
 ↪y_train)):
    X_train_fold, X_val_fold = X_train.iloc[train_index], X_train.
 ↪iloc[test_index]
    y_train_fold, y_val_fold = y_train.iloc[train_index], y_train.
 ↪iloc[test_index]

    svc = SVC(C= 100, degree= 2, kernel= 'rbf', probability=True,␣
 ↪random_state=42)
    svc.fit(X_train_fold, y_train_fold)

    y_pred = svc.predict(X_val_fold)
    y_pred_proba = svc.predict_proba(X_val_fold)[:, 1]
    svc_cv[i+1] = get_all_metrics(y_val_fold, y_pred)
    svc_cv[i+1]['Brier Score'] = np.mean((y_pred_proba - y_val_fold)**2)
    svc_cv[i+1]['Brier Skill Score'] = svc_cv[i+1]['Brier Score'] / (np.
 ↪mean((y_val_fold - np.mean(y_pred_proba))**2))
    svc_cv_models.append(svc)

svc_cv['mean'] = pd.DataFrame(svc_cv).mean(axis=1)
pd.DataFrame(svc_cv).round(4)
```

[ ]:

	1	2	3	4	5	\
TP	263.0000	265.0000	259.0000	260.0000	263.0000	
TN	780.0000	778.0000	785.0000	784.0000	787.0000	
FP	25.0000	27.0000	20.0000	21.0000	18.0000	
FN	21.0000	19.0000	25.0000	24.0000	21.0000	
P	284.0000	284.0000	284.0000	284.0000	284.0000	
N	805.0000	805.0000	805.0000	805.0000	805.0000	
TPR	0.9261	0.9331	0.9120	0.9155	0.9261	
TNR	0.9689	0.9665	0.9752	0.9739	0.9776	
FPR	0.0311	0.0335	0.0248	0.0261	0.0224	
FNR	0.0739	0.0669	0.0880	0.0845	0.0739	
Recall	0.9261	0.9331	0.9120	0.9155	0.9261	
Precision	0.9132	0.9075	0.9283	0.9253	0.9359	
F1 Score	0.9196	0.9201	0.9201	0.9204	0.9310	
Accuracy	0.9578	0.9578	0.9587	0.9587	0.9642	
Error Rate	0.0422	0.0422	0.0413	0.0413	0.0358	
Balanced Accuracy	0.9475	0.9498	0.9436	0.9447	0.9518	
True Skill Statistics	0.8950	0.8996	0.8871	0.8894	0.9037	
Heidke Skill Score	0.8950	0.8996	0.8871	0.8894	0.9037	

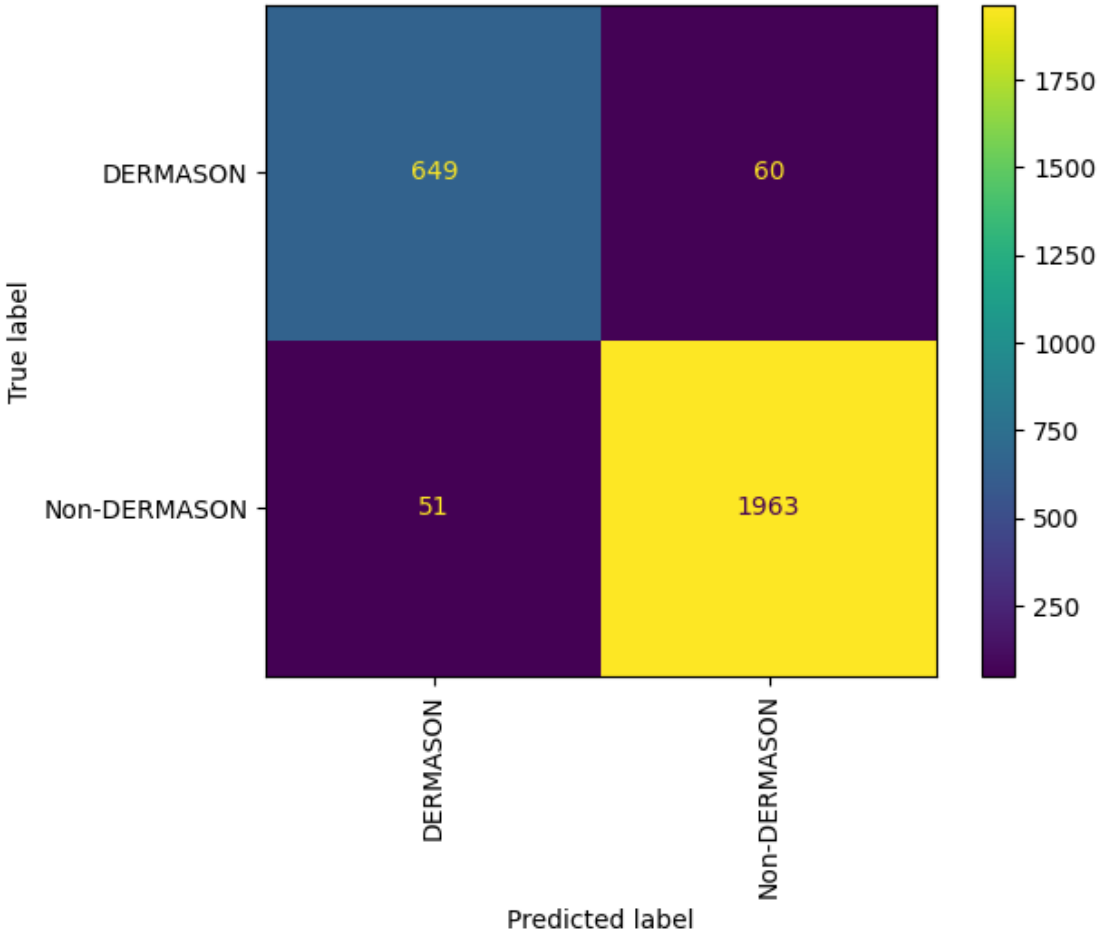
Brier Score	0.0337	0.0310	0.0300	0.0297	0.0265
Brier Skill Score	0.1749	0.1608	0.1556	0.1543	0.1374

	6	7	8	9	10 \
TP	262.0000	261.0000	258.0000	262.0000	265.0000
TN	784.0000	781.0000	781.0000	783.0000	784.0000
FP	21.0000	24.0000	24.0000	22.0000	21.0000
FN	22.0000	23.0000	26.0000	22.0000	19.0000
P	284.0000	284.0000	284.0000	284.0000	284.0000
N	805.0000	805.0000	805.0000	805.0000	805.0000
TPR	0.9225	0.9190	0.9085	0.9225	0.9331
TNR	0.9739	0.9702	0.9702	0.9727	0.9739
FPR	0.0261	0.0298	0.0298	0.0273	0.0261
FNR	0.0775	0.0810	0.0915	0.0775	0.0669
Recall	0.9225	0.9190	0.9085	0.9225	0.9331
Precision	0.9258	0.9158	0.9149	0.9225	0.9266
F1 Score	0.9242	0.9174	0.9117	0.9225	0.9298
Accuracy	0.9605	0.9568	0.9541	0.9596	0.9633
Error Rate	0.0395	0.0432	0.0459	0.0404	0.0367
Balanced Accuracy	0.9482	0.9446	0.9393	0.9476	0.9535
True Skill Statistics	0.8964	0.8892	0.8786	0.8952	0.9070
Heidke Skill Score	0.8964	0.8892	0.8786	0.8952	0.9070
Brier Score	0.0281	0.0308	0.0342	0.0320	0.0264
Brier Skill Score	0.1460	0.1600	0.1774	0.1660	0.1367

	mean
TP	261.8000
TN	782.7000
FP	22.3000
FN	22.2000
P	284.0000
N	805.0000
TPR	0.9218
TNR	0.9723
FPR	0.0277
FNR	0.0782
Recall	0.9218
Precision	0.9216
F1 Score	0.9217
Accuracy	0.9591
Error Rate	0.0409
Balanced Accuracy	0.9471
True Skill Statistics	0.8941
Heidke Skill Score	0.8941
Brier Score	0.0303
Brier Skill Score	0.1569

