CARDEC Trial (Global) - Machine Learning Prediction Models

```
# Install required packages
!pip install scikit-learn numpy pandas scipy \
joblib threadpoolctl cython \
imbalanced-learn xgboost catboost \
keras tensorflow focal-loss shap \
matplotlib seaborn
```

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```

```
# Import necessary libraries
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.model_selection import train_test_split, StratifiedKFold, GridSear
from sklearn.impute import SimpleImputer
from sklearn.preprocessing import StandardScaler
from sklearn.tree import DecisionTreeClassifier
from sklearn.ensemble import RandomForestClassifier
from sklearn.metrics import accuracy_score, precision_score, recall_score, f1_s
from sklearn.pipeline import Pipeline
import xgboost as xgb
import catboost as cb
import tensorflow as tf
from tensorflow.keras.models import Sequential
from tensorflow.keras.layers import Dense, Dropout, BatchNormalization
from tensorflow.keras.callbacks import EarlyStopping, ReduceLROnPlateau
from tensorflow.keras.regularizers import l2
from keras import backend as K
import warnings
warnings.filterwarnings('ignore')

# Set random seed for reproducibility
np.random.seed(42)
tf.random.set_seed(42)

# Set style for plots
plt.style.use('default')
sns.set_palette("husl")
```

Data Loading and Preprocessing

Patient-level train-test split (80:20) - CARDEC methodology

```
# Load the data from Excel file
data = pd.read_excel('2024_corrected_global_CARDEC_3_ML_Vitor.xlsx')

print(f"Dataset shape: {data.shape}")
print(f"Target distribution: {data['Failure'].value_counts()}")
print(f"Failure rate: {data['Failure'].mean():.1%}")
```

```
Dataset shape: (637, 17)
Target distribution: Failure
0    326
1    311
Name: count, dtype: int64
Failure rate: 48.8%
```

```
# Patient-level train-test split (80:20 as per CARDEC methodology)
# Ensures no patient data leakage between train and test sets
unique_n_part = data['IDpac'].unique()
train_n_part, test_n_part = train_test_split(unique_n_part, test_size=0.2, ranc

train_data = data[data['IDpac'].isin(train_n_part)]
test_data = data[data['IDpac'].isin(test_n_part)]

# Separate features and target variable
X_train = train_data.drop(['Failure', 'IDrest', 'IDpac'], axis=1)
y_train = train_data['Failure']
X_test = test_data.drop(['Failure', 'IDrest', 'IDpac'], axis=1)
y_test = test_data['Failure']

print(f"Training set: {len(X_train)} samples, {y_train.sum()} failures ({y_trai
print(f"Test set: {len(X_test)} samples, {y_test.sum()} failures ({y_test.mean(
print(f"Split ratio: {len(X_train)/(len(X_train)+len(X_test)):.1%}:{len(X_test)
```

```
Training set: 507 samples, 251 failures (49.5%)
Test set: 130 samples, 60 failures (46.2%)
Split ratio: 79.6%:20.4%
```

