DISTRIBUTION SHIFT

A Study on Their Effects on Statistical Models and Strategies for Mitigation

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Introduction

Dataset shift

- **Dataset shift** is a common problem in machine learning.
- It occurs when the distribution of the training data differs from the distribution of the test data.
- This can lead to a decrease in the performance of the model.

The two most common and well-studied causes of dataset shift are:

- Sample selection bias
- non stationary environments

Aims of project

This project aims to evaluate the impact of simple **Covariate shift** in the input distribution on the performance of robust models within the context of a synthetic binary classification task.

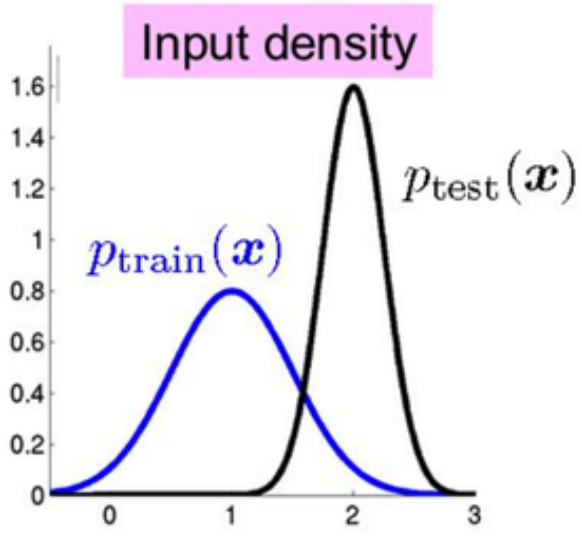
Key questions addressed in this study include:

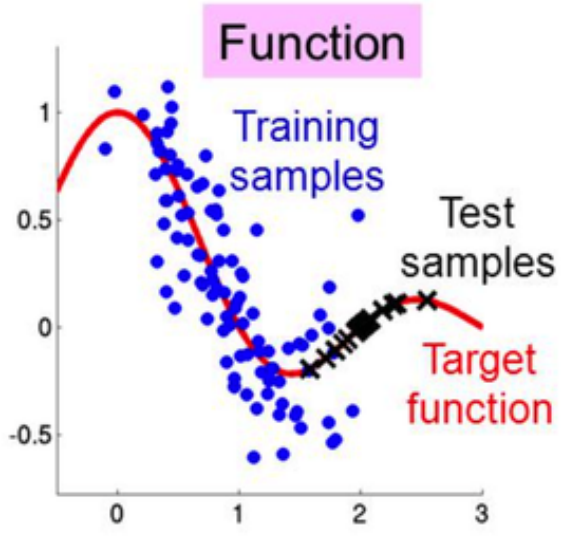
- How do different types of covariate shifts affect the performance of robust models?
- Are certain models inherently more robust to simple covariate shifts?
- What strategies can be employed to improve model performance following such shifts?

Covariate shift

Can be formally defined as follows. Consider an input variable X and a response variable Y, where $X \to Y$ represents the relationship between the two. Let P_{tra} denote the probability distribution of the training data and P_{tst} denote the probability distribution of the test data. A covariate shift occurs when:

$$P_{\text{tra}}(Y \mid X) = P_{\text{tst}}(Y \mid X) \quad \text{but} \quad P_{\text{tra}}(X) \neq P_{\text{tst}}(X)\,.$$

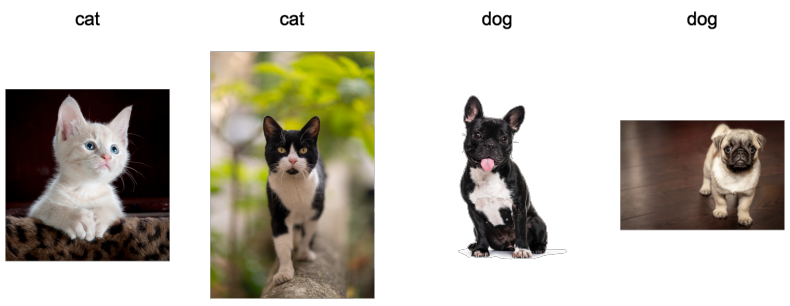




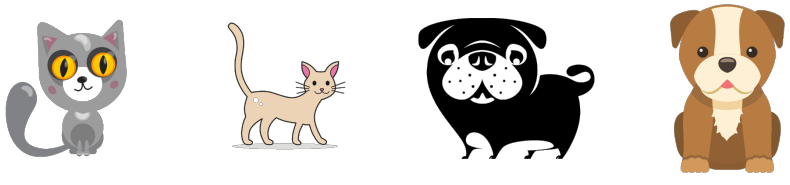
Example

Consider a model designed to distinguish between cats and dogs:

Training set:



Test set:



- Model will not accurately distinguish between cats and dogs because the feature distribution will differ.
- Changes in the input distribution can significantly impact the model's accuracy.

