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DISTRIBUTION SHIFT

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

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Introduction

Aims of project

Models:

- Logistic Regression
- Random Forest
- Gradient Boosting
- XGBoost

Roadmap:

- Creation of synthetic data and data affected by shift
- Evaluation of model performance on the data
- Identification of improvement strategies (R.W.A.)

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.

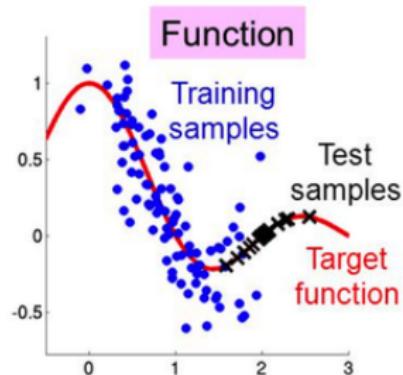
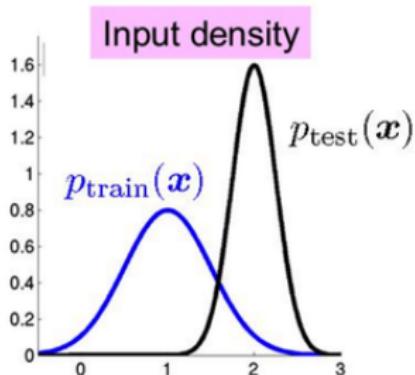
The two most common and well-studied causes of Dataset shift are:

- **Sample selection bias** (e.g. Economic studies)
- **Non stationary environments**

Covariate shift

Consider a target variable X and a response variable Y . 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:

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



Example

Consider a model designed to distinguish between images of cats and dogs:

Training set:

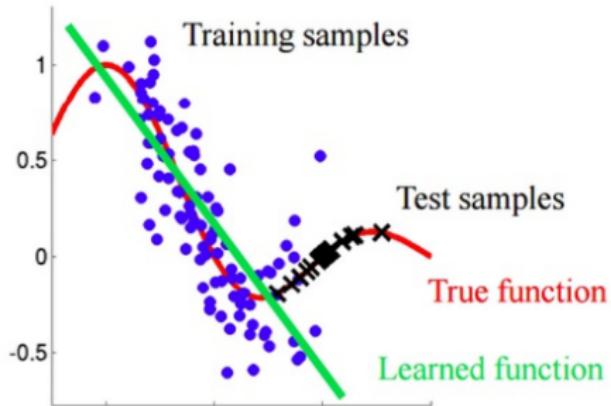


Test set:



Model will not accurately distinguish between cats and dogs because the feature distribution will differ.

Inaccurate Model



Changes in the features distribution can significantly impact the model's accuracy.

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.

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

2.

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

3.

