ISE 625 Project Progress Report

Stable decision trees for suicide experience prediction

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Problem Context and Background

We aim to develop a model to predict suicidal experiences among youth experiencing homelessness (YEH). The provided decision tree (DT) model for the current YEH dataset shows instability with respect to changes in train-test splits. We aim to address the following:

Core Question: Can we design a robust, stable decision tree that remains invariant under shifts in data distributions while still identifying the key features indicative of suicidal ideation and attempts?

Dataset Considerations

Missing data

- (584, 587) samples remaining for each prediction model from initial listwise deletion method form original 940 total samples
- 4% of data set missing for `suicideidea` and `suicideattempt` (36 and 40 samples respectively)

Imbalanced classes

- 83% labeled 2, 16% labeled 1 for `suicideidea` class
- 88% labeled 0, 11% labeled 1 for `suicideattempt` class

Steps to implementing a Stable Decision Tree (Bertsimas et al. 2023)

1. **Initial Training (T0):**
   Train an initial set of decision trees on a subset of the data.
2. **Full Data Training (T):**
   Train a second set of decision trees on the full dataset.
3. **Distance Computation:**
   Calculate the average distance between each tree in **T** and the trees in **T0**. The distance between two trees is defined as:

$$d(\mathcal{T}_1, \mathcal{T}_2) \;=\; \min_{\{x\}} \sum_{p \in \mathcal{P}(\mathcal{T}_1)} \sum_{q \in \mathcal{P}(\mathcal{T}_2)} d(p,q)\, x_{p,q} \;+\; \sum_{p \in \mathcal{P}(\mathcal{T}_1)} w(p)\, x_p$$

4. **Performance Metrics:**
   Compute performance metrics (such as AUC) on a validation/test set.
5. **Pareto Optimization:**
   Select Pareto optimal trees that balance predictive performance and stability. This is expressed as:

$$\mathbb{T}^\star = \operatorname{argmax} f(d_b, \alpha_b)$$

Implementation progress:

final_bertsimas_tree_report

April 22, 2025

1 Notebook implementing the stable tree algorithm in Bertsimas et al. (https://arxiv.org/abs/2305.17299)

[26]:
```
import sys
import itertools
from pathlib import Path
src_path = Path("../src/dt-distance").resolve()
if str(src_path) not in sys.path:
    sys.path.insert(0, str(src_path))

import numpy as np
from sklearn.tree import DecisionTreeClassifier, plot_tree
from sklearn.metrics import roc_auc_score
from sklearn.utils import resample
from sklearn.datasets import load_breast_cancer
from sklearn.model_selection import train_test_split
from dt_distance.data_processor import DataProcessor
from dt_distance.tree_parser import TreeParser
from dt_distance.distance_calculator import DistanceCalculator
from dt_distance.problem_params import ProblemParams
import matplotlib.pyplot as plt
# set seed for reproducibility
np.random.seed(42)
```

Parameters listed in the paper:

[2]:
```
DEPTHS = list(range(3, 13))
MIN_SAMPLES = [3, 5, 10, 30, 50]
```

1.1 Loading the breast cancer dataset

[3]:
```
data_breast_cancer = load_breast_cancer(as_frame=True)
X_full = data_breast_cancer["data"]
y_full = data_breast_cancer["target"]
print("X_full shape: ", X_full.shape)
X_full.head()
```

```
X_full shape:  (569, 30)
```

[3]:
```
   mean radius  mean texture  mean perimeter  mean area  mean smoothness  \
0        17.99         10.38          122.80     1001.0          0.11840
1        20.57         17.77          132.90     1326.0          0.08474
2        19.69         21.25          130.00     1203.0          0.10960
3        11.42         20.38           77.58      386.1          0.14250
4        20.29         14.34          135.10     1297.0          0.10030

   mean compactness  mean concavity  mean concave points  mean symmetry  \
0           0.27760          0.3001              0.14710         0.2419
1           0.07864          0.0869              0.07017         0.1812
2           0.15990          0.1974              0.12790         0.2069
3           0.28390          0.2414              0.10520         0.2597
4           0.13280          0.1980              0.10430         0.1809

   mean fractal dimension  …  worst radius  worst texture  worst perimeter  \
0                 0.07871  …         25.38          17.33           184.60
1                 0.05667  …         24.99          23.41           158.80
2                 0.05999  …         23.57          25.53           152.50
3                 0.09744  …         14.91          26.50            98.87
4                 0.05883  …         22.54          16.67           152.20

   worst area  worst smoothness  worst compactness  worst concavity  \
0      2019.0            0.1622             0.6656           0.7119
1      1956.0            0.1238             0.1866           0.2416
2      1709.0            0.1444             0.4245           0.4504
3       567.7            0.2098             0.8663           0.6869
4      1575.0            0.1374             0.2050           0.4000

   worst concave points  worst symmetry  worst fractal dimension
0                0.2654          0.4601                  0.11890
1                0.1860          0.2750                  0.08902
2                0.2430          0.3613                  0.08758
3                0.2575          0.6638                  0.17300
4                0.1625          0.2364                  0.07678

[5 rows x 30 columns]
```