```
[ ]: # Mode function returns the values that appear most frequently in the array
y_pred = stats.mode([model.predict(X_test) for model in svc_cv_models]).mode
matrix = confusion_matrix(y_test, y_pred)
ConfusionMatrixDisplay.from_predictions(
    y_test,
    y_pred,
    display_labels=encoder.inverse_transform([0, 1]),
    xticks_rotation="vertical",
)

results_comparison['SVM'] = get_all_metrics(y_test, y_pred)
results_comparison.loc["Brier Score", "SVM"] = np.mean((y_pred - y_test) ** 2)
results_comparison.loc["Brier Skill Score", "SVM"] = results_comparison["SVM"][
    "Brier Score"
] / (np.mean((y_test - np.mean(y_pred)) ** 2))
```



4.3 Additional Algorithm - KNN

[ ]:
```
# params = {
#     "n_neighbors": [3, 5, 7],
#     "weights": ["uniform", "distance"],
#     "algorithm": ["ball_tree", "kd_tree", "brute"],
#     "leaf_size": [10, 30, 50],
#     "p": [1, 2, 3],
# }
stratified_split = StratifiedShuffleSplit(n_splits=6, test_size=0.1,␣
 ↪random_state=42)
# gridsearch_knn = GridSearchCV(
#     KNeighborsClassifier(n_jobs=-1),
#     params,
#     cv=stratified_split,
#     n_jobs=-1,
#     verbose=3,
#     scoring=custom_calculate_f1_score
# )
# gridsearch_knn.fit(X_train, y_train)
# gridsearch_knn.best_params_