Inaccurate model

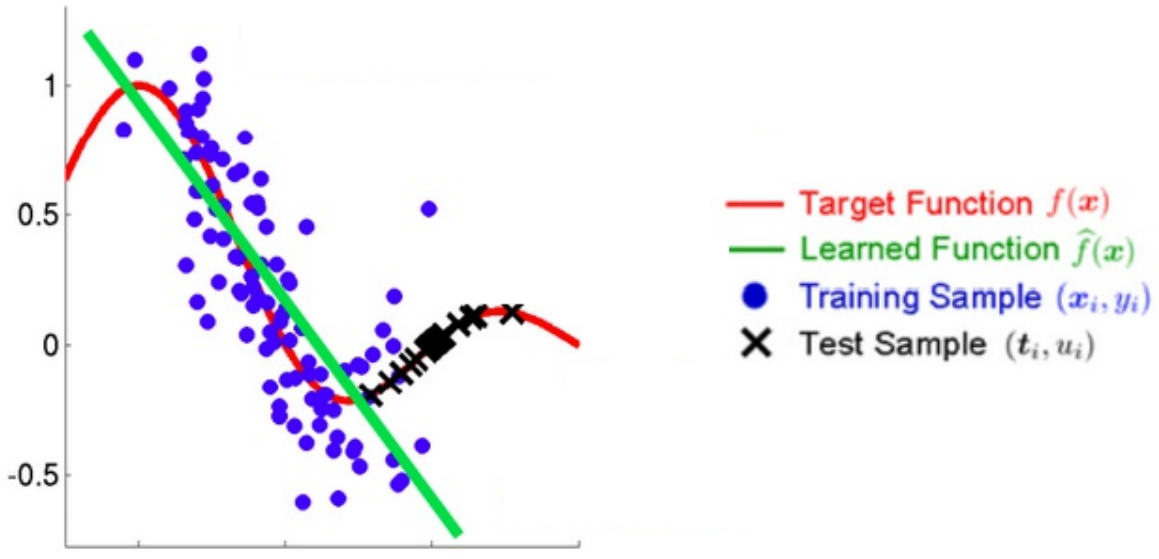


Figure 1: Example of inaccurate model.

In this study, we analyze the effects of distribution shift on different statistical models and propose strategies for its mitigation.

Data Generation

Training Dataset: Features

The dataset consists of $n = 10^4$ observations with 3 features and 1 binary target variable.

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Features:

- $X_{\text{train}} = (X_{\text{train}\,1}, X_{\text{train}\,2}, X_{\text{train}\,3}) \sim \mathcal{N}(\boldsymbol{\mu}_{\text{train}}, \boldsymbol{\Sigma}_{\text{train}})$
- $\mu_{\text{train}\,i} \sim \mathcal{U}_{[0,1]}$ for $i = 1, 2, 3$
- $[\boldsymbol{\Sigma}_{\text{train}}]_{i,j} \sim \mathcal{U}_{[-1,1]}$ for $i, j = 1, 2, 3$

Note: The $\boldsymbol{\Sigma}$ randomly generated has been transformed to a symmetric and positive semidefinite matrix by computing $\boldsymbol{\Sigma}\boldsymbol{\Sigma}^T$.

Training Dataset: Target Variable

Building the **target variable** $Y \in \{0, 1\}$:

1. $$z = \beta_0 + \sum_{i=1}^{3} \beta_i x_i + \sum_{i=1}^{3} \beta_{ii} x_i^2 + \sum_{i=1}^{2} \sum_{j=i+1}^{3} \beta_{ij} x_i x_j \,, \quad \beta_\cdot \sim \mathcal{U}_{[-1,1]}$$