[4]:
```python
print("y_full shape: ", y_full.shape)
y_full.head()
```

```
y_full shape:  (569,)
```

[4]:
```
0    0
1    0
2    0
3    0
4    0
Name: target, dtype: int64
```

```
[5]: X_train, X_test, y_train, y_test = train_test_split(X_full, y_full, test_size=0.
     ↪2, random_state=42)

     print("X_train shape: {}, X_test shape: {}".format(X_train.shape, X_test.shape))
     print("y_train shape: {}, y_test shape: {}".format(y_train.shape, y_test.shape))
```

```
X_train shape: (455, 30), X_test shape: (114, 30)
y_train shape: (455,), y_test shape: (114,)
```

1.2 Step 1: Split Training set into X0 and X1

```
[6]: def random_train_split(X,y):
         N = X.shape[0]
         indices = np.random.permutation(N)
         X0, y0 = X[indices[:N // 2]], y[indices[:N // 2]]
         return X0, y0

     X0, y0 = random_train_split(X_train.values, y_train.values)
     X0.shape, y0.shape
```

```
[6]: ((227, 30), (227,))
```

1.3 Step 3: Bootstrap and Train (T_0) Tree Set

```
[7]: def train_decision_tree(X, y, depth, min_samples_leaf):
         clf = DecisionTreeClassifier(max_depth=depth,␣
     ↪min_samples_leaf=min_samples_leaf)
         clf.fit(X, y)
         return clf

     def bootstrap_trees(X, y, depths, min_samples, B):
         '''
         Create B bootstrap trees by sampling with replacement from X_0
         '''
         trees = []
         for _ in range(B):
             X_sample, y_sample = resample(X, y, replace= True)
             depth = np.random.choice(depths)
             min_leaf = np.random.choice(min_samples)
             tree = train_decision_tree(X_sample, y_sample, depth, min_leaf)
             trees.append(tree)
         return trees

     T0 = bootstrap_trees(X0, y0, DEPTHS, MIN_SAMPLES, 100)
     print("Number of trees in T0:", len(T0))
```

```
Number of trees in T0: 100
```

1.4 Step 4: Train Second Tree Collection: $\mathcal{T}$

Train the second tree collection $\mathcal{T}$ using the same method but on the entire training set.

[8]:
```
T = bootstrap_trees(X_train.values, y_train.values, DEPTHS, MIN_SAMPLES, 100)
print("Number of trees in T:", len(T))
```

```
Number of trees in T: 100
```

1.5 Step 5.1: Compute Mean distance for each $T \in T$

- For each tree in $\mathcal{T}$, compute `dt-distance` for all $T \in T_0$ and average over all B
- Compute AUC score from Test Data to get out-of-sample predictive power
- Return B average distances
- Intuition for larger set: Say we get new data in the future-> how much do these new trees (entire set)$\mathcal{T}$ deviate from the previosuly smaller set of trees T_0?
- Only structural differences (via path definitions) matter for problem params, so the path_converstion does not care about the dataset, but the bounds on features, quantification of categories, and assigned class labels as a sequence of splits

[17]:
```
def compute_average_distances(T0, T, X_train, y_train):
    X_train_values = X_train.values if hasattr(X_train, 'values') else X_train

    distances = []
    for i, tree_b in enumerate(T):
        d_b = 0.0
        for tree_beta in T0:
            distance_calculator = DistanceCalculator(tree_beta, tree_b,␣
 ↪X=X_train_values, y=y_train)
            d_b += distance_calculator.compute_tree_distance()
        d_b /= len(T0)
        distances.append(d_b)

    return distances
distances = compute_average_distances(T0, T, X_train, y_train)
print("Number of distances computed:", len(distances))
```

```
Number of distances computed: 100
Average of all distances: 0.049360019999999999
```

1.6 Step 5.2: Compute out-of-sample Predicitive Performance

Calculate the AUC score for each tree in $\mathcal{T}$ using the test set.