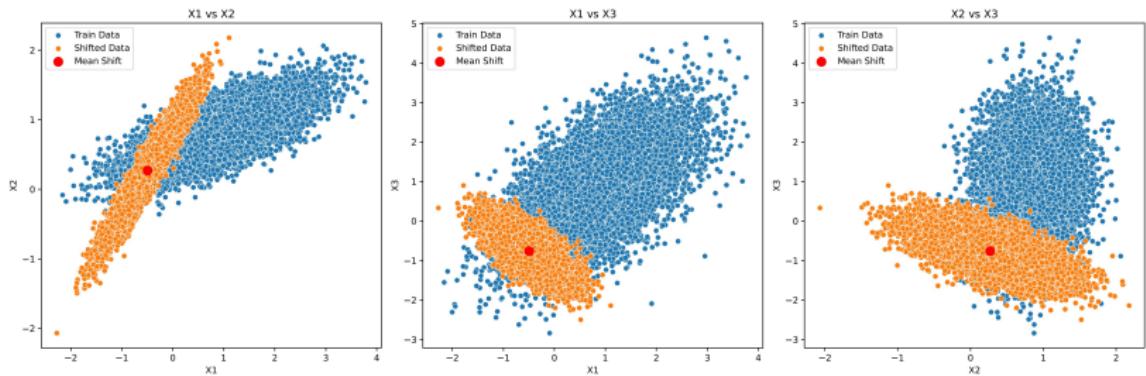
$$Y \sim \text{Be}(p)$$

Testing Dataset

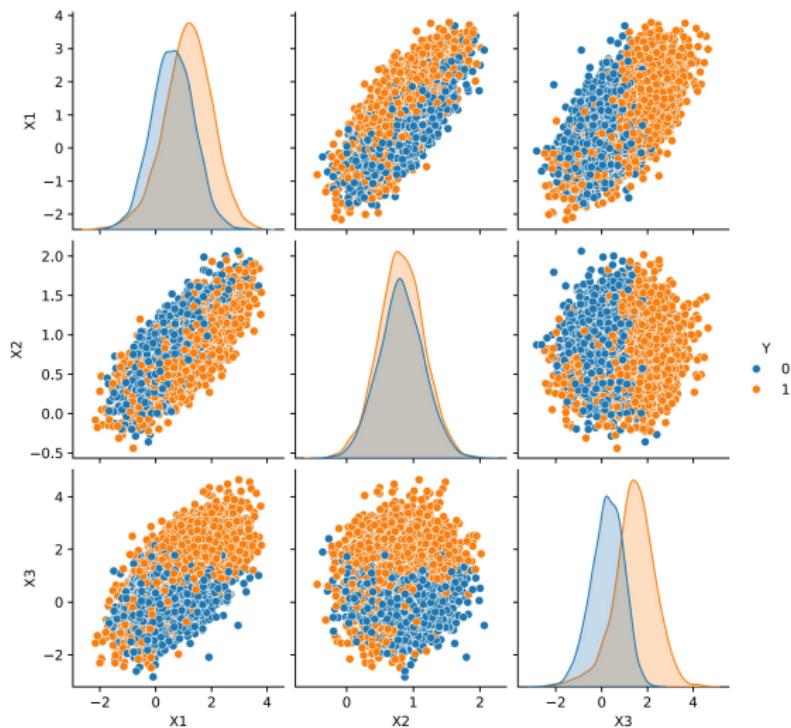
Same dataset structure as the train set, but:

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

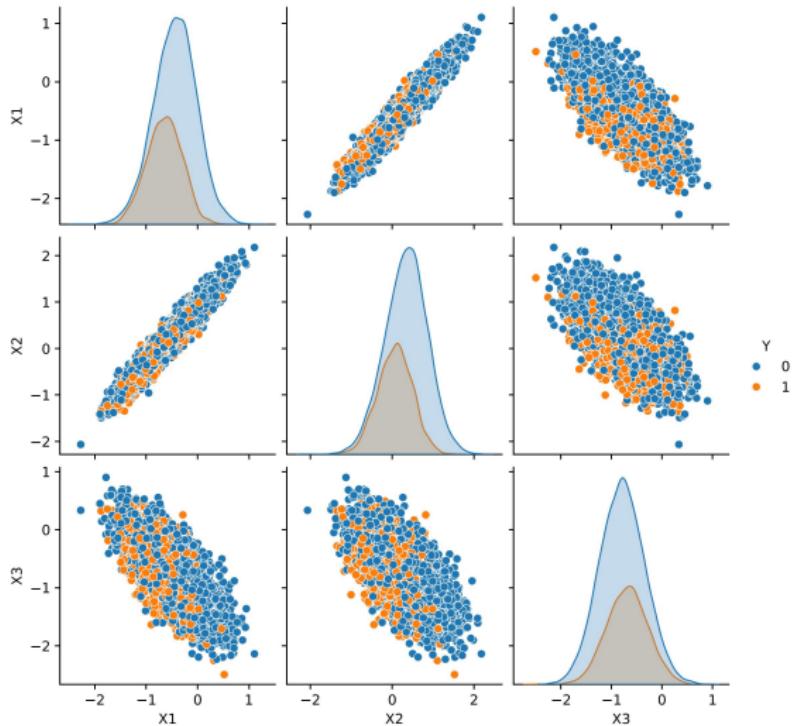
Original and Shifted Features



Label Distribution in Train Set



Label Distribution in Shifted Test Set



Note: IR from 1.19 to 2.36

Testing Mixture

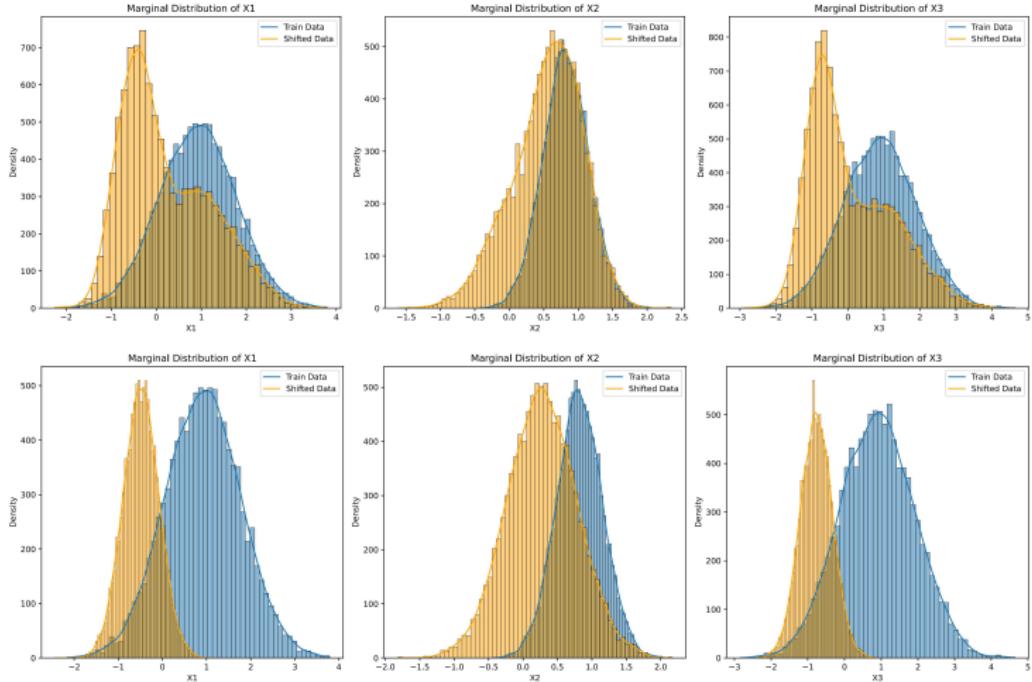
Series of datasets using **statistical mixtures** of the training features distribution and the fully shifted distribution.

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

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

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

Below are summarized the coefficients, significance ($P>|z|$), and confidence intervals for the logistic regression baseline model.

	coef	std err	z	P> z	[0.025	0.975]
Intercept	-0.9761	0.122	-8.022	0.000	-1.215	-0.738
X1	-0.6550	0.120	-5.462	0.000	-0.890	-0.420
X2	-0.2049	0.180	-1.139	0.255	-0.558	0.148
X1:X2	-0.2653	0.125	-2.118	0.034	-0.511	-0.020
X3	1.3187	0.115	11.478	0.000	1.094	1.544
X1:X3	1.3248	0.106	12.453	0.000	1.116	1.533
X2:X3	-0.3253	0.172	-1.894	0.058	-0.662	-0.011
X1:X2:X3	0.0510	0.120	0.427	0.670	-0.183	0.285