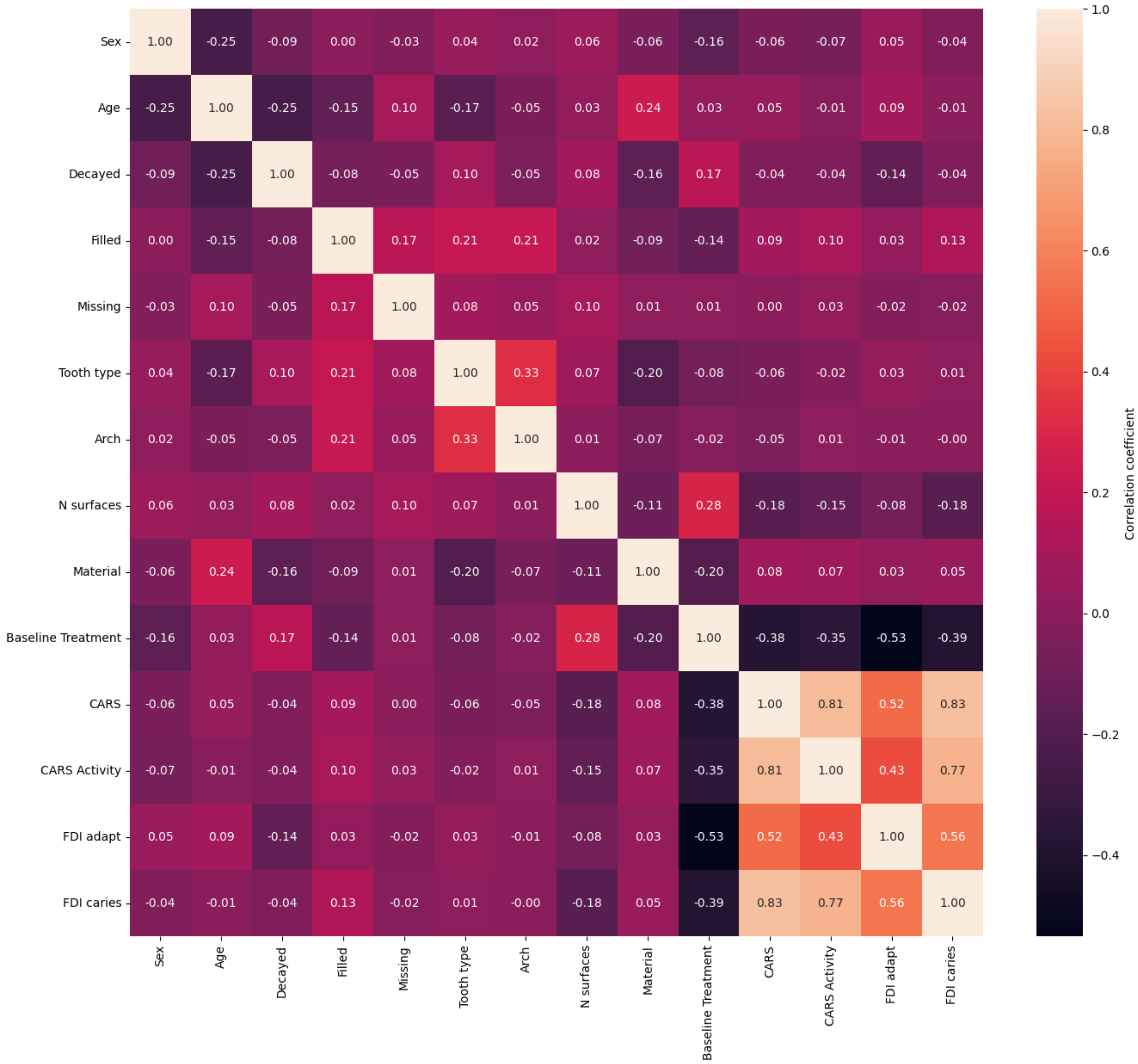
```
import seaborn as sns
import matplotlib.pyplot as plt

# Calculate the correlation matrix of the training data.
# The correlation matrix quantifies the linear relationships between the variat
corr_matrix = X_train.corr()

# Initialize a matplotlib figure with a specified size (width=16 inches, height
# This size is chosen to make the heatmap large enough to be easily readable.
plt.figure(figsize=(16, 14))
```

```
# Draw the heatmap using seaborn to visualize the correlation matrix.
sns.heatmap(corr_matrix, annot=True, annot_kws={"size": 10}, fmt=".2f", cbar_kw

# Display the plot on the screen. This command is necessary to show the figure
plt.show()
```



```
import pandas as pd

# Define lists for each type of variable in the dataset: numeric, binary, and or
numeric_vars = ['Age', 'Decayed', 'Filled', 'Missing']
binary_vars = ['Sex', 'Tooth type', 'Arch', 'Failure', 'CARS Activity']
categorical_vars = ['N surfaces', 'Material', 'Baseline Treatment', 'CARS', 'FDI

def descriptive_statistics(train_data, test_data):
    # Print a heading for the descriptive statistics of numeric variables.
    print("Descriptive Statistics for Numeric Variables:")
    # Display descriptive statistics (like count, mean, std, min, max, etc.) for
    print("\nTraining Set:")
    print(train_data[numeric_vars].describe())
    # Repeat the process for the test set.
    print("\nTest Set:")
    print(test_data[numeric_vars].describe())

    # Initialize an empty dictionary to store statistics for binary and ordinal
    stats = {}
    # Loop through each variable in the binary and ordinal lists to calculate th
    for var in binary_vars + categorical_vars:
        stats[var] = {
            "Training Set": {
                "Count": train_data[var].value_counts().to_dict(),  # Count occu
                "Percentage": (train_data[var].value_counts(normalize=True) * 10
            },
            "Test Set": {
                "Count": test_data[var].value_counts().to_dict(),  # Count occur
                "Percentage": (test_data[var].value_counts(normalize=True) * 100
            }
        }

    # Loop through the stats dictionary to print the statistics for each categor
    for var, data in stats.items():
        print(f"\n{var} Statistics:")  # Print the variable name.
        for dataset, values in data.items():
            print(f"\n{dataset}:")  # Print which dataset (training or test) the
            for metric, metric_values in values.items():
                print(f"{metric}: {metric_values}")  # Print the count and perce
```

```
# Call the function with the training and test datasets as arguments to display
descriptive_statistics(train_data, test_data)
```

```
N surfaces Statistics:

Training Set:
Count: {1: 207, 2: 139, 3: 72, 4: 60, 5: 29}
Percentage: {1: 40.828402366863905, 2: 27.416173570019726, 3: 14.20118343

Test Set:
Count: {1: 56, 2: 27, 3: 20, 4: 14, 5: 13}
Percentage: {1: 43.07692307692308, 2: 20.76923076923077, 3: 15.384615384

Material Statistics:

Training Set:
Count: {1: 304, 0: 189, 2: 14}
Percentage: {1: 59.96055226824457, 0: 37.278106508875744, 2: 2.761341222

Test Set:
Count: {1: 74, 0: 51, 2: 5}
Percentage: {1: 56.92307692307692, 0: 39.23076923076923, 2: 3.846153846

Baseline Treatment Statistics:

Training Set:
Count: {0: 292, 1: 167, 2: 48}
Percentage: {0: 57.59368836291914, 1: 32.938856015779095, 2: 9.467455621

Test Set:
Count: {0: 75, 1: 34, 2: 21}
Percentage: {0: 57.692307692307686, 1: 26.153846153846157, 2: 16.1538461

CARS Statistics:

Training Set:
Count: {0: 399, 2: 62, 1: 46}
Percentage: {0: 78.69822485207101, 2: 12.22879684418146, 1: 9.072978303

Test Set:
Count: {0: 99, 2: 20, 1: 11}
Percentage: {0: 76.15384615384615, 2: 15.384615384615385, 1: 8.461538461

FDI adapt Statistics:

Training Set:
Count: {0: 333, 1: 155, 2: 19}
Percentage: {0: 65.68047337278107, 1: 30.57199211045365, 2: 3.747534516

Test Set:
Count: {0: 82, 1: 43, 2: 5}
```

```
Percentage: {0: 63.07692307692307, 1: 33.07692307692307, 2: 3.84615384615З

FDI caries Statistics:

Training Set:
Count: {0: 401, 1: 98, 2: 8}
Percentage: {0: 79.09270216962526, 1: 19.32938856015779, 2: 1.57790927021

Test Set:
Count: {0: 97, 1: 30, 2: 3}
```

```
# Data preprocessing
from sklearn.impute import SimpleImputer
from sklearn.preprocessing import StandardScaler
import pandas as pd

# Display basic info about the dataset
print("Dataset columns:", X_train.columns.tolist())
print("\nData types:")
print(X_train.dtypes)
print("\nMissing values:")
print(X_train.isnull().sum())

# Handle missing values if any
if X_train.isnull().sum().sum() > 0:
    # Impute missing values
    numeric_columns = X_train.select_dtypes(include=[np.number]).columns
    categorical_columns = X_train.select_dtypes(exclude=[np.number]).columns

    if len(numeric_columns) > 0:
        imputer_num = SimpleImputer(strategy='median')
        X_train[numeric_columns] = imputer_num.fit_transform(X_train[numeric_cc
        X_test[numeric_columns] = imputer_num.transform(X_test[numeric_columns]

    if len(categorical_columns) > 0:
        imputer_cat = SimpleImputer(strategy='most_frequent')
        X_train[categorical_columns] = imputer_cat.fit_transform(X_train[catego
        X_test[categorical_columns] = imputer_cat.transform(X_test[categorical_

# Scale numerical features if needed
numeric_columns = X_train.select_dtypes(include=[np.number]).columns
if len(numeric_columns) > 0:
    scaler = StandardScaler()
    X_train[numeric_columns] = scaler.fit_transform(X_train[numeric_columns])
    X_test[numeric_columns] = scaler.transform(X_test[numeric_columns])

# Final data check
X_train = X_train.fillna(0)
```

```
X_test = X_test.fillna(0)

print(f"\nFinal feature shape: {X_train.shape}")
print(f"NaN check - Train: {X_train.isnull().sum().sum()}, Test: {X_test.isnull
print(f"Feature names: {list(X_train.columns)}")
```

```
Dataset columns: ['Sex', 'Age', 'Decayed', 'Filled', 'Missing', 'Tooth type

Data types:
Sex                    int64
Age                  float64
Decayed                int64
Filled                 int64
Missing                int64
Tooth type             int64
Arch                   int64
N surfaces             int64
Material               int64
Baseline Treatment     int64
CARS                   int64
CARS Activity          int64
FDI adapt              int64
FDI caries             int64
dtype: object

Missing values:
Sex                  0
Age                  0
Decayed              0
Filled               0
Missing              0
Tooth type           0
Arch                 0
N surfaces           0
Material             0
Baseline Treatment   0
CARS                 0
CARS Activity        0
FDI adapt            0
FDI caries           0
dtype: int64

Final feature shape: (507, 14)
NaN check - Train: 0, Test: 0
Feature names: ['Sex', 'Age', 'Decayed', 'Filled', 'Missing', 'Tooth type',
```