# If you uncomment the commented code above, you will get the following output
# Output - {'algorithm': 'ball_tree',
#  'leaf_size': 10,
#  'n_neighbors': 5,
#  'p': 2,
#  'weights': 'distance'}
```

[ ]:
```
knn_cv = {}
knn_cv_models = []

for i, (train_index, test_index) in enumerate(stratified_split.split(X_train,␣
 ↪y_train)):
    X_train_fold, X_val_fold = X_train.iloc[train_index], X_train.
 ↪iloc[test_index]
    y_train_fold, y_val_fold = y_train.iloc[train_index], y_train.
 ↪iloc[test_index]

    knn = KNeighborsClassifier(
        algorithm="ball_tree",
        leaf_size=10,
        n_neighbors=5,
        p=2,
        weights="distance",
        n_jobs=-1,
    )
```

```
    knn.fit(X_train_fold, y_train_fold)

    y_pred = knn.predict(X_val_fold)
    y_pred_proba = knn.predict_proba(X_val_fold)[:, 1]
    knn_cv[i + 1] = get_all_metrics(y_val_fold, y_pred)
    knn_cv[i+1]['Brier Score'] = np.mean((y_pred_proba - y_val_fold)**2)
    knn_cv[i+1]['Brier Skill Score'] = knn_cv[i+1]['Brier Score'] / (np.
 ↪mean((y_val_fold - np.mean(y_pred_proba))**2))
    knn_cv_models.append(knn)

knn_cv["mean"] = pd.DataFrame(knn_cv).mean(axis=1)
pd.DataFrame(knn_cv).round(4)
```

[ ]:

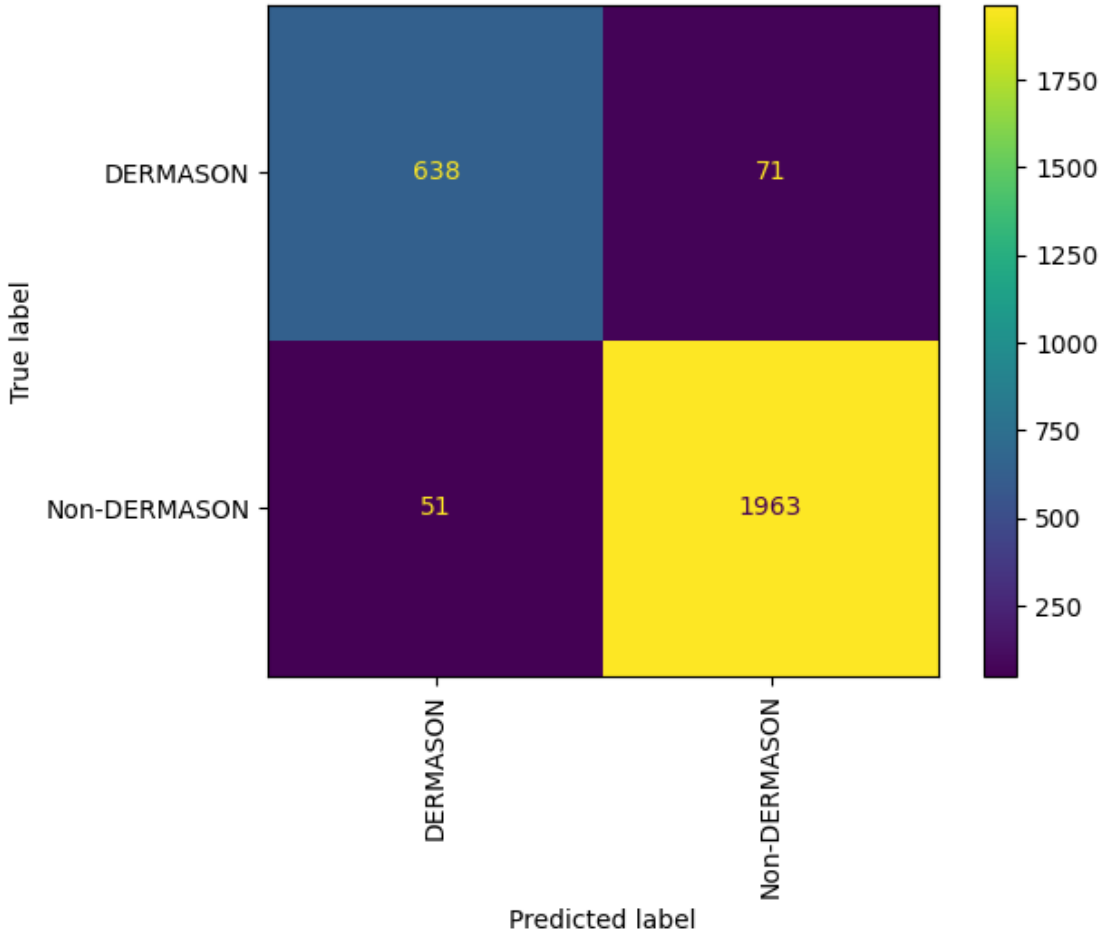
	1	2	3	4	5	\
TP	261.0000	264.0000	257.0000	255.0000	260.0000	
TN	780.0000	775.0000	783.0000	785.0000	779.0000	
FP	25.0000	30.0000	22.0000	20.0000	26.0000	
FN	23.0000	20.0000	27.0000	29.0000	24.0000	
P	284.0000	284.0000	284.0000	284.0000	284.0000	
N	805.0000	805.0000	805.0000	805.0000	805.0000	
TPR	0.9190	0.9296	0.9049	0.8979	0.9155	
TNR	0.9689	0.9627	0.9727	0.9752	0.9677	
FPR	0.0311	0.0373	0.0273	0.0248	0.0323	
FNR	0.0810	0.0704	0.0951	0.1021	0.0845	
Recall	0.9190	0.9296	0.9049	0.8979	0.9155	
Precision	0.9126	0.8980	0.9211	0.9273	0.9091	
F1 Score	0.9158	0.9135	0.9130	0.9123	0.9123	
Accuracy	0.9559	0.9541	0.9550	0.9550	0.9541	
Error Rate	0.0441	0.0459	0.0450	0.0450	0.0459	
Balanced Accuracy	0.9440	0.9462	0.9388	0.9365	0.9416	
True Skill Statistics	0.8880	0.8923	0.8776	0.8730	0.8832	
Heidke Skill Score	0.8880	0.8923	0.8776	0.8730	0.8832	
Brier Score	0.0379	0.0343	0.0335	0.0356	0.0326	
Brier Skill Score	0.1965	0.1780	0.1736	0.1844	0.1690	

	6	mean
TP	265.0000	260.3333
TN	786.0000	781.3333
FP	19.0000	23.6667
FN	19.0000	23.6667
P	284.0000	284.0000
N	805.0000	805.0000
TPR	0.9331	0.9167
TNR	0.9764	0.9706
FPR	0.0236	0.0294
FNR	0.0669	0.0833
Recall	0.9331	0.9167