[19]:
```
def evaluate_predictive_power(trees, X_holdout, y_holdout):
    auc_scores = []
    for tree in trees:
        y_proba = tree.predict_proba(X_holdout)[:, 1]
        auc = roc_auc_score(y_holdout, y_proba)
        auc_scores.append(auc)
```

```
    return auc_scores

auc_scores = evaluate_predictive_power(T, X_test.values, y_test.values)
print("Average AUC score:", np.mean(auc_scores))
```

```
Average AUC score: 0.9595316082541763
```

1.7 Step 6: Find the Pareto Optimal Set $\mathcal{T}^*$ from $\mathcal{T}$

- Multi-objective function to find pareto optimal tree set from $\mathcal{T}$ based on average distance, d_b , $\forall b \in \mathcal{T}$ and the out-of-sample AUC_ROC score a_b, $\forall b \in \mathcal{T}$
- **Pareto Optimal Definition:** $(d_{b'} \leq d_b$ and $\alpha_{b'} > \alpha_b)$ or $(d_{b'} < d_b$ and $\alpha_{b'} \geq \alpha_b)$

[21]:
```
def pareto_optimal_trees(distances, auc_scores):
    pareto_trees = []
    for i, (d_i, a_i) in enumerate(zip(distances, auc_scores)):
        dominated = False
        for j, (d_j, a_j) in enumerate(zip(distances, auc_scores)):
            if i != j and ((d_j <= d_i and a_j > a_i) or (d_j < d_i and a_j >=␣
 ↪a_i)):
                dominated = True
                break
        if not dominated:
            pareto_trees.append(i)
    return pareto_trees

pareto_trees = pareto_optimal_trees(distances, auc_scores)
print("Number of Pareto optimal trees:", len(pareto_trees))
```

```
Number of Pareto optimal trees: 7
```

1.8 Step 7: Find the Optimal Tree from the Pareto Optimal Set, $\mathcal{T}^*$

- $\mathbb{T}^\star = \underset{\mathbb{T}_b \in \mathcal{T}^\star}{\operatorname{argmax}} f(d_b, \alpha_b)$
- Need to consider here what we value: stability or predicitve power.
- Current function is most stable model among all "good enough" performers.
- Can modify to find optimal trade-off for accuracy-stability
- Indicator function where:
  - 1 if α_b is within of the best score
  - 0 otherwise

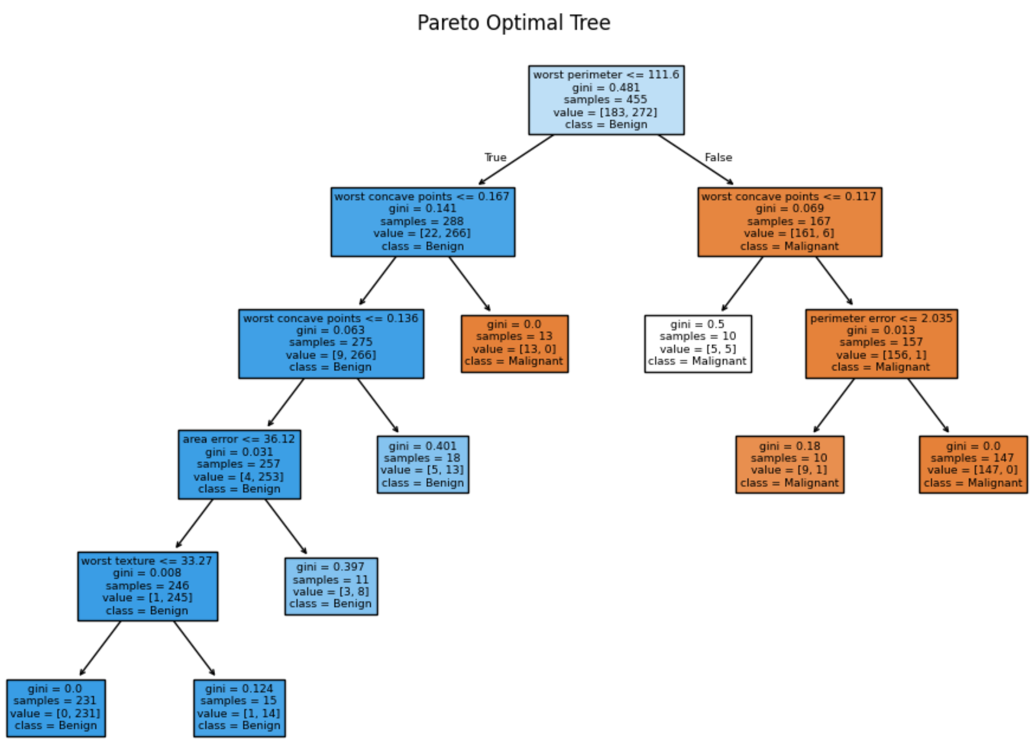
[27]:
```
def select_final_tree(distances, auc_scores, pareto_indices, epsilon=0.01):
    best_auc = max(auc_scores)
    candidates = [i for i in pareto_indices if auc_scores[i] >= (1 - epsilon) *␣
 ↪best_auc]
    if not candidates:
        candidates = pareto_indices
    best_idx = max(candidates, key=lambda i: auc_scores[i] - distances[i])
```

```
    return best_idx

selected_tree_index = select_final_tree(distances, auc_scores, pareto_trees)
print("Selected tree index:", selected_tree_index)
```

```
Selected tree index: 47
```