2. $$p = \frac{1}{1 + e^{-z}}$$

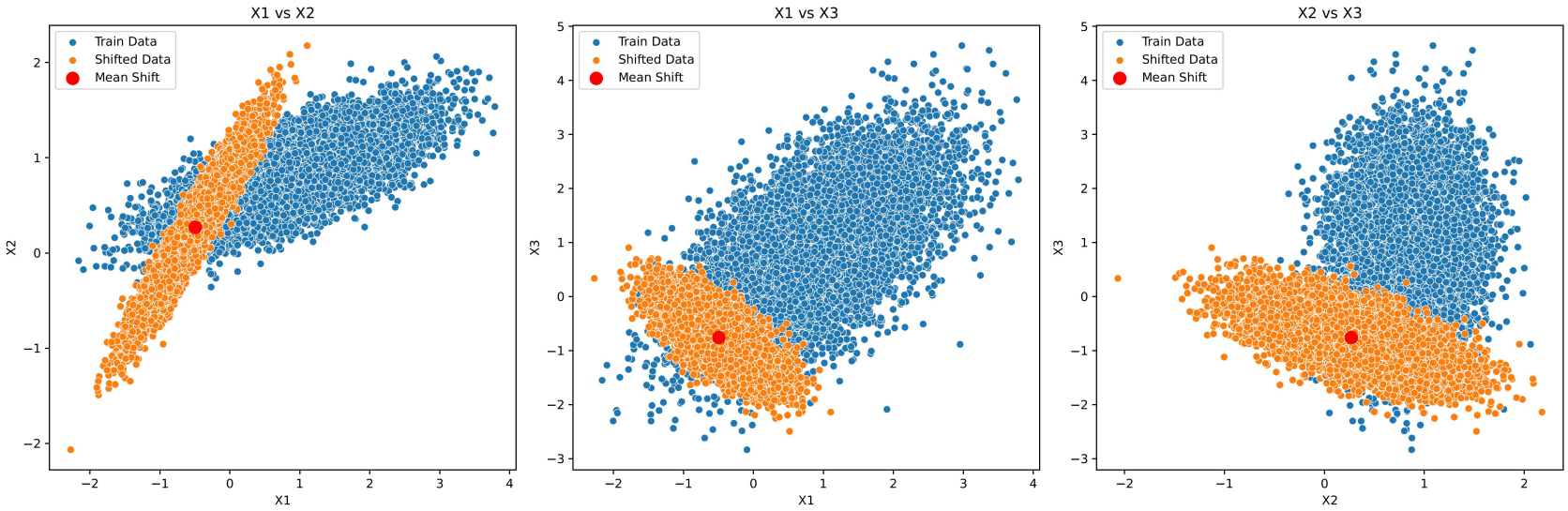
3. $$Y \sim \mathrm{Be}(p)$$

Testing Dataset

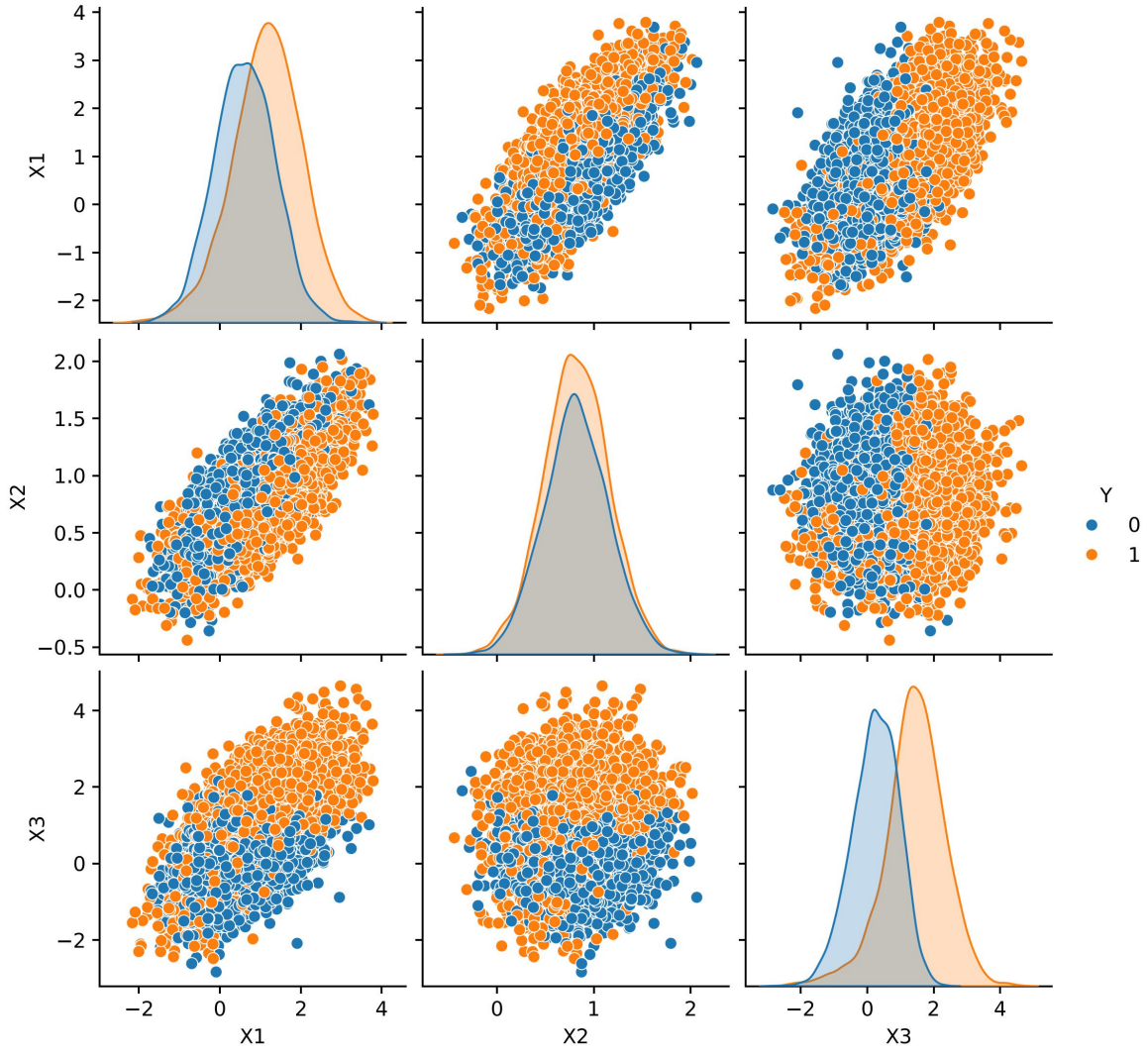
Same dataset structure as the train set, but:

- $X_{\text{shift}} = (X_{\text{shift}\,1}, X_{\text{shift}\,2}, X_{\text{shift}\,3}) \sim \mathcal{N}(\boldsymbol{\mu}_{\text{shift}}, \boldsymbol{\Sigma}_{\text{shift}})$
- $\boldsymbol{\mu}_{\text{shift}} = \mathcal{Q}_{0.05}(X_{\text{train}})$
- $[\boldsymbol{\Sigma}_{\text{shift}}]_{i,j} \sim \mathcal{U}_{[-0.5,0.5]}$ for $i, j = 1, 2, 3$

