UNIVERSITÀ
DEGLI STUDI
DI TRIESTE

# DISTRIBUTION SHIFT

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

Andrea Spinelli, Giacomo Amerio,
Giovanni Lucarelli, Tommaso Piscitelli

University of Trieste

# Table of contents

# 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.A.W.)

# 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.

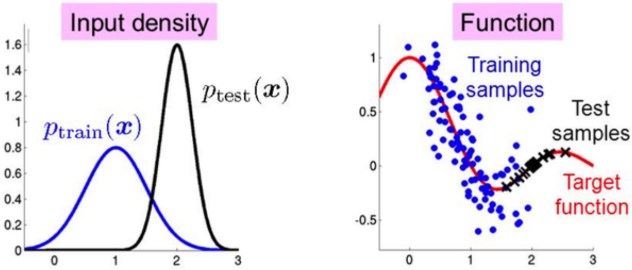
The two most common and well-studied causes of Dataset shift are:

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

# Covariate shift

Consider a target variable $X$ and a response variable $Y$. Let $P_{\text{tra}}$ denote the probability distribution of the training data and $P_{\text{tst}}$ denote the probability distribution of the test data. A **covariate shift** occurs when:

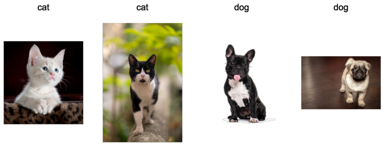
$$P_{\text{tra}}(Y \mid X) = P_{\text{tst}}(Y \mid X) \quad \text{but} \quad P_{\text{tra}}(X) \neq P_{\text{tst}}(X)$$



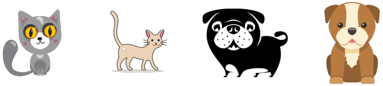
# Example

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

**Training set:**

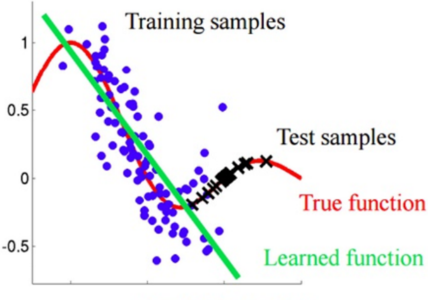



**Test set:**



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.

Features:

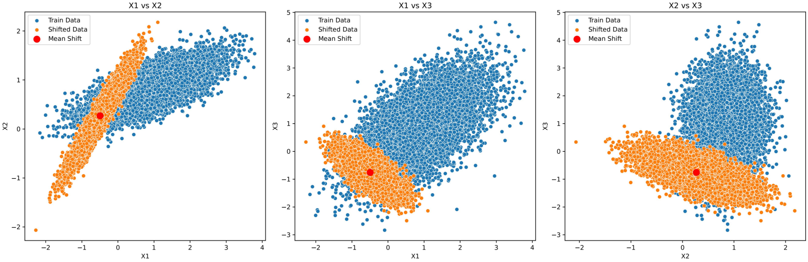
- $X_{\text{train}} = (X_{\text{train}\,1}, X_{\text{train}\,2}, X_{\text{train}\,3}) \sim \mathcal{N}(\boldsymbol{\mu}_{\text{train}}, \boldsymbol{\Sigma}_{\text{train}})$
- $\mu_{\text{train}\,i} \sim \mathcal{U}_{[0,1]}$ for $i = 1, 2, 3$
- $[\boldsymbol{\Sigma}_{\text{train}}]_{i,j} \sim \mathcal{U}_{[-1,1]}$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

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

# 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 $i, j = 1, 2, 3$



# Target Variable

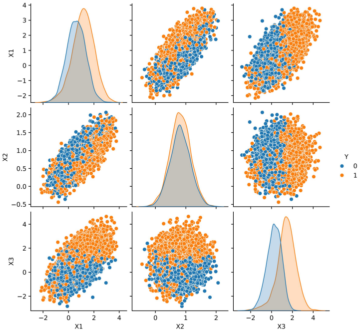
Building the **target variable** $Y \in \{0, 1\}$:

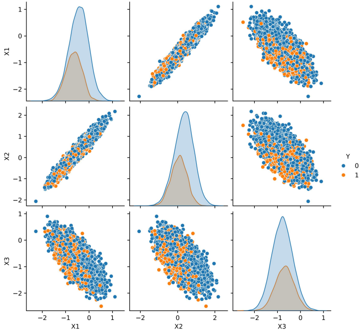
1. $$z = \beta_0 + \sum_{i=1}^{3} \beta_i x_i + \sum_{i=1}^{3} \beta_{ii} x_i^2 + \sum_{i=1}^{2} \sum_{j=i+1}^{3} \beta_{ij} x_i x_j \, , \quad \beta_{\cdot} \sim \mathcal{U}_{[-1,1]}$$