1.8.1 Plot the Pareto optimal tree:

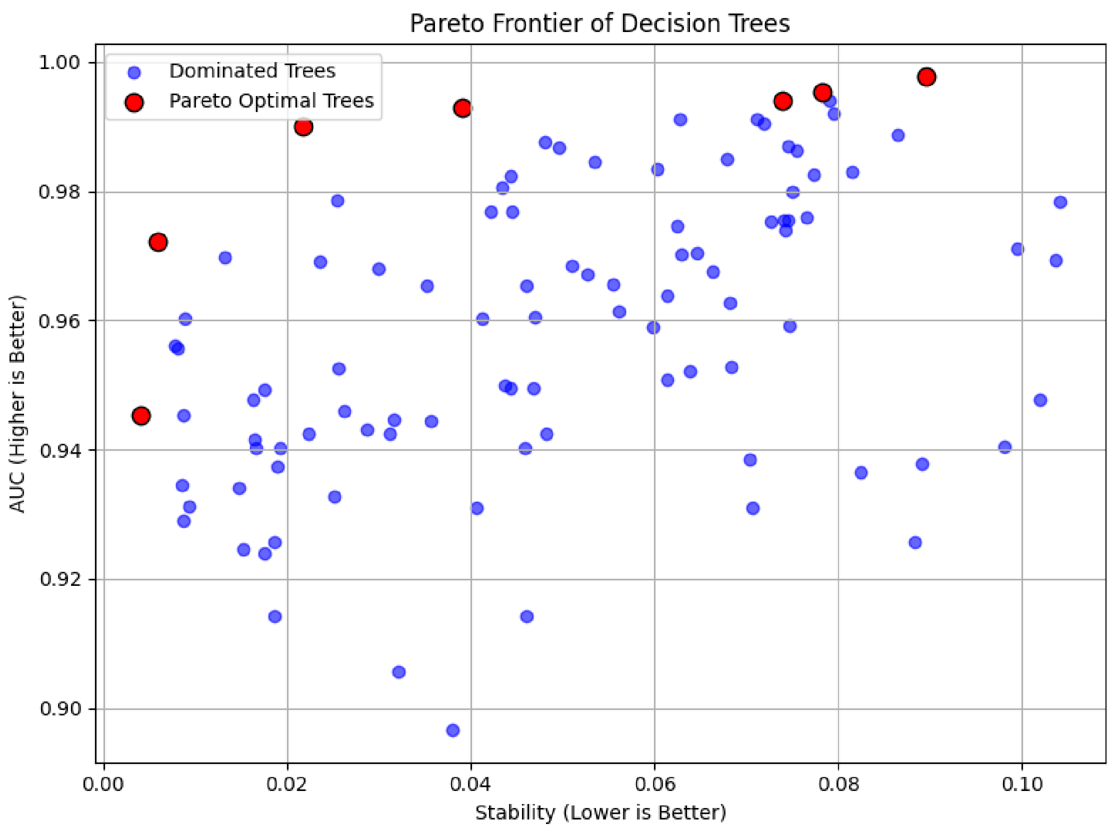
[29]:
```
selected_tree = T[selected_tree_index]
plt.figure(figsize=(12, 8))
plot_tree(selected_tree,
          feature_names=X_full.columns,
          class_names=["Malignant", "Benign"],
          filled=True)
plt.title("Pareto Optimal Tree")
plt.show()
```