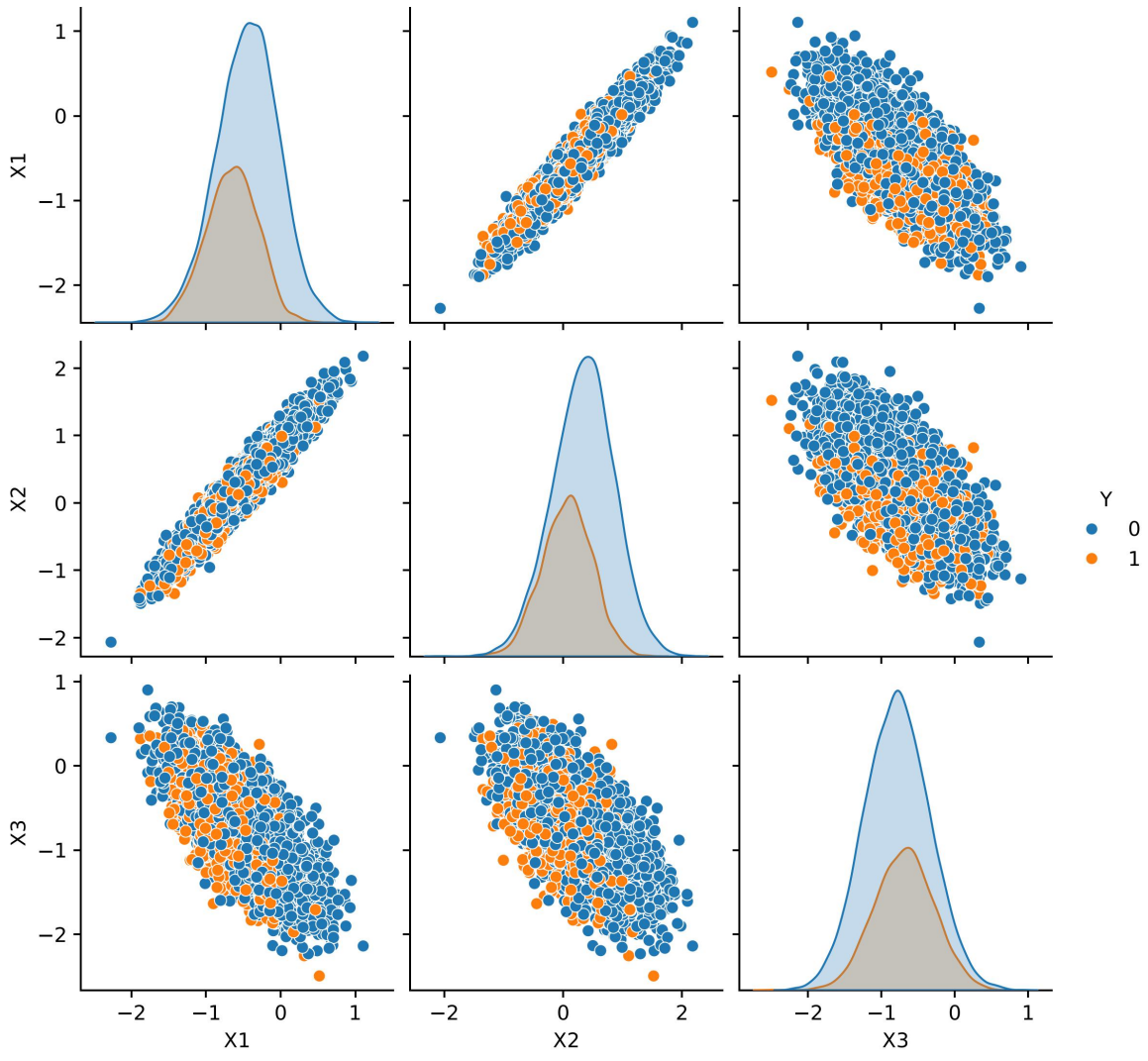
Original and Shiftd Features



Label Distribution in Train Set



Label Distribution in Shifted Test Set



Note: IR from 1.19 to 2.36

Testing Mixture

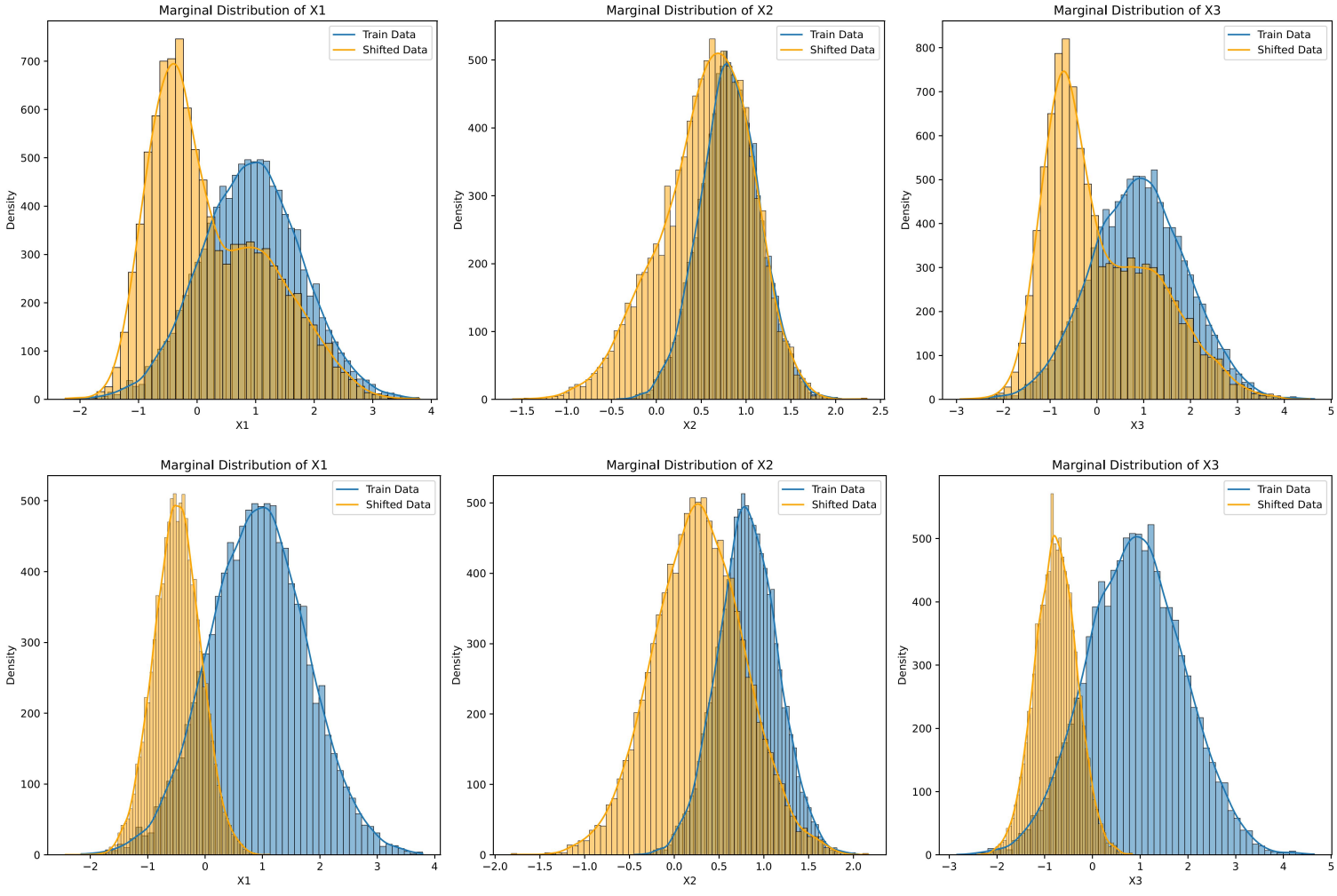
Series of datasets using **statistical mixtures** of the training features distribution and the fully shifted distribution.

$$X_\alpha \sim \alpha \cdot \mathcal{N}(\boldsymbol{\mu}_{\text{shift}}, \boldsymbol{\Sigma}_{\text{shift}}) + (1-\alpha) \cdot \mathcal{N}(\boldsymbol{\mu}_{\text{train}}, \boldsymbol{\Sigma}_{\text{train}})$$

$$\alpha \in \{0.0, 0.1, \ldots, 1.0\}$$

Y_α generated as before

Note: $X_{0.0}$ and X_{train} come from the same distribution, but the former are used as fresh new data.