Utility Functions

Consistent threshold optimization and model evaluation

```
# Optimal threshold selection based on F1-score maximization
import numpy as np
from sklearn.metrics import (
    f1_score, accuracy_score, precision_score, recall_score,
    roc_auc_score
)
from sklearn.model_selection import StratifiedKFold, GridSearchCV

def find_optimal_threshold(y_true, y_proba):
    """Find optimal threshold based on F1-score maximization."""
    thresholds = np.arange(0.1, 1.01, 0.05)
    best_f1 = 0
    best_threshold = 0.5

    for threshold in thresholds:
        y_pred = (y_proba >= threshold).astype(int)
        f1 = f1_score(y_true, y_pred, zero_division=0)
        if f1 > best_f1:
            best_f1 = f1
            best_threshold = threshold

    return best_threshold


def evaluate_model_with_seeds(pipeline, param_grid, X_train, y_train, X_test, y
    """Evaluate model with multiple seeds for robustness."""
    seeds = [40, 41, 42, 43, 44, 45, 46, 47, 48, 49]
    all_results = []
    all_predictions = []  # Store all predictions for averaging

    print(f"\nTraining {model_name} with {n_seeds} seeds...")

    for i, seed in enumerate(seeds[:n_seeds]):
        print(f"  Seed {i+1}/{n_seeds}: {seed}")

        # Set random states
        np.random.seed(seed)

        # Update pipeline random states
        if hasattr(pipeline.named_steps['classifier'], 'random_state'):
            pipeline.set_params(**{f'classifier__random_state': seed})
```

```
        # Cross-validation setup
        cv = StratifiedKFold(n_splits=5, shuffle=True, random_state=seed)

        # Grid search with cross-validation
        grid_search = GridSearchCV(
            pipeline, param_grid, cv=cv, scoring='f1', n_jobs=-1, verbose=0
        )

        # Fit model
        grid_search.fit(X_train, y_train)

        # Get predictions
        y_pred_proba = grid_search.predict_proba(X_test)[:, 1]
        all_predictions.append(y_pred_proba)  # Store for averaging

        # Find optimal threshold
        optimal_threshold = find_optimal_threshold(y_test, y_pred_proba)
        y_pred = (y_pred_proba >= optimal_threshold).astype(int)

        # Calculate metrics
        seed_results = {
            'seed': seed,
            'accuracy': accuracy_score(y_test, y_pred),
            'precision': precision_score(y_test, y_pred, zero_division=0),
            'recall': recall_score(y_test, y_pred, zero_division=0),
            'f1': f1_score(y_test, y_pred, zero_division=0),
            'auc': roc_auc_score(y_test, y_pred_proba),
            'threshold': optimal_threshold,
            'cv_score': grid_search.best_score_,
            'best_params': grid_search.best_params_,
            'model': grid_search.best_estimator_,
            'y_pred_proba': y_pred_proba
        }

        all_results.append(seed_results)

    # Calculate averaged predictions across all seeds
    avg_predictions = np.mean(all_predictions, axis=0)

    # Calculate statistics across seeds
    metrics = ['accuracy', 'precision', 'recall', 'f1', 'auc', 'threshold', 'cv
    final_results = {}

    for metric in metrics:
        values = [r[metric] for r in all_results]
        final_results[f'{metric}_mean'] = np.mean(values)
        final_results[f'{metric}_std'] = np.std(values)
```

```
    # Best individual result (for SHAP analysis)
    best_result = max(all_results, key=lambda x: x['auc'])
    final_results['best_model'] = best_result['model']
    final_results['best_params'] = best_result['best_params']

    # Use averaged predictions for consistent reporting
    final_results['avg_predictions'] = avg_predictions
    final_results['all_results'] = all_results

    return final_results, all_results


def display_model_summary(results, model_name):
    """Display comprehensive model summary with consistent metrics."""
    print(f"\n{'='*60}")
    print(f"{model_name.upper()} RESULTS SUMMARY (10 Seeds)")
    print(f"{'='*60}")

    # Display mean ± std for all metrics
    if 'cv_score_mean' in results:
        print(f"Mean CV F1 Score: {results['cv_score_mean']:.4f} ± {results['cv
        print(f"Mean Test AUC: {results['auc_mean']:.4f} ± {results['auc_std']:
        print(f"Mean Test F1: {results['f1_mean']:.4f} ± {results['f1_std']:.4f
        print(f"Mean Test Accuracy: {results['accuracy_mean']:.4f} ± {results['
        print(f"Mean Test Precision: {results['precision_mean']:.4f} ± {results
        print(f"Mean Test Recall: {results['recall_mean']:.4f} ± {results['reca
        print(f"Mean Optimal Threshold: {results['threshold_mean']:.4f} ± {resu

    if 'best_params' in results:
        print(f"Best Parameters: {results['best_params']}")

    # Show threshold evaluation using AVERAGED predictions
    print(f"\nThreshold evaluation using averaged predictions across 10 seeds:"
    avg_predictions = results['avg_predictions']

    # Calculate AUC with averaged predictions
    avg_auc = roc_auc_score(y_test, avg_predictions)
    print(f"AUC with averaged predictions: {avg_auc:.4f}")

    # Find optimal threshold with averaged predictions
    optimal_threshold = find_optimal_threshold(y_test, avg_predictions)
    y_pred_optimal = (avg_predictions >= optimal_threshold).astype(int)

    # Calculate metrics with optimal threshold
    optimal_accuracy = accuracy_score(y_test, y_pred_optimal)
    optimal_precision = precision_score(y_test, y_pred_optimal, zero_division=0
    optimal_recall = recall_score(y_test, y_pred_optimal, zero_division=0)
```

```
    optimal_f1 = f1_score(y_test, y_pred_optimal, zero_division=0)

    print(f"Optimal threshold: {optimal_threshold:.3f}")
    print(f"Performance at optimal threshold:")
    print(f"  Accuracy: {optimal_accuracy:.4f}")
    print(f"  Precision: {optimal_precision:.4f}")
    print(f"  Recall: {optimal_recall:.4f}")
    print(f"  F1-Score: {optimal_f1:.4f}")

    return avg_predictions
```

Decision Tree Model

Parameter grid optimization with CARDEC hyperparameters

```
# Decision Tree with CARDEC-specific parameter grid
print("Training Decision Tree...")

# Create pipeline
dt_pipeline = Pipeline([
    ('classifier', DecisionTreeClassifier())
])

# CARDEC-specific parameter grid
dt_param_grid = {
    'classifier__max_depth': [5, 10, 15, 20, None],
    'classifier__criterion': ['gini', 'entropy'],
    'classifier__min_samples_split': [2, 5, 10],
    'classifier__min_samples_leaf': [1, 2, 4]
}

print(f"Parameter combinations: {np.prod([len(v) for v in dt_param_grid.values(

# Evaluate with multiple seeds
dt_results, dt_detailed = evaluate_model_with_seeds(
    dt_pipeline, dt_param_grid, X_train, y_train, X_test, y_test, 'Decision Tre
)

# Display results
dt_avg_predictions = display_model_summary(dt_results, 'Decision Tree')
```

```
Training Decision Tree...
Parameter combinations: 90

Training Decision Tree with 10 seeds...
  Seed 1/10: 40
  Seed 2/10: 41
  Seed 3/10: 42
  Seed 4/10: 43
  Seed 5/10: 44
  Seed 6/10: 45
  Seed 7/10: 46
  Seed 8/10: 47
  Seed 9/10: 48
  Seed 10/10: 49

============================================================
DECISION TREE RESULTS SUMMARY (10 Seeds)
============================================================
Mean CV F1 Score: 0.6524 ± 0.0165
Mean Test AUC: 0.6701 ± 0.0094
Mean Test F1: 0.6623 ± 0.0063
Mean Test Accuracy: 0.6085 ± 0.0276
Mean Test Precision: 0.5526 ± 0.0232
Mean Test Recall: 0.8317 ± 0.0540
Mean Optimal Threshold: 0.3550 ± 0.0350
Best Parameters: {'classifier__criterion': 'gini', 'classifier__max_depth':

Threshold evaluation using averaged predictions across 10 seeds:
AUC with averaged predictions: 0.7064
Optimal threshold: 0.250
Performance at optimal threshold:
  Accuracy: 0.5308
  Precision: 0.4957
  Recall: 0.9667
  F1-Score: 0.6554
```