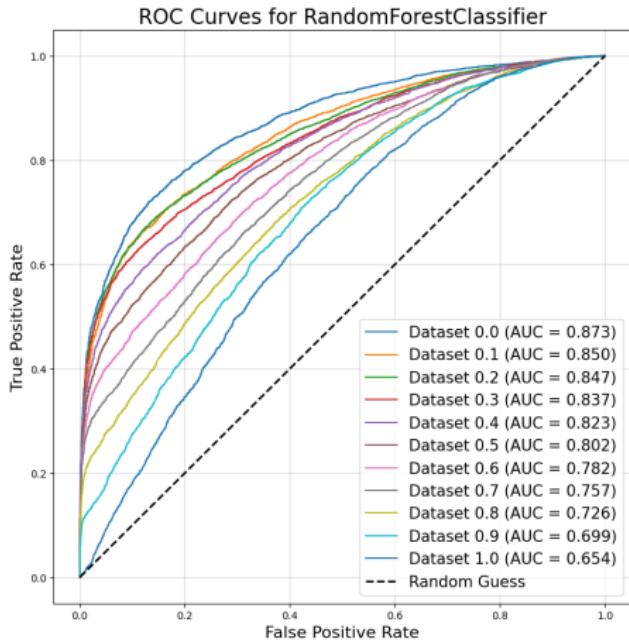
$$\log \left(\frac{p}{1-p} \right) = \sigma(-0.976 - 0.655 \cdot X_1 - 0.265 \cdot X_1 X_2 + 1.319 \cdot X_3 + 1.325 \cdot X_1 X_3)$$

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
<i>n_estimators</i>	125
<i>criterion</i>	<i>gini</i>
<i>max_depth</i>	5
<i>min_samples_split</i>	5
<i>min_samples_leaf</i>	1



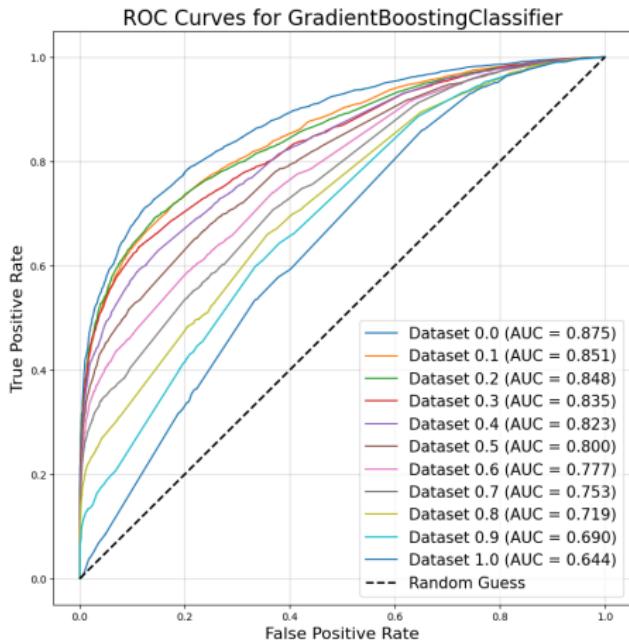
Note: We set `random_state` to 0 for reproducibility.

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.

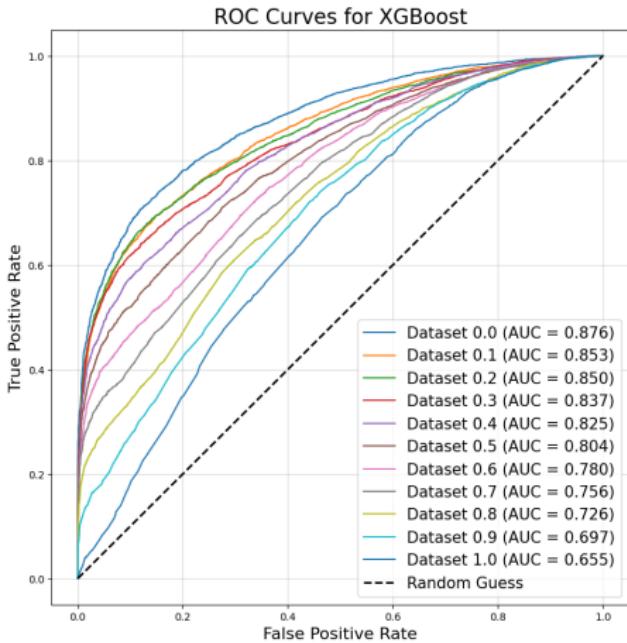
Hyperparameter	Values
<i>n_estimators</i>	125
<i>learning_rate</i>	0.025
<i>max_depth</i>	3
<i>subsample</i>	0.4