Top: $\alpha = 0.5$. Bottom: $\alpha = 1.0$.

Performance Degradation

Performance Degradation

Models

- Random Forest
- Gradient Boosting
- XGBoost
- **Logistic Regression** [baseline]

Performance Metric

We used the **Area Under the Receiver Operating Characteristic Curve (ROC-AUC)** as the performance metric for our models.

Fine Tuning

We performed a **hyperparameter tuning** to optimise the performance of our models. to do this, we used the **Grid Search** method with 5-fold cross-validation.

Logistic Regression

Logistic Regression is a simple linear model used for binary classification.

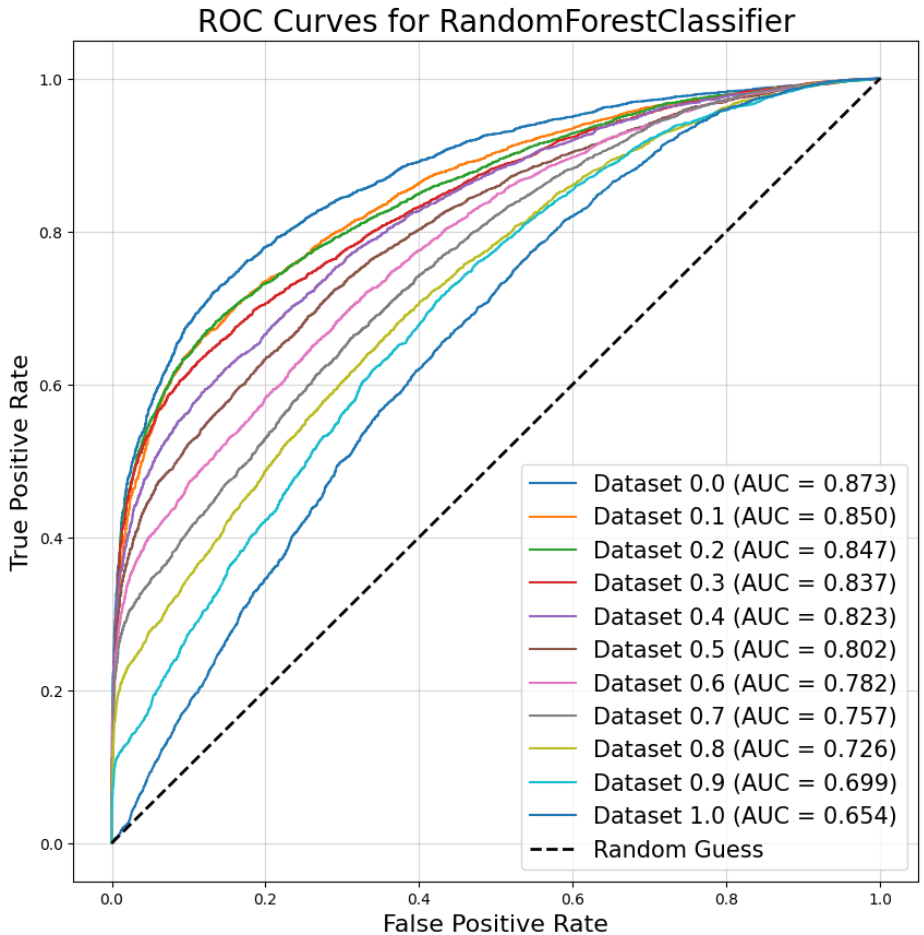
TODO

Random Forests

Random Forest is an ensemble learning method that builds multiple decision trees during training.

It outputs the class that is the majority vote of the individual trees.

Hyperparameter	Value
n_estimators	125
criterion	*gini*
max_depth	5
min_samples_split	5
min_samples_leaf	1



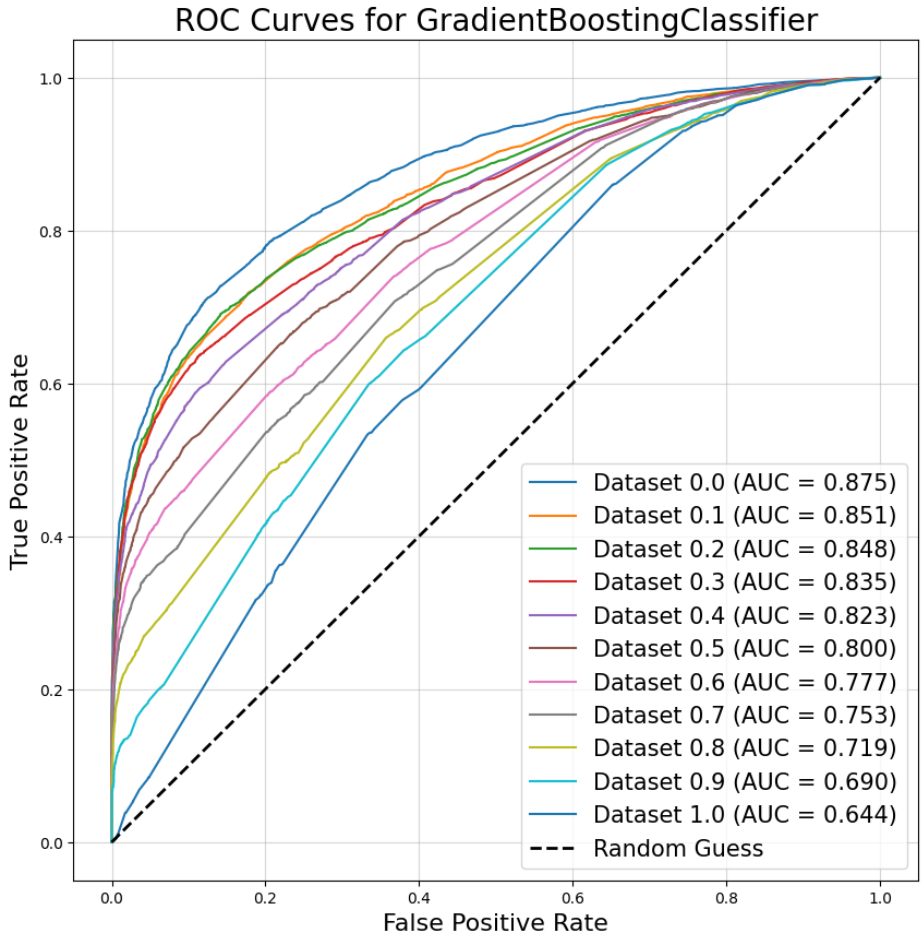
Note: We set `random_state` to `0` for reproducibility.