Random Forest Model

Parameter grid optimization with CARDEC hyperparameters

```
# Random Forest with CARDEC-specific parameter grid
print("Training Random Forest...")

# Create pipeline
rf_pipeline = Pipeline([
    ('classifier', RandomForestClassifier())
])
```

```
# CARDEC-specific parameter grid
rf_param_grid = {
    'classifier__n_estimators': [100, 200, 300],
    'classifier__max_depth': [5, 10, 15],
    'classifier__min_samples_split': [2, 5, 10],
    'classifier__min_samples_leaf': [1, 2, 4]
}

print(f"Parameter combinations: {np.prod([len(v) for v in rf_param_grid.values(

# Evaluate with multiple seeds
rf_results, rf_detailed = evaluate_model_with_seeds(
    rf_pipeline, rf_param_grid, X_train, y_train, X_test, y_test, 'Random Fores
)

# Display results
rf_avg_predictions = display_model_summary(rf_results, 'Random Forest')
```

```
Training Random Forest...
Parameter combinations: 81

Training Random Forest with 10 seeds...
  Seed 1/10: 40
  Seed 2/10: 41
  Seed 3/10: 42
  Seed 4/10: 43
  Seed 5/10: 44
  Seed 6/10: 45
  Seed 7/10: 46
  Seed 8/10: 47
  Seed 9/10: 48
  Seed 10/10: 49

============================================================
RANDOM FOREST RESULTS SUMMARY (10 Seeds)
============================================================
Mean CV F1 Score: 0.6703 ± 0.0144
Mean Test AUC: 0.7551 ± 0.0056
Mean Test F1: 0.7152 ± 0.0115
Mean Test Accuracy: 0.6846 ± 0.0349
Mean Test Precision: 0.6186 ± 0.0391
Mean Test Recall: 0.8550 ± 0.0533
Mean Optimal Threshold: 0.4700 ± 0.0400
Best Parameters: {'classifier__max_depth': 5, 'classifier__min_samples_leaf

Threshold evaluation using averaged predictions across 10 seeds:
AUC with averaged predictions: 0.7590
Optimal threshold: 0.500
Performance at optimal threshold:
  Accuracy: 0.7154
  Precision: 0.6575
  Recall: 0.8000
  F1-Score: 0.7218
```

XGBoost Model

Parameter grid optimization with CARDEC hyperparameters

```
# XGBoost with CARDEC-specific parameter grid
print("Training XGBoost...")

# Create pipeline
xgb_pipeline = Pipeline([
    ('classifier', xgb.XGBClassifier(eval_metric='logloss'))
])
```

```
# CARDEC-specific parameter grid
xgb_param_grid = {
    'classifier__n_estimators': [100, 200, 300],
    'classifier__max_depth': [3, 6, 9],
    'classifier__learning_rate': [0.01, 0.1, 0.2],
    'classifier__subsample': [0.8, 0.9, 1.0]
}

print(f"Parameter combinations: {np.prod([len(v) for v in xgb_param_grid.values

# Evaluate with multiple seeds
xgb_results, xgb_detailed = evaluate_model_with_seeds(
    xgb_pipeline, xgb_param_grid, X_train, y_train, X_test, y_test, 'XGBoost',
)

# Display results
xgb_avg_predictions = display_model_summary(xgb_results, 'XGBoost')
```

```
Training XGBoost...
Parameter combinations: 81

Training XGBoost with 10 seeds...
  Seed 1/10: 40
  Seed 2/10: 41
  Seed 3/10: 42
  Seed 4/10: 43
  Seed 5/10: 44
  Seed 6/10: 45
  Seed 7/10: 46
  Seed 8/10: 47
  Seed 9/10: 48
  Seed 10/10: 49

============================================================
XGBOOST RESULTS SUMMARY (10 Seeds)
============================================================
Mean CV F1 Score: 0.6747 ± 0.0103
Mean Test AUC: 0.7374 ± 0.0207
Mean Test F1: 0.7156 ± 0.0066
Mean Test Accuracy: 0.6869 ± 0.0129
Mean Test Precision: 0.6168 ± 0.0152
Mean Test Recall: 0.8533 ± 0.0233
Mean Optimal Threshold: 0.4950 ± 0.0150
Best Parameters: {'classifier__learning_rate': 0.01, 'classifier__max_depth

Threshold evaluation using averaged predictions across 10 seeds:
AUC with averaged predictions: 0.7440
Optimal threshold: 0.500
Performance at optimal threshold:
  Accuracy: 0.7000
  Precision: 0.6296
  Recall: 0.8500
  F1-Score: 0.7234
```

Neural Network Model

Custom implementation with CARDEC hyperparameters

```
# Neural Network with CARDEC-specific architecture
print("Training Neural Network...")

def create_nn_model(input_dim, hidden_units=64, dropout_rate=0.3, l2_reg=0.01):
    """Create neural network model with CARDEC specifications."""
    model = Sequential([
        Dense(hidden_units, activation='relu', input_dim=input_dim,
              kernel_regularizer=l2(l2_reg)),
```

```
        BatchNormalization(),
        Dropout(dropout_rate),
        Dense(hidden_units//2, activation='relu',
              kernel_regularizer=l2(l2_reg)),
        BatchNormalization(),
        Dropout(dropout_rate),
        Dense(1, activation='sigmoid')
    ])

    model.compile(
        optimizer='adam',
        loss='binary_crossentropy',
        metrics=['accuracy']
    )

    return model

def evaluate_nn_with_seeds(X_train, y_train, X_test, y_test, n_seeds=10):
    """Evaluate Neural Network with multiple seeds."""
    seeds = [40, 41, 42, 43, 44, 45, 46, 47, 48, 49]
    all_results = []
    all_predictions = []

    for i, seed in enumerate(seeds[:n_seeds]):
        print(f"  Seed {i+1}/{n_seeds}: {seed}")

        # Set random seeds
        np.random.seed(seed)
        tf.random.set_seed(seed)

        # Create and train model
        model = create_nn_model(X_train.shape[1])

        # Callbacks
        early_stopping = EarlyStopping(monitor='val_loss', patience=10, restore_
        reduce_lr = ReduceLROnPlateau(monitor='val_loss', factor=0.2, patience=5

        # Train model
        history = model.fit(
            X_train, y_train,
            epochs=100,
            batch_size=32,
            validation_split=0.2,
            callbacks=[early_stopping, reduce_lr],
            verbose=0
        )

        # Get predictions
```

```
        y_pred_proba = model.predict(X_test, verbose=0).ravel()
        all_predictions.append(y_pred_proba)

        # Find optimal threshold
        optimal_threshold = find_optimal_threshold(y_test, y_pred_proba)
        y_pred = (y_pred_proba >= optimal_threshold).astype(int)

        # Calculate metrics
        seed_results = {
            'seed': seed,
            'accuracy': accuracy_score(y_test, y_pred),
            'precision': precision_score(y_test, y_pred, zero_division=0),
            'recall': recall_score(y_test, y_pred, zero_division=0),
            'f1': f1_score(y_test, y_pred, zero_division=0),
            'auc': roc_auc_score(y_test, y_pred_proba),
            'threshold': optimal_threshold,
            'model': model,
            'y_pred_proba': y_pred_proba
        }

        all_results.append(seed_results)

    # Calculate averaged predictions
    avg_predictions = np.mean(all_predictions, axis=0)

    # Calculate statistics
    metrics = ['accuracy', 'precision', 'recall', 'f1', 'auc', 'threshold']
    final_results = {}

    for metric in metrics:
        values = [r[metric] for r in all_results]
        final_results[f'{metric}_mean'] = np.mean(values)
        final_results[f'{metric}_std'] = np.std(values)

    # Best individual result
    best_result = max(all_results, key=lambda x: x['auc'])
    final_results['best_model'] = best_result['model']
    final_results['avg_predictions'] = avg_predictions
    final_results['all_results'] = all_results

    return final_results, all_results

# Evaluate Neural Network
nn_results, nn_detailed = evaluate_nn_with_seeds(X_train, y_train, X_test, y_tes

# Display results
def display_nn_summary(results, model_name):
    """Display Neural Network summary."""
    print(f"\n{'='*60}")
```

```
    print(f"\n{'='*60}")
    print(f"{model_name.upper()} RESULTS SUMMARY (10 Seeds)")
    print(f"{'='*60}")

    print(f"Mean Test AUC: {results['auc_mean']:.4f} ± {results['auc_std']:.4f}"
    print(f"Mean Test F1: {results['f1_mean']:.4f} ± {results['f1_std']:.4f}")
    print(f"Mean Test Accuracy: {results['accuracy_mean']:.4f} ± {results['accur
    print(f"Mean Test Precision: {results['precision_mean']:.4f} ± {results['pre
    print(f"Mean Test Recall: {results['recall_mean']:.4f} ± {results['recall_st
    print(f"Mean Optimal Threshold: {results['threshold_mean']:.4f} ± {results['

    # Show threshold evaluation using AVERAGED predictions
    print(f"\nThreshold evaluation using averaged predictions across 10 seeds:")
    avg_predictions = results['avg_predictions']

    # Calculate AUC with averaged predictions
    avg_auc = roc_auc_score(y_test, avg_predictions)
    print(f"AUC with averaged predictions: {avg_auc:.4f}")

    # Find optimal threshold with averaged predictions
    optimal_threshold = find_optimal_threshold(y_test, avg_predictions)
    y_pred_optimal = (avg_predictions >= optimal_threshold).astype(int)

    # Calculate metrics with optimal threshold
    optimal_accuracy = accuracy_score(y_test, y_pred_optimal)
    optimal_precision = precision_score(y_test, y_pred_optimal, zero_division=0)
    optimal_recall = recall_score(y_test, y_pred_optimal, zero_division=0)
    optimal_f1 = f1_score(y_test, y_pred_optimal, zero_division=0)

    print(f"Optimal threshold: {optimal_threshold:.3f}")
    print(f"Performance at optimal threshold:")
    print(f"  Accuracy: {optimal_accuracy:.4f}")
    print(f"  Precision: {optimal_precision:.4f}")
    print(f"  Recall: {optimal_recall:.4f}")
    print(f"  F1-Score: {optimal_f1:.4f}")

    return avg_predictions

nn_avg_predictions = display_nn_summary(nn_results, 'Neural Network')
```

```
Training Neural Network...
  Seed 1/10: 40
  Seed 2/10: 41
  Seed 3/10: 42
WARNING:tensorflow:5 out of the last 11 calls to <function TensorFlowTrainer
WARNING:tensorflow:5 out of the last 11 calls to <function TensorFlowTrainer
  Seed 4/10: 43
  Seed 5/10: 44
  Seed 6/10: 45
  Seed 7/10: 46
  Seed 8/10: 47
  Seed 9/10: 48
  Seed 10/10: 49

============================================================
NEURAL NETWORK RESULTS SUMMARY (10 Seeds)
============================================================
Mean Test AUC: 0.7453 ± 0.0256
Mean Test F1: 0.7158 ± 0.0282
Mean Test Accuracy: 0.6731 ± 0.0550
Mean Test Precision: 0.6048 ± 0.0497
Mean Test Recall: 0.8850 ± 0.0497
Mean Optimal Threshold: 0.3400 ± 0.0860

Threshold evaluation using averaged predictions across 10 seeds:
AUC with averaged predictions: 0.7633
Optimal threshold: 0.350
Performance at optimal threshold:
  Accuracy: 0.6692
  Precision: 0.5934
  Recall: 0.9000
  F1-Score: 0.7152
```