```
Precision                0.9331    0.9169
F1 Score                 0.9331    0.9167
Accuracy                 0.9651    0.9565
Error Rate               0.0349    0.0435
Balanced Accuracy        0.9547    0.9436
True Skill Statistics    0.9095    0.8873
Heidke Skill Score       0.9095    0.8873
Brier Score              0.0278    0.0336
Brier Skill Score        0.1443    0.1743
```

[ ]:
```python
# Mode function returns the values that appear most frequently in the array
y_pred = stats.mode([model.predict(X_test) for model in knn_cv_models]).mode
matrix = confusion_matrix(y_test, y_pred)
ConfusionMatrixDisplay.from_predictions(
    y_test,
    y_pred,
    display_labels=encoder.inverse_transform([0, 1]),
    xticks_rotation="vertical",
)

results_comparison['KNN'] = get_all_metrics(y_test, y_pred)
results_comparison.loc["Brier Score", "KNN"] = np.mean((y_pred - y_test) ** 2)
results_comparison.loc["Brier Skill Score", "KNN"] = results_comparison["KNN"][
    "Brier Score"
] / (np.mean((y_test - np.mean(y_pred)) ** 2))
```



4.4 Additional Deep Learning Algorithm - Conv1D

[ ]:
```
device = (
    "cuda"
    if torch.cuda.is_available()
    else "mps" if torch.backends.mps.is_available() else "cpu"
)
print(f"Using {device} device for torch models")
```

```
Using mps device for torch models
```

[ ]:
```
class Conv1DNNModel(nn.Module):
    def __init__(self, *args, **kwargs) -> None:
        super().__init__(*args, **kwargs)
        self.conv1d_relu_stack = nn.Sequential(
            nn.Conv1d(in_channels=1, out_channels=128, kernel_size=3),
            nn.ReLU(),
```

```
            nn.BatchNorm1d(128),
            nn.Conv1d(in_channels=128, out_channels=64, kernel_size=3),
            nn.ReLU(),
            nn.BatchNorm1d(64),
            nn.Conv1d(in_channels=64, out_channels=32, kernel_size=3),
            nn.ReLU(),
            nn.BatchNorm1d(32),
            nn.Flatten(),
            nn.Linear(32 * 10, 64),
            nn.ReLU(),
            nn.BatchNorm1d(64),
            nn.Linear(64, 2),
            nn.Sigmoid(),
        )

    def forward(self, x):
        return self.conv1d_relu_stack(x)
```

[ ]:
```
learning_rate = 1e-2
batch_size = 64
epochs = 20

conv1d_model = Conv1DNNModel()
loss_fn = nn.BCEWithLogitsLoss()
summary(conv1d_model, input_size=(batch_size, 1, 16))
```

[ ]:
```
==========================================================================================
Layer (type:depth-idx)                   Output Shape              Param #
==========================================================================================
Conv1DNNModel                            [64, 2]                   --
 Sequential: 1-1                         [64, 2]                   --
      Conv1d: 2-1                        [64, 128, 14]             512
      ReLU: 2-2                          [64, 128, 14]             --
      BatchNorm1d: 2-3                   [64, 128, 14]             256
      Conv1d: 2-4                        [64, 64, 12]              24,640
      ReLU: 2-5                          [64, 64, 12]              --
      BatchNorm1d: 2-6                   [64, 64, 12]              128
      Conv1d: 2-7                        [64, 32, 10]              6,176
      ReLU: 2-8                          [64, 32, 10]              --
      BatchNorm1d: 2-9                   [64, 32, 10]              64
      Flatten: 2-10                      [64, 320]                 --
      Linear: 2-11                       [64, 64]                  20,544
      ReLU: 2-12                         [64, 64]                  --
      BatchNorm1d: 2-13                  [64, 64]                  128
      Linear: 2-14                       [64, 2]                   130
```