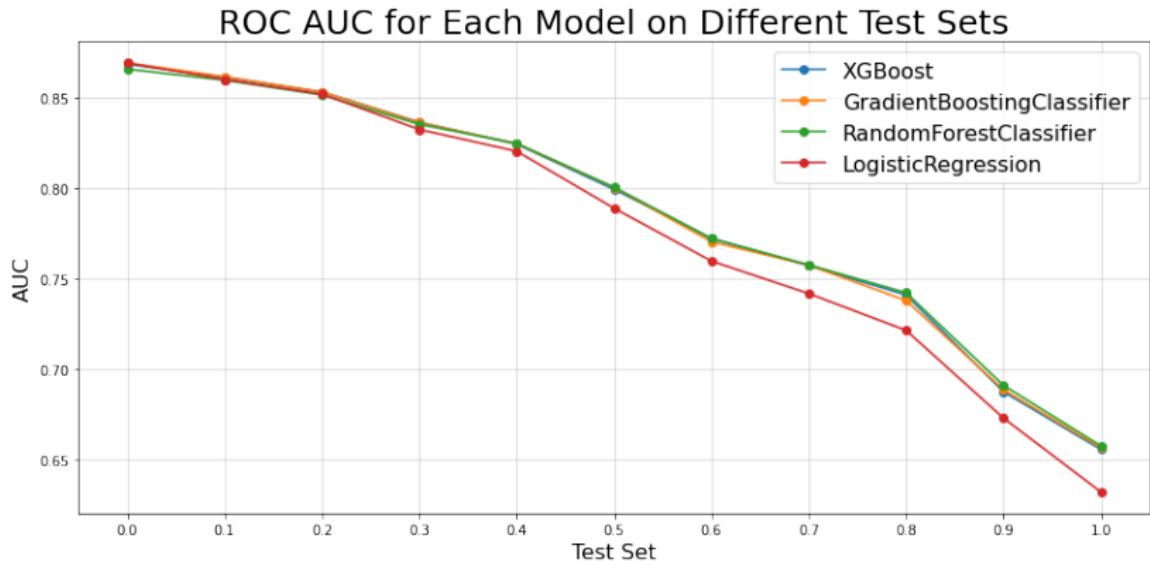
Extreme Gradient Boosting

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

Hyperparameter	Values
<i>n_estimators</i>	100
<i>learning_rate</i>	0.1
<i>max_depth</i>	6
<i>subsample</i>	0.7
<i>gamma</i>	5



Performance Comparison



The figure illustrates how model performance (AUC) decreases as α increases, reflecting greater covariate shift.