CatBoost Model

Parameter grid optimization with CARDEC hyperparameters

```
# CatBoost with CARDEC-specific parameter grid
print("Training CatBoost...")

# Prepare data for CatBoost
X_train_cb = X_train.copy()
X_test_cb = X_test.copy()

# Convert categorical and boolean columns to numeric
for col in X_train_cb.columns:
    if X_train_cb[col].dtype in ['category', 'bool', 'object']:
```

```
        X_train_cb[col] = X_train_cb[col].astype('int')
        X_test_cb[col] = X_test_cb[col].astype('int')

X_train_cb = X_train_cb.fillna(0)
X_test_cb = X_test_cb.fillna(0)

# Create pipeline
cb_pipeline = Pipeline([
    ('classifier', cb.CatBoostClassifier(verbose=False))
])

# CARDEC-specific parameter grid (from original CARDEC CatBoost)
cb_param_grid = {
    'classifier__iterations': [100, 200, 300],
    'classifier__depth': [4, 6, 8],
    'classifier__learning_rate': [0.01, 0.1, 0.2],
    'classifier__l2_leaf_reg': [1, 3, 5],
    'classifier__border_count': [64, 128, 254]
}

print(f"Parameter combinations: {np.prod([len(v) for v in cb_param_grid.values(

# Evaluate with multiple seeds
cb_results, cb_detailed = evaluate_model_with_seeds(
    cb_pipeline, cb_param_grid, X_train_cb, y_train, X_test_cb, y_test, 'CatBoc
)

# Display results
cb_avg_predictions = display_model_summary(cb_results, 'CatBoost')
```

```
Training CatBoost...
Parameter combinations: 243

Training CatBoost with 10 seeds...
  Seed 1/10: 40
  Seed 2/10: 41
  Seed 3/10: 42
  Seed 4/10: 43
  Seed 5/10: 44
  Seed 6/10: 45
  Seed 7/10: 46
  Seed 8/10: 47
  Seed 9/10: 48
  Seed 10/10: 49

============================================================
CATBOOST RESULTS SUMMARY (10 Seeds)
============================================================
Mean CV F1 Score: 0.6598 ± 0.0132
Mean Test AUC: 0.7588 ± 0.0186
Mean Test F1: 0.7115 ± 0.0126
Mean Test Accuracy: 0.6938 ± 0.0255
Mean Test Precision: 0.6339 ± 0.0358
Mean Test Recall: 0.8183 ± 0.0643
Mean Optimal Threshold: 0.4800 ± 0.0714
Best Parameters: {'classifier__border_count': 64, 'classifier__depth': 4, '

Threshold evaluation using averaged predictions across 10 seeds:
AUC with averaged predictions: 0.7698
Optimal threshold: 0.400
Performance at optimal threshold:
  Accuracy: 0.6692
  Precision: 0.5859
  Recall: 0.9667
  F1-Score: 0.7296
```