```
      Sigmoid: 2-15                          [64, 2]                   --
==========================================================================================
==========
Total params: 52,578
Trainable params: 52,578
Non-trainable params: 0
Total mult-adds (Units.MEGABYTES): 24.69
==========================================================================================
==========
Input size (MB): 0.00
Forward/backward pass size (MB): 3.02
Params size (MB): 0.21
Estimated Total Size (MB): 3.23
==========================================================================================
==========
```

[ ]:
```
y_train_one_hot = pd.get_dummies(y_train.values, dtype=np.float32)
y_test_one_hot = pd.get_dummies(y_test.values, dtype=np.float32)

test_dataset = TensorDataset(
    torch.tensor(X_test.values.reshape((-1, 1, 16)), dtype=torch.float32),
    torch.tensor(y_test.values, dtype=torch.float32),
)
```

[ ]:
```
stratified_cv_split = StratifiedShuffleSplit(n_splits=10, test_size=0.1,␣
 ↪random_state=42)

conv1d_cv = TorchKFoldCrossValidation(
    model_class=Conv1DNNModel,
    loss_fn=loss_fn,
    learning_rate=learning_rate,
    batch_size=batch_size,
    epochs=epochs,
    cv=stratified_cv_split,
    device=device
)
conv1d_cv.fit(X_train.values.reshape(-1,1,16), y_train_one_hot.values)

## Load models, it is faster than to train the model again
## If you want to train the model then comment out the below line and uncomment␣
 ↪the above code line
# conv1d_cv.load_models()
```

```
Cross validation step 1

Epoch 1
------------------------------
Model saved with F1 Score: 0.9205776173285198
```

```
Epoch 1 completed

Epoch 2
------------------------------
Epoch 2 completed

Epoch 3
------------------------------
Model saved with F1 Score: 0.9228070175438596
Epoch 3 completed

Epoch 4
------------------------------
Model saved with F1 Score: 0.924693520140105
Epoch 4 completed

Epoch 5
------------------------------
Model saved with F1 Score: 0.9261261261261261
Epoch 5 completed

Epoch 6
------------------------------
Model saved with F1 Score: 0.9311594202898551
Epoch 6 completed

Epoch 7
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Epoch 7 completed

Epoch 8
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Epoch 10
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Epoch 11 completed

Epoch 12
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Epoch 12 completed

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Epoch 18 completed

Epoch 19
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Epoch 19 completed

Epoch 20
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Epoch 20 completed

Cross validation step 2

Epoch 1
------------------------------
Model saved with F1 Score: 0.921985815602837
Epoch 1 completed

Epoch 2
------------------------------
Model saved with F1 Score: 0.9236111111111112
Epoch 2 completed