Gradient Boosting

Gradient Boosting combines weak predictive models (in our case decision trees) in an iterative manner.

Each model corrects the errors of its predecessor, making it highly effective but sensitive to hyperparameter tuning.

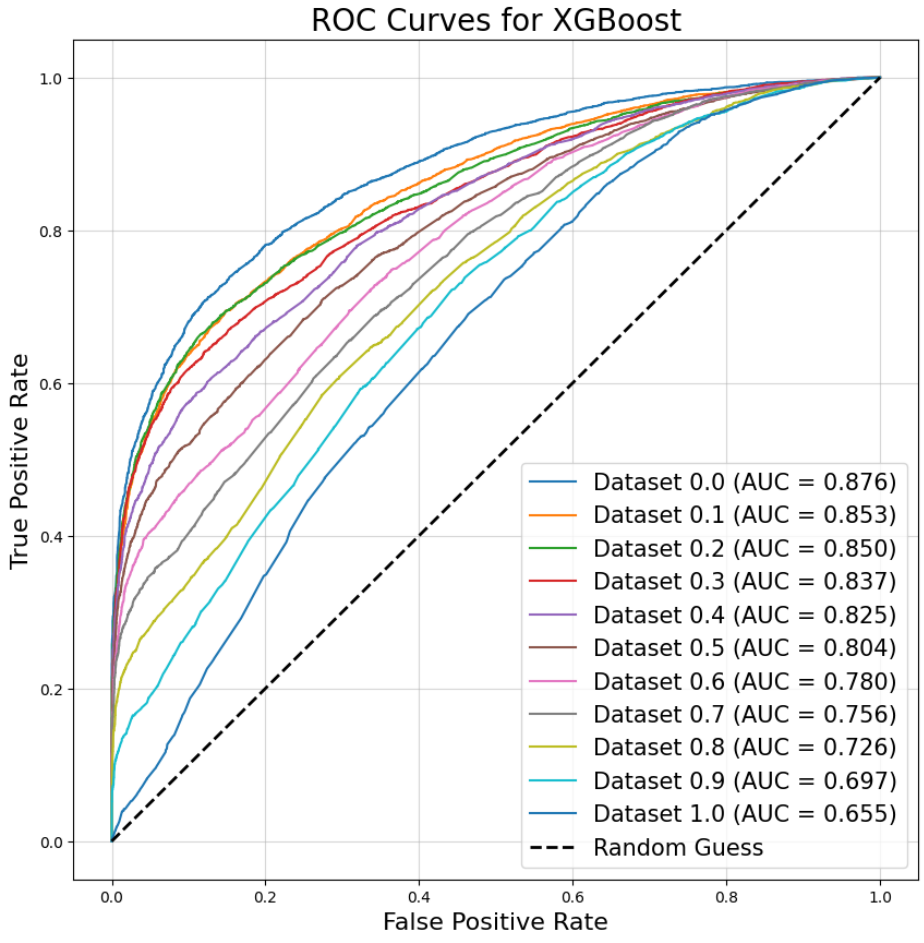
Hyperparameter	Values
n_estimators	125
learning_rate	0.025
max_depth	3
subsample	0.4