Model Comparison and ROC Curves

Comprehensive comparison of all models

```
import matplotlib.pyplot as plt
import pandas as pd
from sklearn.metrics import roc_curve, roc_auc_score, accuracy_score, precisior
import numpy as np

# Create comprehensive comparison table and ROC curves
print("\n" + "="*80)
```

```
print("COMPREHENSIVE MODEL COMPARISON - CARDEC DATASET")
print("="*80)

# Collect all models and their performance metrics
# IMPORTANTE: Agora usamos o auc_mean (média dos AUCs dos 10 seeds) para compar
models_comparison = {
    'Decision Tree': {
        'avg_predictions': dt_avg_predictions,
        'auc_mean': dt_results['auc_mean'],
        'auc_std': dt_results['auc_std'],
        'accuracy_mean': dt_results['accuracy_mean'],
        'precision_mean': dt_results['precision_mean'],
        'recall_mean': dt_results['recall_mean'],
        'f1_mean': dt_results['f1_mean'],
        'threshold_mean': dt_results['threshold_mean']
    },
    'Random Forest': {
        'avg_predictions': rf_avg_predictions,
        'auc_mean': rf_results['auc_mean'],
        'auc_std': rf_results['auc_std'],
        'accuracy_mean': rf_results['accuracy_mean'],
        'precision_mean': rf_results['precision_mean'],
        'recall_mean': rf_results['recall_mean'],
        'f1_mean': rf_results['f1_mean'],
        'threshold_mean': rf_results['threshold_mean']
    },
    'XGBoost': {
        'avg_predictions': xgb_avg_predictions,
        'auc_mean': xgb_results['auc_mean'],
        'auc_std': xgb_results['auc_std'],
        'accuracy_mean': xgb_results['accuracy_mean'],
        'precision_mean': xgb_results['precision_mean'],
        'recall_mean': xgb_results['recall_mean'],
        'f1_mean': xgb_results['f1_mean'],
        'threshold_mean': xgb_results['threshold_mean']
    },
    'Neural Network': {
        'avg_predictions': nn_avg_predictions,
        'auc_mean': nn_results['auc_mean'],
        'auc_std': nn_results['auc_std'],
        'accuracy_mean': nn_results['accuracy_mean'],
        'precision_mean': nn_results['precision_mean'],
        'recall_mean': nn_results['recall_mean'],
        'f1_mean': nn_results['f1_mean'],
        'threshold_mean': nn_results['threshold_mean']
    },
    'CatBoost': {
        'avg_predictions': cb_avg_predictions,
```

```
        'auc_mean': cb_results['auc_mean'],
        'auc_std': cb_results['auc_std'],
        'accuracy_mean': cb_results['accuracy_mean'],
        'precision_mean': cb_results['precision_mean'],
        'recall_mean': cb_results['recall_mean'],
        'f1_mean': cb_results['f1_mean'],
        'threshold_mean': cb_results['threshold_mean']
    }
}

# Create comparison table using Mean Test AUC
comparison_data = []
for model_name, metrics in models_comparison.items():
    # Calculate metrics using averaged predictions for display consistency
    avg_pred = metrics['avg_predictions']
    optimal_threshold = metrics['threshold_mean']
    y_pred_optimal = (avg_pred >= optimal_threshold).astype(int)

    comparison_data.append({
        'Model': model_name,
        'Mean AUC': f"{metrics['auc_mean']:.4f}",  # Mean Test AUC
        'Accuracy': f"{accuracy_score(y_test, y_pred_optimal):.4f}",
        'Precision': f"{precision_score(y_test, y_pred_optimal, zero_division=0
        'Recall': f"{recall_score(y_test, y_pred_optimal, zero_division=0):.4f}
        'F1-Score': f"{f1_score(y_test, y_pred_optimal, zero_division=0):.4f}",
        'Threshold': f"{optimal_threshold:.3f}"
    })

comparison_df = pd.DataFrame(comparison_data)
print("\nFinal Model Performance (Mean Test AUC ± SD):")
print(comparison_df.to_string(index=False))

# Create ROC curves plot
plt.figure(figsize=(12, 8))

# Plot ROC curve for each model
colors = ['#1f77b4', '#ff7f0e', '#2ca02c', '#9467bd', '#d62728']
model_names = ['Decision Tree', 'Random Forest', 'XGBoost', 'Neural Network', '

for i, model_name in enumerate(model_names):
    model_data = models_comparison[model_name]

    # Calculate FPR and TPR using averaged predictions (for smooth curve)
    fpr, tpr, _ = roc_curve(y_test, model_data['avg_predictions'])

    # MUDANÇA PRINCIPAL: Usar auc_mean ± auc_std no label
    auc_mean = model_data['auc_mean']
    auc_std = model_data['auc_std']
```

```
    plt.plot(fpr, tpr, linewidth=3, color=colors[i],
             label=f'{model_name} (AUC = {auc_mean:.3f} ± {auc_std:.3f})')

# Plot diagonal line (random classifier)
plt.plot([0, 1], [0, 1], 'k--', linewidth=2, alpha=0.7, label='Random Classifie

# Formatting
plt.xlim([0.0, 1.0])
plt.ylim([0.0, 1.05])
plt.xlabel('False Positive Rate', fontsize=14, fontweight='bold')
plt.ylabel('True Positive Rate', fontsize=14, fontweight='bold')
plt.title('ROC Curves - CARDEC Restoration Failure Prediction Models\nMean Test
          fontsize=16, fontweight='bold', pad=20)
plt.legend(loc="lower right", fontsize=12, frameon=True, fancybox=True, shadow=
plt.grid(True, alpha=0.3, linestyle='-', linewidth=0.5)

# Add text box with dataset information
textstr = (
    f'Dataset: CARDEC Trial\n'
    f'Test samples: {len(y_test)}\n'
    f'Failure rate: {y_test.mean():.1%}\n'
    f'Patient-level split: 80:20\n'
    f'Methodology: 10 seeds, Mean AUC reported'
)
props = dict(boxstyle='round,pad=0.5', facecolor='lightgreen', alpha=0.8)
plt.text(0.02, 0.98, textstr, transform=plt.gca().transAxes, fontsize=11,
         verticalalignment='top', bbox=props)

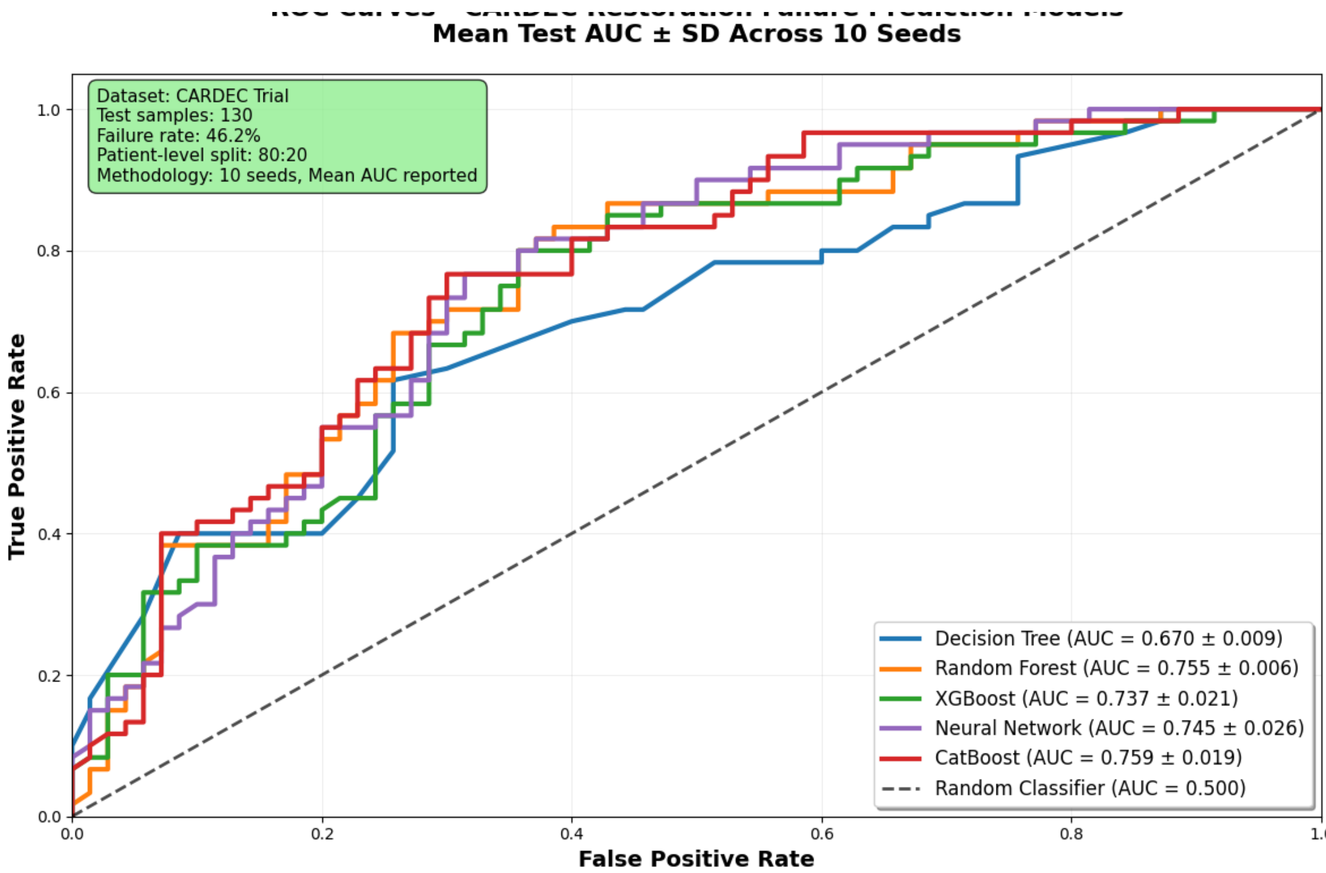
plt.tight_layout()
plt.savefig('roc_curves_cardec_mean_test_auc.png', dpi=300, bbox_inches='tight'
plt.show()

print("ROC curves saved as 'roc_curves_cardec_mean_test_auc.png'")
print("\nNote: ROC curves now display Mean Test AUC ± SD across 10 seeds in the
print("Curves are plotted using averaged predictions for smooth visualization."
```

```
================================================================================
COMPREHENSIVE MODEL COMPARISON - CARDEC DATASET
================================================================================

Final Model Performance (Mean Test AUC ± SD):
```