Epoch 3
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```

```
Model saved with F1 Score: 0.9249999999999999
Epoch 3 completed

Epoch 4
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Epoch 4 completed

Epoch 5
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Epoch 5 completed

Epoch 6
------------------------------
Model saved with F1 Score: 0.9384885764499121
Epoch 6 completed

Epoch 7
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Epoch 7 completed

Epoch 8
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Epoch 8 completed

Epoch 9
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Epoch 9 completed

Epoch 10
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Epoch 10 completed

Epoch 11
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Epoch 11 completed

Epoch 12
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Epoch 12 completed

Epoch 13
------------------------------
Model saved with F1 Score: 0.9390681003584229
Epoch 13 completed

Epoch 14
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Epoch 14 completed
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Epoch 15
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Epoch 15 completed

Epoch 16
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Epoch 16 completed

Epoch 17
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Epoch 17 completed

Epoch 18
------------------------------
Model saved with F1 Score: 0.9391304347826086
Epoch 18 completed

Epoch 19
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Epoch 19 completed

Epoch 20
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Epoch 20 completed

Cross validation step 3

Epoch 1
------------------------------
Model saved with F1 Score: 0.928082191780822
Epoch 1 completed

Epoch 2
------------------------------
Model saved with F1 Score: 0.93015332197615
Epoch 2 completed

Epoch 3
------------------------------
Model saved with F1 Score: 0.9397590361445785
Epoch 3 completed

Epoch 4
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Epoch 4 completed

Epoch 5
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Epoch 5 completed

Epoch 6
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Epoch 6 completed

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Epoch 9 completed

Epoch 10
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Epoch 10 completed

Epoch 11
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Epoch 11 completed

Epoch 12
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Epoch 12 completed

Epoch 13
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Model saved with F1 Score: 0.9444444444444444
Epoch 13 completed

Epoch 14
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Epoch 14 completed

Epoch 15
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Epoch 15 completed

Epoch 16
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Epoch 16 completed
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Epoch 17
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Epoch 17 completed

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Epoch 18 completed

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Epoch 19 completed

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Epoch 20 completed

Cross validation step 4

Epoch 1
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Model saved with F1 Score: 0.9184397163120568
Epoch 1 completed

Epoch 2
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Epoch 2 completed

Epoch 3
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Epoch 3 completed

Epoch 4
------------------------------
Model saved with F1 Score: 0.9273356401384083
Epoch 4 completed

Epoch 5
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Epoch 5 completed

Epoch 6
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Epoch 6 completed

Epoch 7
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Epoch 7 completed
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Epoch 8
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Epoch 8 completed

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Epoch 11 completed

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Epoch 12 completed

Epoch 13
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Epoch 13 completed

Epoch 14
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Epoch 14 completed

Epoch 15
------------------------------
Model saved with F1 Score: 0.9312169312169312
Epoch 15 completed

Epoch 16
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Epoch 16 completed

Epoch 17
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Epoch 17 completed

Epoch 18
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Epoch 18 completed

Epoch 19
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Epoch 19 completed
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Epoch 20
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Epoch 20 completed

Cross validation step 5

Epoch 1
------------------------------
Model saved with F1 Score: 0.9192982456140351
Epoch 1 completed

Epoch 2
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Epoch 2 completed

Epoch 3
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Epoch 3 completed

Epoch 4
------------------------------
Model saved with F1 Score: 0.9249999999999999
Epoch 4 completed

Epoch 5
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Epoch 5 completed

Epoch 6
------------------------------
Model saved with F1 Score: 0.9342560553633218
Epoch 6 completed

Epoch 7
------------------------------
Model saved with F1 Score: 0.9383561643835617
Epoch 7 completed

Epoch 8
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Epoch 8 completed

Epoch 9
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Epoch 9 completed

Epoch 10
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Epoch 10 completed

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Epoch 20 completed

Cross validation step 6

Epoch 1
------------------------------
Model saved with F1 Score: 0.9094138543516875
```

```
Epoch 1 completed

Epoch 2
------------------------------
Model saved with F1 Score: 0.9135802469135803
Epoch 2 completed

Epoch 3
------------------------------
Model saved with F1 Score: 0.9244288224956063
Epoch 3 completed

Epoch 4
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Epoch 4 completed

Epoch 5
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Epoch 5 completed

Epoch 6
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Epoch 6 completed

Epoch 7
------------------------------
Model saved with F1 Score: 0.9269949066213922
Epoch 7 completed

Epoch 8
------------------------------
Model saved with F1 Score: 0.9312169312169312
Epoch 8 completed

Epoch 9
------------------------------
Model saved with F1 Score: 0.9349736379613356
Epoch 9 completed

Epoch 10
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Epoch 10 completed

Epoch 11
------------------------------
Model saved with F1 Score: 0.9389179755671903
Epoch 11 completed
```

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Epoch 12
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Epoch 12 completed

Epoch 13
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Epoch 13 completed

Epoch 14
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Epoch 14 completed

Epoch 15
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Model saved with F1 Score: 0.9413793103448277
Epoch 15 completed

Epoch 16
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Epoch 16 completed

Epoch 17
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Epoch 17 completed

Epoch 18
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Epoch 18 completed

Epoch 19
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Epoch 19 completed

Epoch 20
------------------------------
Model saved with F1 Score: 0.9428076256499133
Epoch 20 completed

Cross validation step 7

Epoch 1
------------------------------
Model saved with F1 Score: 0.903448275862069
Epoch 1 completed

Epoch 2
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Epoch 2 completed
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Epoch 3
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Model saved with F1 Score: 0.9075342465753424
Epoch 3 completed

Epoch 4
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Epoch 4 completed

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Epoch 12 completed

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Epoch 13 completed

Epoch 14
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```
Model saved with F1 Score: 0.9090909090909091
Epoch 14 completed

Epoch 15
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Epoch 18 completed

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Epoch 19 completed

Epoch 20
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Epoch 20 completed

Cross validation step 8

Epoch 1
------------------------------
Model saved with F1 Score: 0.9050847457627118
Epoch 1 completed

Epoch 2
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Model saved with F1 Score: 0.9100719424460433
Epoch 2 completed

Epoch 3
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Epoch 3 completed

Epoch 4
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Model saved with F1 Score: 0.9133574007220218
Epoch 4 completed
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Epoch 5
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Epoch 5 completed

Epoch 6
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Model saved with F1 Score: 0.9184397163120568
Epoch 6 completed

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Epoch 20 completed

Cross validation step 9

Epoch 1
------------------------------
Model saved with F1 Score: 0.8816793893129771
Epoch 1 completed

Epoch 2
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Model saved with F1 Score: 0.9041591320072333
Epoch 2 completed

Epoch 3
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Epoch 3 completed

Epoch 4
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Epoch 4 completed

Epoch 5
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Epoch 5 completed

Epoch 6
------------------------------
Model saved with F1 Score: 0.9148936170212766
Epoch 6 completed