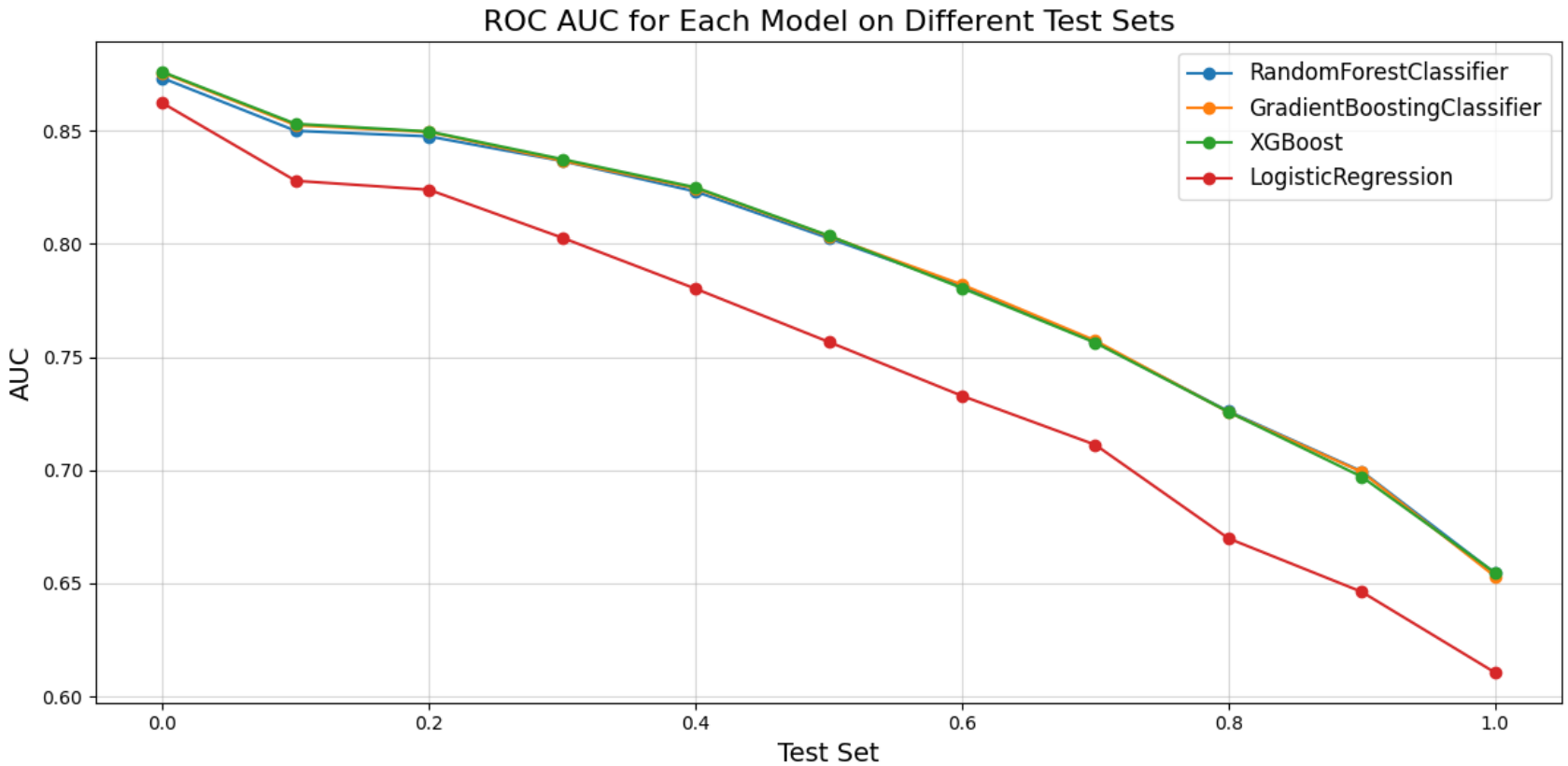
Extreme Gradient Boosting

XGBoost (*Extreme Gradient Boosting*) is a scalable and efficient gradient boosting framework known for its regularization capabilities and speed.

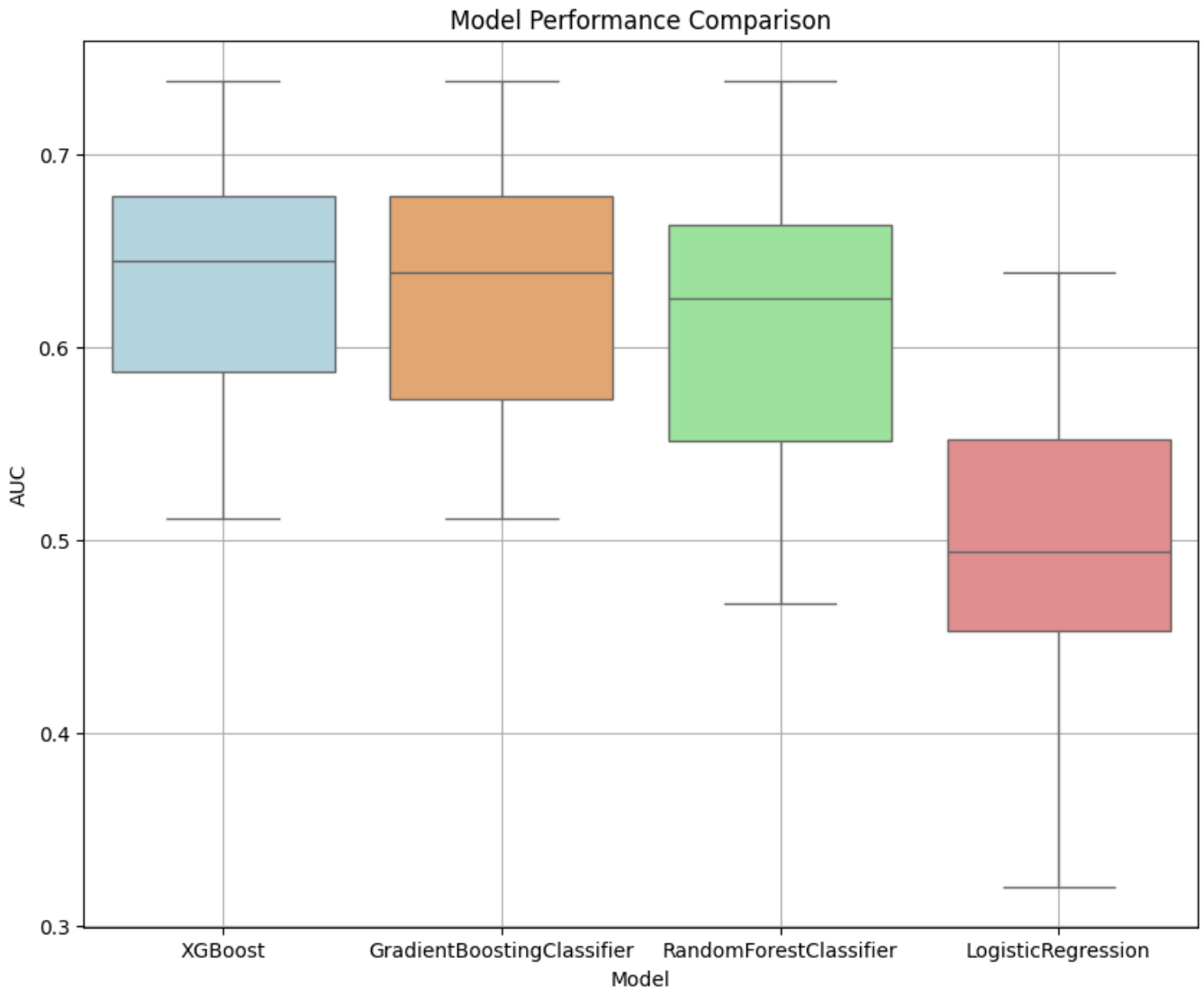
Hyperparameter	Values
n_estimators	100
learning_rate	0.1
max_depth	6
subsample	0.7
gamma	5



Performance Comparison



Performance Comparison



Performance Enhancement

A Novel Pre-Processing Method Against Covariate Shift

1. **No Prior Shift Knowledge Needed**
   - Simplifies implementation by eliminating the need for shift estimation.
   - Adaptable to various datasets without additional shift information.
2. **Built-in Regularization**
   - Prevents overfitting by introducing controlled noise.
   - Enhances model generalization on unseen data.