Model	Mean AUC	Accuracy	Precision	Recall	F1-Score	Threshold
Decision Tree	0.6701	0.5692	0.5217	0.8000	0.6316	0.355
Random Forest	0.7551	0.6923	0.6190	0.8667	0.7222	0.470
XGBoost	0.7374	0.6769	0.6071	0.8500	0.7083	0.495
Neural Network	0.7453	0.6692	0.5914	0.9167	0.7190	0.340
CatBoost	0.7588	0.7000	0.6364	0.8167	0.7153	0.480




```
ROC curves saved as 'roc_curves_cardec_mean_test_auc.png'

Note: ROC curves now display Mean Test AUC ± SD across 10 seeds in the lege
Curves are plotted using averaged predictions for smooth visualization.
```

SHAP Analysis

Feature importance analysis for the best model

```
# SHAP Analysis for the best performing model
```

```
import shap
from imblearn.over_sampling import SMOTE

# Find best model by mean AUC from the models_comparison dictionary
best_model_name = max(models_comparison.keys(), key=lambda x: models_comparisor
best_model_data = models_comparison[best_model_name]
best_model_obj = None

# Get the actual trained model object
if best_model_name == 'Decision Tree':
    # Get the best model object from the detailed results for this model
    best_model_obj = dt_results['best_model']
elif best_model_name == 'Random Forest':
    best_model_obj = rf_results['best_model']
elif best_model_name == 'XGBoost':
    best_model_obj = xgb_results['best_model']
elif best_model_name == 'CatBoost':
    best_model_obj = cb_results['best_model']
elif best_model_name == 'Neural Network':
    best_model_obj = nn_results['best_model']

print(f"Creating SHAP analysis for best model: {best_model_name}")
print(f"Best model Mean Test AUC: {best_model_data['auc_mean']:.3f}")


# For Neural Network, we need to use a different approach
if best_model_name == 'Neural Network':
    print("Note: SHAP analysis for Neural Network requires special handling.")
    print("Using the best tree-based model for SHAP analysis instead based on M

    # Use best tree-based model for SHAP based on Mean Test AUC
    tree_models = {}
    if 'dt_results' in locals():
         tree_models['Decision Tree'] = {'auc_mean': dt_results['auc_mean'], 'b
    if 'rf_results' in locals():
         tree_models['Random Forest'] = {'auc_mean': rf_results['auc_mean'], 'b
    if 'xgb_results' in locals():
         tree_models['XGBoost'] = {'auc_mean': xgb_results['auc_mean'], 'best_m
    if 'cb_results' in locals():
         tree_models['CatBoost'] = {'auc_mean': cb_results['auc_mean'], 'best_m


    best_tree_model_name = max(tree_models.keys(), key=lambda x: tree_models[x]
    best_model_obj = tree_models[best_tree_model_name]['best_model']
    best_model_name = best_tree_model_name
    print(f"Using {best_model_name} for SHAP analysis (Mean Test AUC: {tree_moc
```

```
# Get the trained classifier from the pipeline (for pipeline models)
if hasattr(best_model_obj, 'named_steps'):
    classifier = best_model_obj.named_steps['classifier']
else:
    classifier = best_model_obj

# Create SHAP explainer
print("Creating SHAP explainer...")