Epoch 7
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Epoch 7 completed

Epoch 8
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Epoch 8 completed

Epoch 9
------------------------------
Model saved with F1 Score: 0.9150090415913201
Epoch 9 completed

Epoch 10
------------------------------
Model saved with F1 Score: 0.9179755671902269
Epoch 10 completed

Epoch 11
------------------------------
Model saved with F1 Score: 0.9198606271777003
Epoch 11 completed

Epoch 12
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Epoch 12 completed

Epoch 13
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Epoch 13 completed

Epoch 14
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Model saved with F1 Score: 0.9270833333333333
Epoch 14 completed

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Epoch 18 completed

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Epoch 20 completed

Cross validation step 10

Epoch 1
------------------------------
Model saved with F1 Score: 0.9264957264957264
Epoch 1 completed

Epoch 2
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Model saved with F1 Score: 0.9282136894824707
Epoch 2 completed

Epoch 3
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Epoch 3 completed

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Epoch 19 completed

Epoch 20
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Epoch 20 completed
```

[ ]:

	1	2	3	4	\
TP	259	263	270	266	
TN	788	791	782	780	
FP	17	14	23	25	
FN	25	21	14	18	
P	284	284	284	284	
N	805	805	805	805	
TPR	0.911972	0.926056	0.950704	0.93662	
TNR	0.978882	0.982609	0.971429	0.968944	
FPR	0.021118	0.017391	0.028571	0.031056	
FNR	0.088028	0.073944	0.049296	0.06338	
Recall	0.911972	0.926056	0.950704	0.93662	
Precision	0.938406	0.949458	0.921502	0.914089	
F1 Score	0.925	0.937611	0.935875	0.925217	
Accuracy	0.961433	0.96786	0.966024	0.960514	
Error Rate	0.038567	0.03214	0.033976	0.039486	
Balanced Accuracy	0.945427	0.954333	0.961066	0.952782	
True Skill Statistics	0.890854	0.908665	0.922133	0.905564	
Heidke Skill Score	0.890854	0.908665	0.922133	0.905564	
Brier Score	0.03626052	0.027723107	0.032477267	0.03672747	
Brier Skill Score	0.18809225	0.14372244	0.1678883	0.19019704	

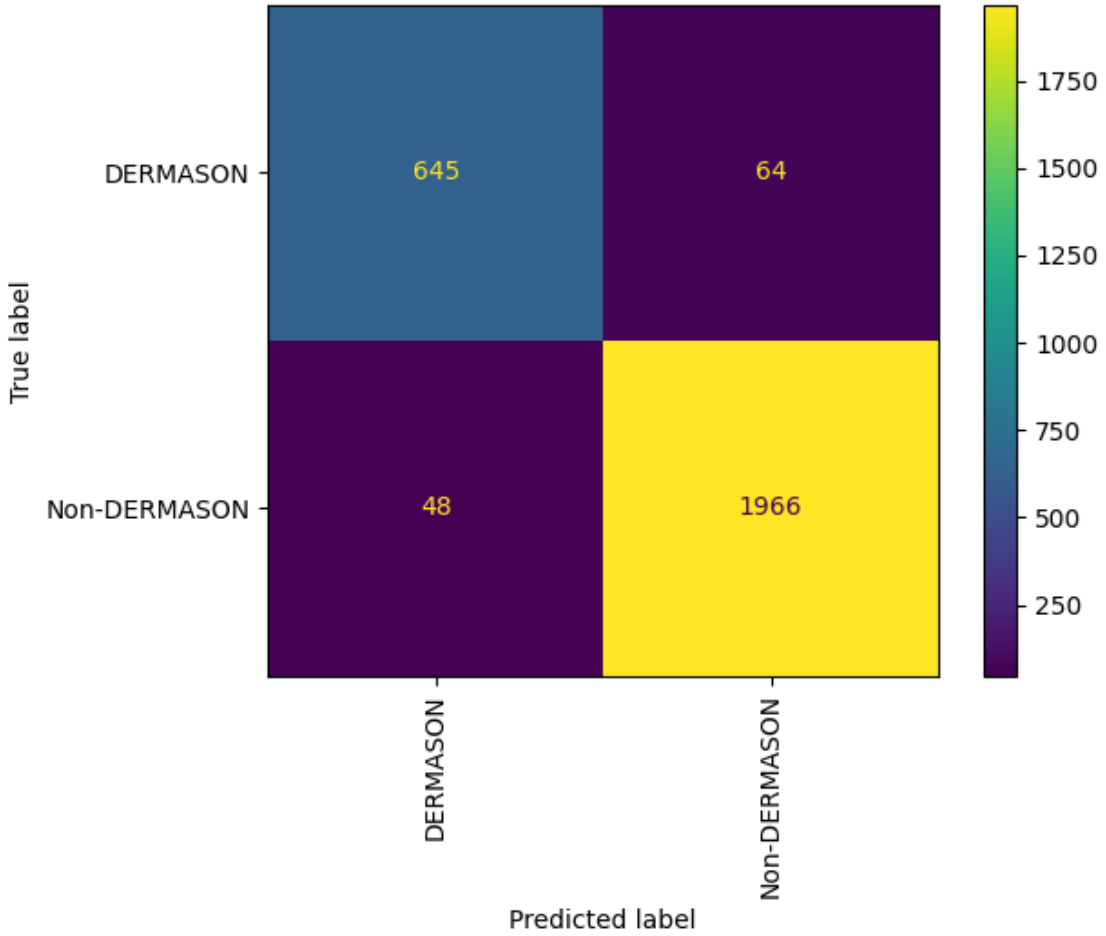
	5	6	7	8	\
TP	267	272	261	258	
TN	784	784	774	781	
FP	21	21	31	24	
FN	17	12	23	26	
P	284	284	284	284	
N	805	805	805	805	
TPR	0.940141	0.957746	0.919014	0.908451	
TNR	0.973913	0.973913	0.961491	0.970186	
FPR	0.026087	0.026087	0.038509	0.029814	
FNR	0.059859	0.042254	0.080986	0.091549	
Recall	0.940141	0.957746	0.919014	0.908451	
Precision	0.927083	0.928328	0.893836	0.914894	
F1 Score	0.933566	0.942808	0.90625	0.911661	
Accuracy	0.965106	0.969697	0.950413	0.954086	
Error Rate	0.034894	0.030303	0.049587	0.045914	
Balanced Accuracy	0.957027	0.96583	0.940252	0.939319	
True Skill Statistics	0.914054	0.93166	0.880505	0.878637	
Heidke Skill Score	0.914054	0.93166	0.880505	0.878637	
Brier Score	0.030710528	0.032167133	0.047392946	0.0379227	
Brier Skill Score	0.15915726	0.16652358	0.24557215	0.19665918	

	9	10	mean
TP	261	265	264.2
TN	782	776	782.2

FP	23	29	22.8
FN	23	19	19.8
P	284	284	284.0
N	805	805	805.0
TPR	0.919014	0.933099	0.930282
TNR	0.971429	0.963975	0.971677
FPR	0.028571	0.036025	0.028323
FNR	0.080986	0.066901	0.069718
Recall	0.919014	0.933099	0.930282
Precision	0.919014	0.901361	0.920797
F1 Score	0.919014	0.916955	0.925396
Accuracy	0.957759	0.955923	0.960882
Error Rate	0.042241	0.044077	0.039118
Balanced Accuracy	0.945221	0.948537	0.950979
True Skill Statistics	0.890443	0.897074	0.901959
Heidke Skill Score	0.890443	0.897074	0.901959
Brier Score	0.034135036	0.039550167	0.035507
Brier Skill Score	0.1769855	0.20468687	0.183948

[ ]:
```
y_pred = conv1d_cv.predict(test_dataset.tensors[0]).argmax(axis=1)
matrix = confusion_matrix(y_test, y_pred)
ConfusionMatrixDisplay.from_predictions(
    y_test,
    y_pred,
    display_labels=encoder.inverse_transform([0, 1]),
    xticks_rotation="vertical",
)