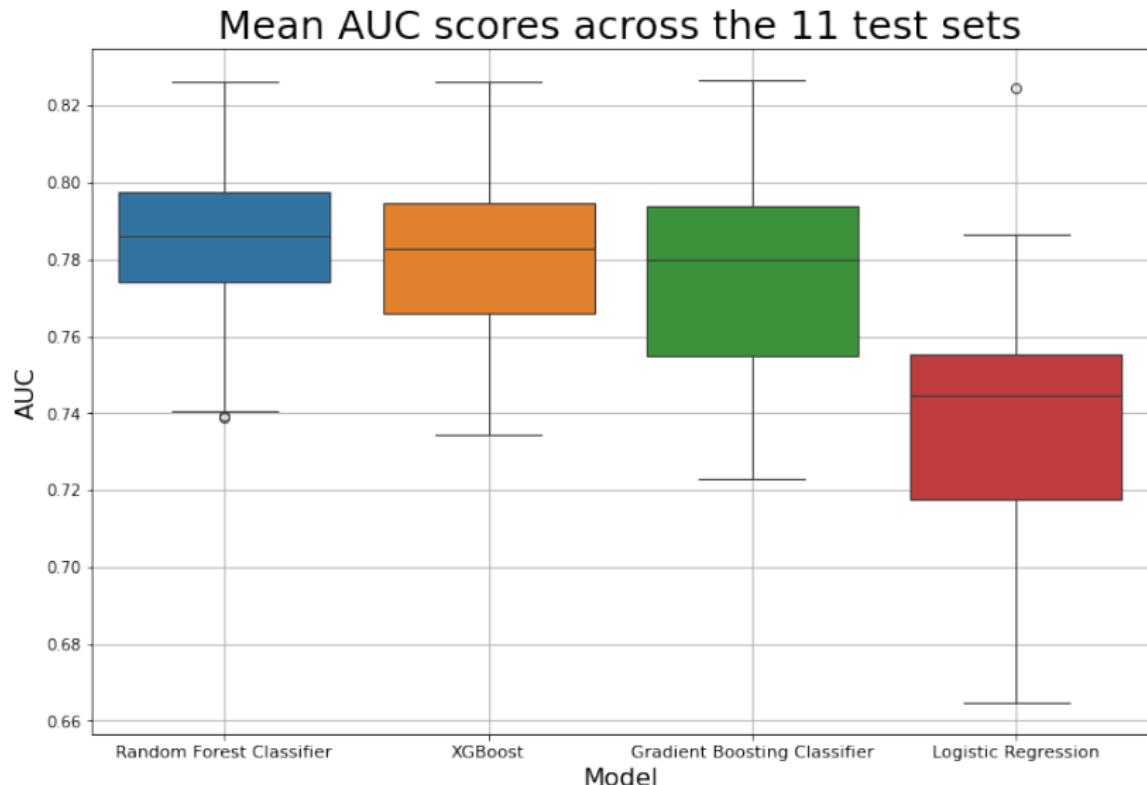
Ensemble models demonstrate higher robustness compared to the Logistic Regression baseline.

Statistical Performance Comparison

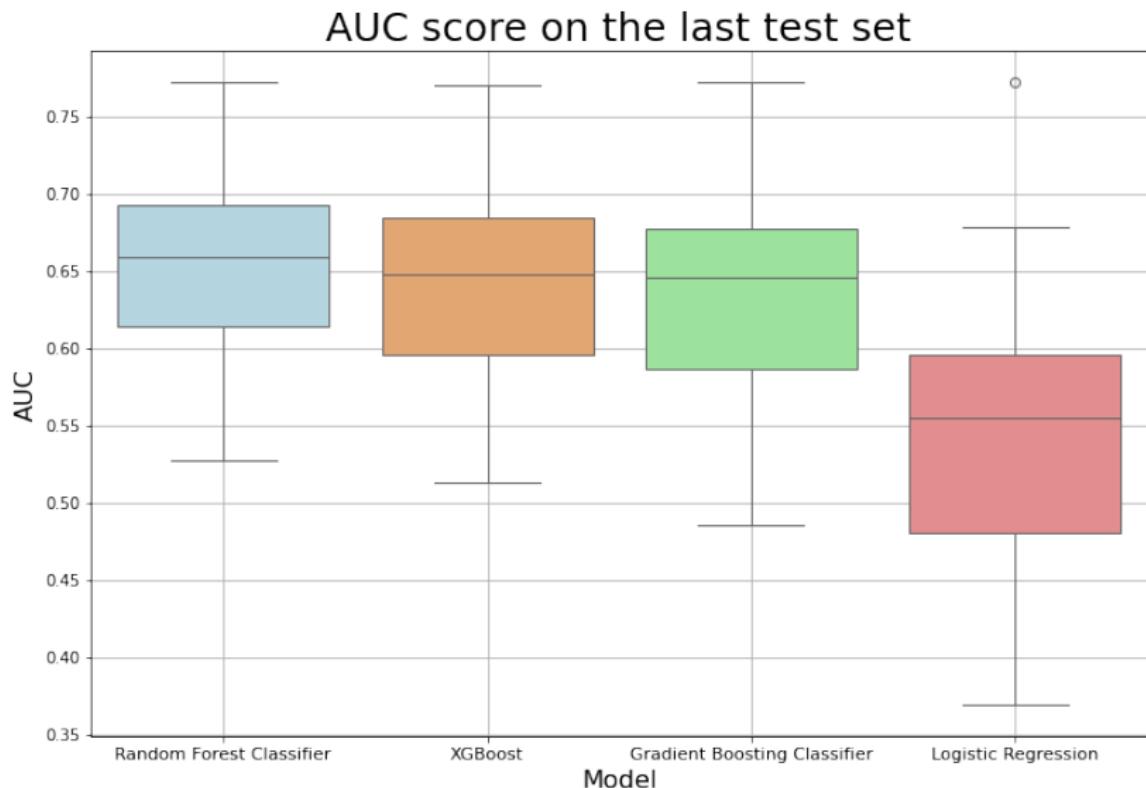
To give statistical support to our study we repeated this experiment $N = 50$ times. Keeping always the same training set (in order to not train the models several times), for each repetition we:

1. defined a new shifted distribution $\mathcal{N}(\boldsymbol{\mu}_{\text{shift}}, \boldsymbol{\Sigma}_{\text{shift}})$
2. created 11 **testing** datasets \mathcal{D}_α with $\alpha \in \{0.0, 0.1, \dots, 1.0\}$, where α represents the mixing probability as before
3. computed the ROC-AUC score for each model on each testing dataset

Statistical Performance Comparison



Statistical Performance Comparison



Performance Enhancement

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.

- Random
- Augmentation
- Walk

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

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

For x_i in $Data\%$

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

$y'_i \leftarrow y_i$

End For

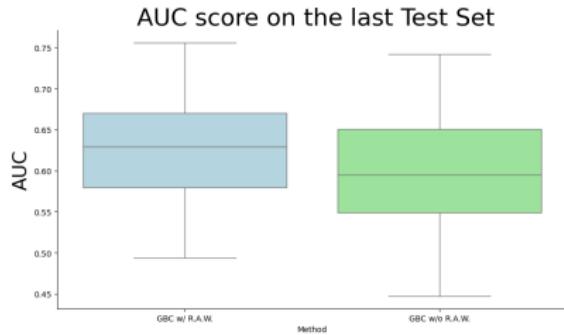
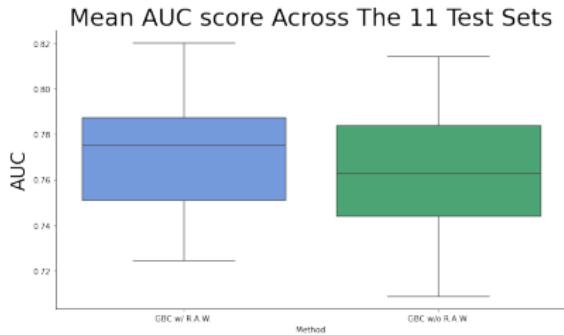
$Data_{aug} \leftarrow Data_{train} \cup Data\%$

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

Return $Data_{final}$

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

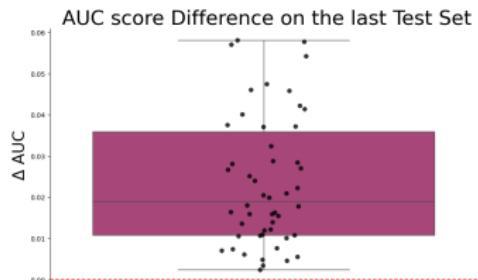
- H_0 :

$$\Delta_{AUC} = AUC_{R.A.W.} - AUC_{base} = 0$$

- H_1 :

$$\Delta_{AUC} = AUC_{R.A.W.} - AUC_{base} \neq 0$$

- **Test:** Two samples t-test on 50 independent Δ_{AUC} .



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

* Mean AUC score difference across all 11 shifted test sets.

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

Conclusion

How can we address the initial questions posed?

- Covariate shift was explored via synthetic data and repeated simulations.
- Performance degradation highlights the need for "fine-tuned" robust models.
- Every tuned model performed equally across each shift, with the exception of the Logistic Regression.
- **Future work:** Since augmentation showed mitigation potential, we are think about how to further improve the R.A.W. algorithm.

Thank You!