explainer = shap.TreeExplainer(classifier)

# Calculate SHAP values for test set (use subset for speed)
print("Calculating SHAP values...")
# Ensure X_test is a pandas DataFrame for SHAP
X_test_df = pd.DataFrame(X_test, columns=X_train.columns)

shap_values = explainer.shap_values(X_test_df[:100])  # Use first 100 samples

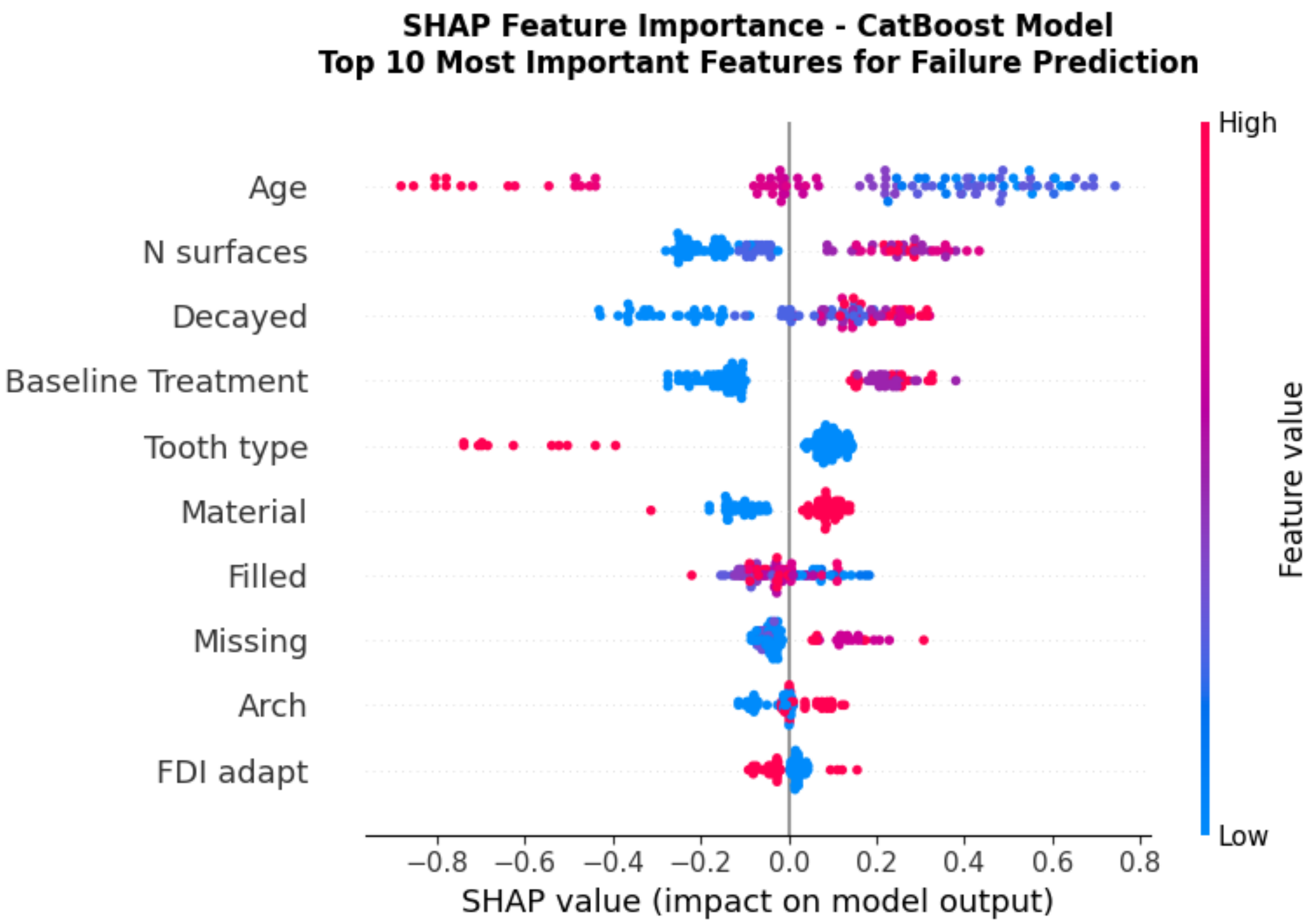
if isinstance(shap_values, list):
    shap_values = shap_values[1]  # For binary classification, take positive cl

print(f"SHAP values shape: {shap_values.shape}")
```

```
Creating SHAP analysis for best model: CatBoost
Best model Mean Test AUC: 0.759
Creating SHAP explainer...
Calculating SHAP values...
SHAP values shape: (100, 14)
```

```
# Create SHAP summary plot (beeswarm plot)
plt.figure(figsize=(8, 5.5))
shap.summary_plot(shap_values, X_test[:100], max_display=10, show=False)
plt.title(f'SHAP Feature Importance - {best_model_name} Model\nTop 10 Most Impor
          fontsize=12, fontweight='bold', pad=20)
plt.tight_layout()
plt.savefig('shap_summary_plot_failure.png', dpi=300, bbox_inches='tight')
plt.show()

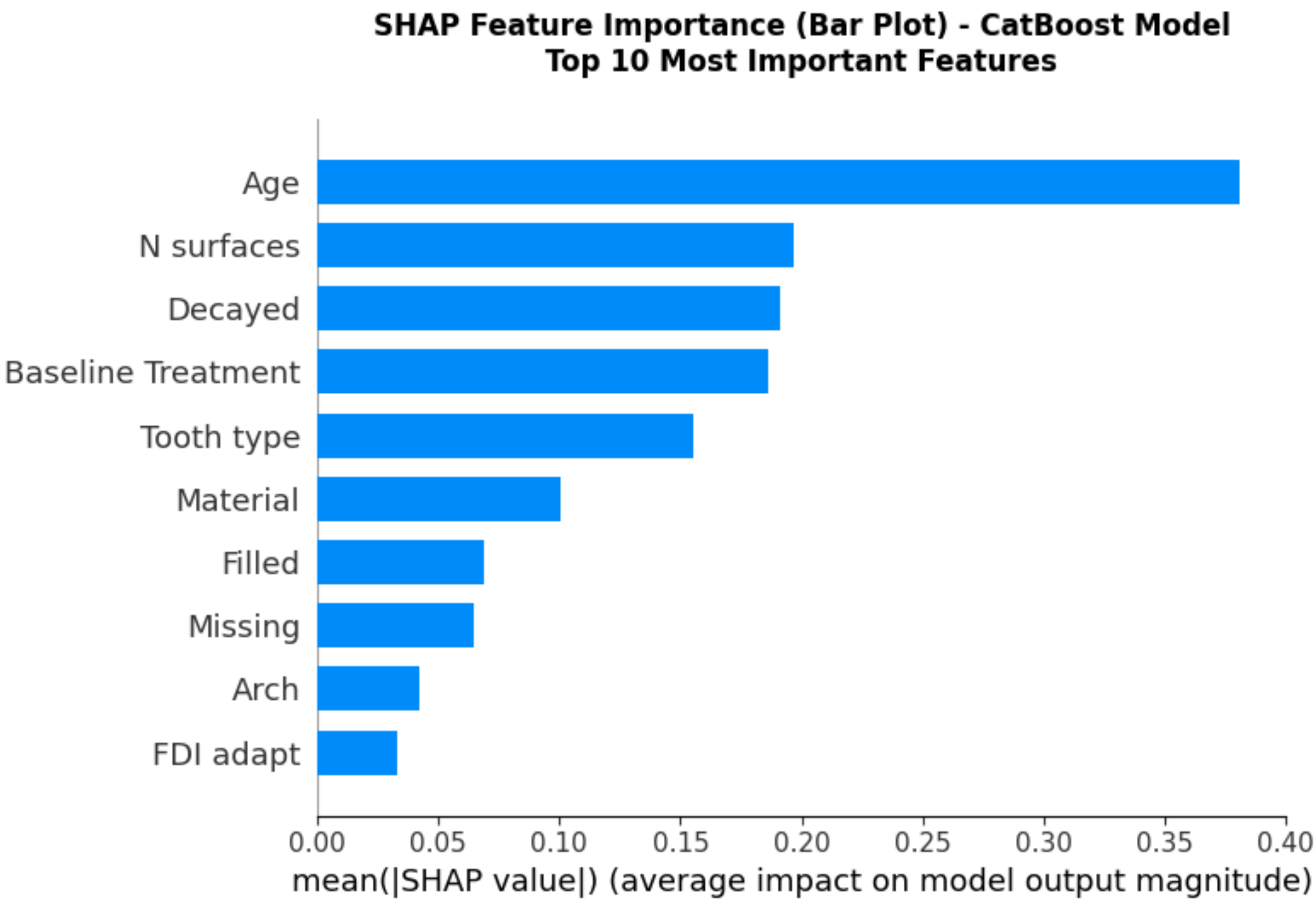
print("SHAP summary plot saved as 'shap_summary_plot_failure.png'")
```




```
SHAP summary plot saved as 'shap_summary_plot_failure.png'
```

```
# Create SHAP bar plot (feature importance)
plt.figure(figsize=(8, 5.5))
shap.summary_plot(shap_values, X_test[:100], plot_type="bar", max_display=10, s
plt.title(f'SHAP Feature Importance (Bar Plot) - {best_model_name} Model\nTop 1
          fontsize=12, fontweight='bold', pad=20)
plt.tight_layout()
plt.savefig('shap_bar_plot_failure.png', dpi=300, bbox_inches='tight')
plt.show()

print("SHAP bar plot saved as 'shap_bar_plot_failure.png'")
```




```
SHAP bar plot saved as 'shap_bar_plot_failure.png'
```

```
# Calculate and save feature importance
feature_importance = np.abs(shap_values).mean(0)

# Create DataFrame with feature names and importance
feature_names = X_test.columns if hasattr(X_test, 'columns') else [f'Feature_{i
importance_df = pd.DataFrame({
    'Feature': feature_names,
    'Importance': feature_importance
})

# Sort by importance
importance_df = importance_df.sort_values('Importance', ascending=False)

print("\nTop 10 Most Important Features (SHAP):")
print(importance_df.head(10).to_string(index=False))

# Save to CSV
importance_df.to_csv('feature_importance_shap_failure.csv', index=False)
print("\nFeature importance saved as 'feature_importance_shap_failure.csv'")
```

```
Top 10 Most Important Features (SHAP):
           Feature  Importance
               Age    0.381079
        N surfaces    0.196680
           Decayed    0.191021
Baseline Treatment    0.186226
        Tooth type    0.155592
          Material    0.100384
            Filled    0.068889
           Missing    0.064613
              Arch    0.042152
         FDI adapt    0.032912

Feature importance saved as 'feature_importance_shap_failure.csv'
```