results_comparison["Conv1D-NN"] = get_all_metrics(y_test, y_pred)
results_comparison.loc["Brier Score", "Conv1D-NN"] = np.mean((y_pred - y_test)␣
 ↪** 2)
results_comparison.loc["Brier Skill Score", "Conv1D-NN"] =␣
 ↪results_comparison["Conv1D-NN"][
    "Brier Score"
] / (np.mean((y_test - np.mean(y_pred)) ** 2))
```



5 Results

[ ]:
```
# Result comparison on the test dataset for all the models
results_comparison.round(4)
```

[ ]:

	RandomForest	SVM	KNN	Conv1D-NN
TP	637.0000	649.0000	638.0000	645.0000
TN	1961.0000	1963.0000	1963.0000	1966.0000
FP	53.0000	51.0000	51.0000	48.0000
FN	72.0000	60.0000	71.0000	64.0000
P	709.0000	709.0000	709.0000	709.0000
N	2014.0000	2014.0000	2014.0000	2014.0000
TPR	0.8984	0.9154	0.8999	0.9097
TNR	0.9737	0.9747	0.9747	0.9762
FPR	0.0263	0.0253	0.0253	0.0238
FNR	0.1016	0.0846	0.1001	0.0903

Recall	0.8984	0.9154	0.8999	0.9097
Precision	0.9232	0.9271	0.9260	0.9307
F1 Score	0.9107	0.9212	0.9127	0.9201
Accuracy	0.9541	0.9592	0.9552	0.9589
Error Rate	0.0459	0.0408	0.0448	0.0411
Balanced Accuracy	0.9361	0.9450	0.9373	0.9429
True Skill Statistics	0.8721	0.8901	0.8745	0.8859
Heidke Skill Score	0.8721	0.8901	0.8745	0.8859
Brier Score	0.0459	0.0408	0.0448	0.0411
Brier Skill Score	0.2383	0.2117	0.2326	0.2135