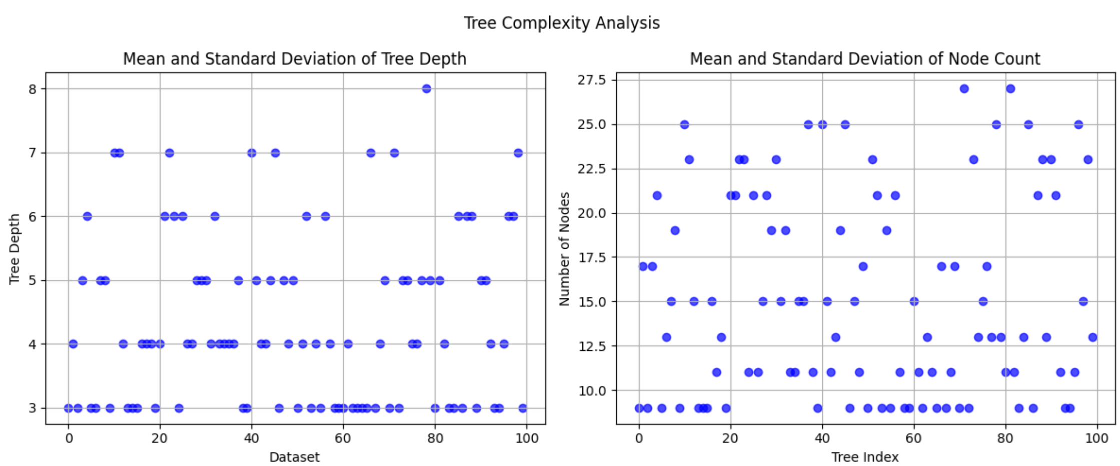
1.8.2 Pareto Frontier Visualization

- Plotting pareto frontier from a collection of trees based on average distance, d_b , $\forall b \in \mathcal{T}$ and the out-of-sample AUC_ROC score a_b, $\forall b \in \mathcal{T}$

[32]:
```
def plot_pareto_frontier(distances, auc_scores, pareto_indices):
    distances = np.array(distances)
    auc_scores = np.array(auc_scores)
    pareto_indices = set(pareto_indices)
    is_pareto = np.array([i in pareto_indices for i in range(len(distances))])
    # Plotting
    plt.figure(figsize=(8, 6))
    plt.scatter(distances[~is_pareto], auc_scores[~is_pareto], c='blue',␣
 ↪label='Dominated Trees', alpha=0.6)
    plt.scatter(distances[is_pareto], auc_scores[is_pareto], c='red',␣
 ↪edgecolors='black', s=80, label='Pareto Optimal Trees')
    plt.xlabel("Stability (Lower is Better)")
    plt.ylabel("AUC (Higher is Better)")
    plt.title("Pareto Frontier of Decision Trees")
    plt.legend()
    plt.grid(True)
    plt.tight_layout()
    plt.show()

plot_pareto_frontier(distances, auc_scores, pareto_trees)
```



[34]:
```
def plot_tree_complexity_metrics(trees):

    depths = [tree.get_depth() for tree in trees]
    node_counts = [tree.tree_.node_count for tree in trees]

    fig, axs = plt.subplots(1, 2, figsize=(12, 5))

    # Tree Depth Plot
    axs[0].scatter(range(len(trees)), depths, color='blue', alpha=0.7)
    axs[0].set_title("Mean and Standard Deviation of Tree Depth")
    axs[0].set_xlabel("Dataset")
    axs[0].set_ylabel("Tree Depth")
    axs[0].grid(True)

    # Node Count Plot
    axs[1].scatter(range(len(trees)), node_counts, color='blue', alpha=0.7)
    axs[1].set_title("Mean and Standard Deviation of Node Count")
    axs[1].set_xlabel("Tree Index")
    axs[1].set_ylabel("Number of Nodes")
    axs[1].grid(True)

    plt.suptitle("Tree Complexity Analysis")
    plt.tight_layout()
    plt.show()
plot_tree_complexity_metrics(T)
```



Project Outcomes

- A robust, stable decision tree model that minimizes the variability in tree structure due to random train-test splits
- Empirical evidence supporting the stability of the model through consistent feature selection and comparable performance metrics
- **Impact:** Better interpretability of decision trees to predict suicide risk among YEHs