The R.A.W. Method

- Random
- Augmentation
- Walk

Input: $Data_{\text{train}}$, $Size$, N, ε.

$Data_{\%} \leftarrow$random subset of N% of Data_{train}

For x_i in $\text{Data}_{\%}$

$$x_i' \leftarrow \begin{cases} X_i + \varepsilon & \text{with probability 0.5} \\ X_i - \varepsilon & \text{with probability 0.5} \end{cases}$$

$y_i' \leftarrow y_i$

End For

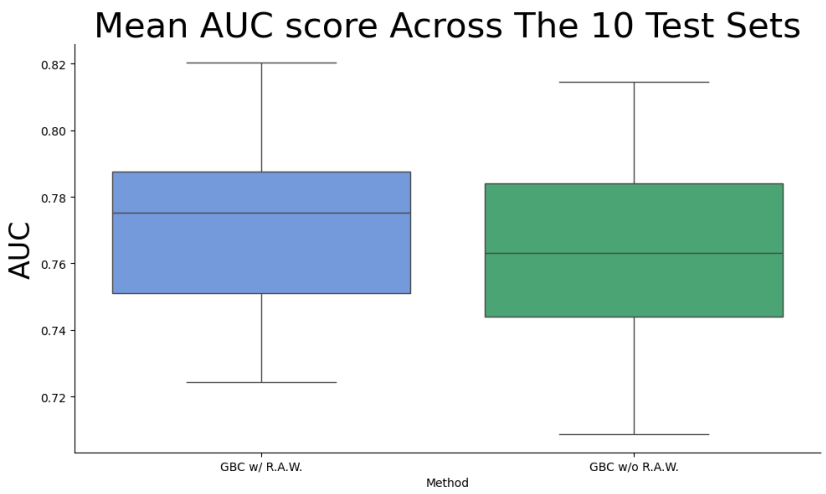
$Data_{\text{aug}} \leftarrow \text{Data}_{train} \cup Data_{\%}$

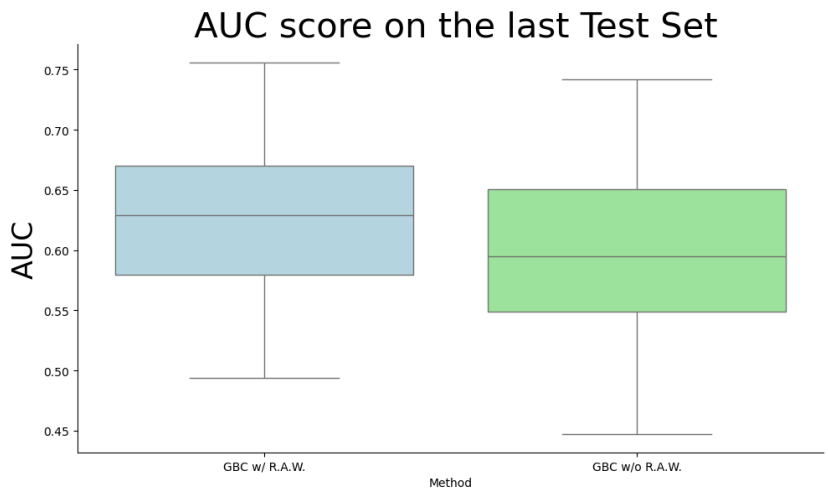
$Data_{\text{final}} \leftarrow \text{Downsample}(\text{Data}_{\text{aug}}, Size)$

Return $Data_{\text{final}}$

Classify With Gradient Boosting Using R.A.W.

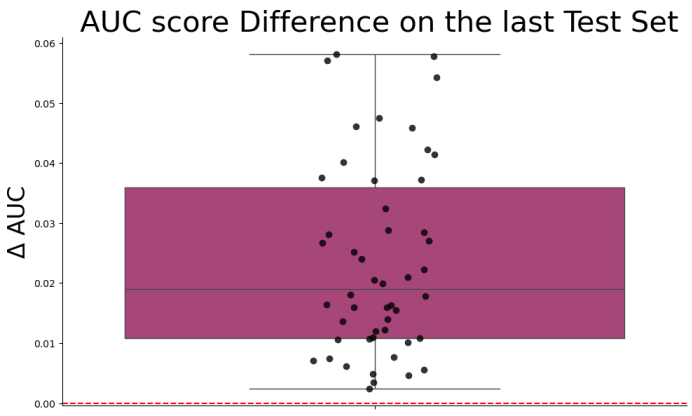
1. Apply the R.A.W. pre-processing method to the training data to address covariate shift.
2. Train a Gradient Boosting Classifier on the augmented dataset.
3. Evaluate the model's performance on shifted test sets.





A Statistical Analysis Of The Results

- H_0: $\Delta\mu = \overline{\text{AUC}}_{\text{R.A.W.}} - \overline{\text{AUC}}_{\text{base}} = 0$
- H_1: $\Delta\mu = \overline{\text{AUC}}_{\text{R.A.W.}} - \overline{\text{AUC}}_{\text{base}} \neq 0$
- **Test:** Two samples t-test on 50 independent $\Delta\overline{\text{AUC}}$ differences.



	$\Delta\mu$	t-stat	p-value	95% CI
$\Delta\overline{\text{AUC}}$*	0.0083	8.75	1.39×10^{-11}	[0.006, 0.010]
$\Delta\text{AUC}_{\text{last}}$**	0.0235	10.59	2.86×10^{-14}	[0.019, 0.028]

* Mean AUC score difference across all 10 shifted test sets.

** AUC score difference on the most shifted test set.

Questions?

References i