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

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

# Label Distributions




**Note:** **IR** from 1.19 to 2.36

# Testing Mixture

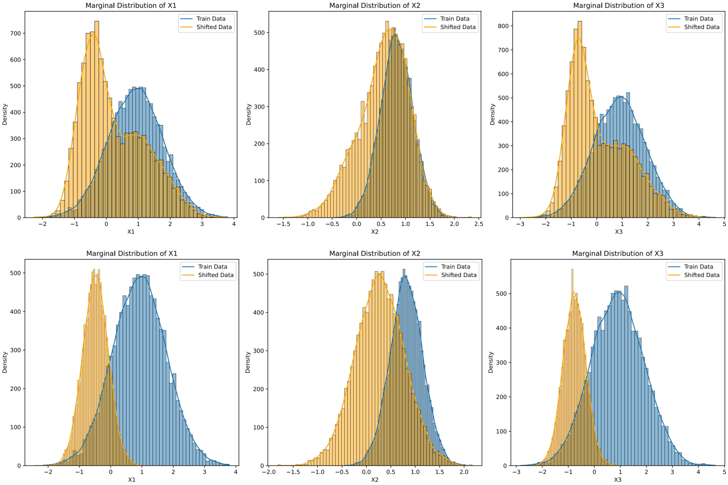
Series of datasets using **statistical mixtures** of the training features distribution and the fully shifted distribution.

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

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

$$Y_\alpha \text{ generated as before}$$

Note: $X_{0.0}$ and $X_{\text{train}}$ 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 |

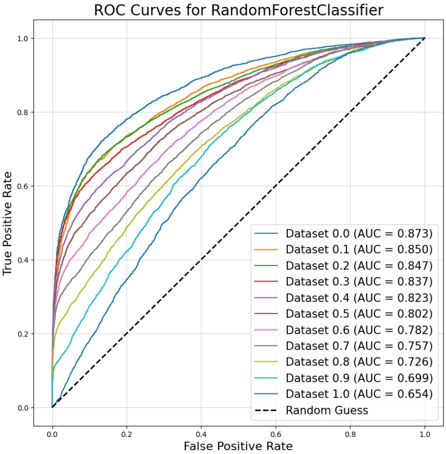
$$\log\left(\frac{p}{1-p}\right) = \sigma(-0.976 - 0.655 \cdot X_1 - 0.265 \cdot X_1 X_2 + 1.319 \cdot X_3 + 1.325 \cdot X_1 X_3)$$

# 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 |
|---|---|
| *n_estimators* | 125 |
| *criterion* | *gini* |
| *max_depth* | 5 |
| *min_samples_split* | 5 |
| *min_samples_leaf* | 1 |
| *bootstrap* | *True* |



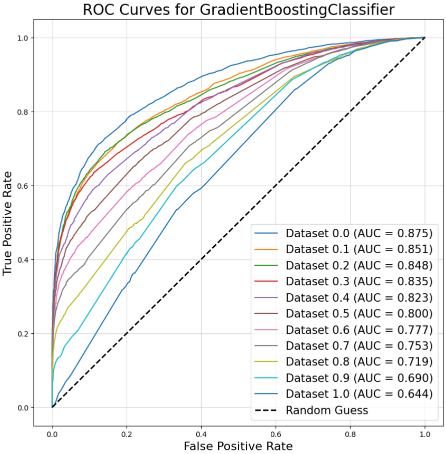

**Note:** We set `random_state` to `0` for reproducibility.

# 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.

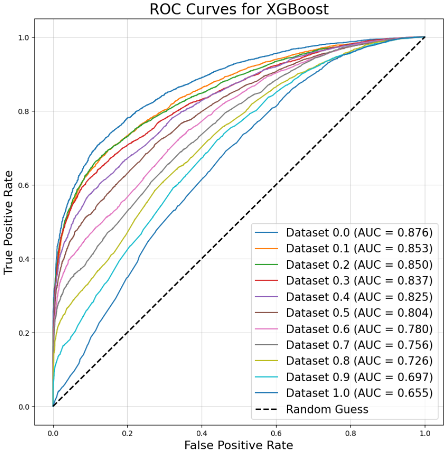
| Hyperparameter | Values |
|---|---|
| *n_estimators* | 125 |
| *learning_rate* | 0.025 |
| *max_depth* | 3 |
| *subsample* | 0.4 |



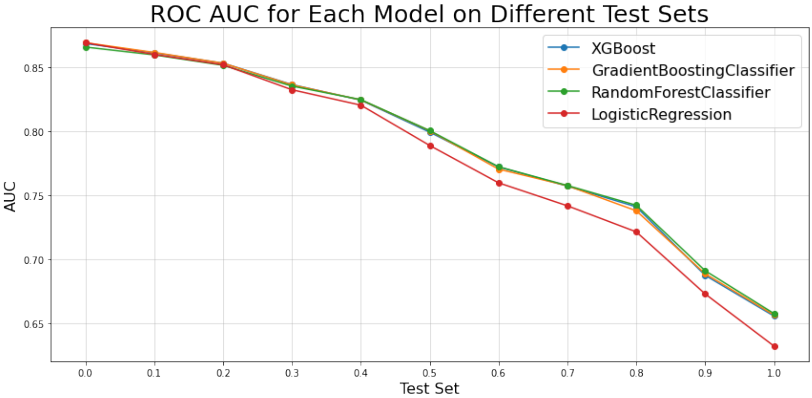
# Extreme Gradient Boosting

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




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

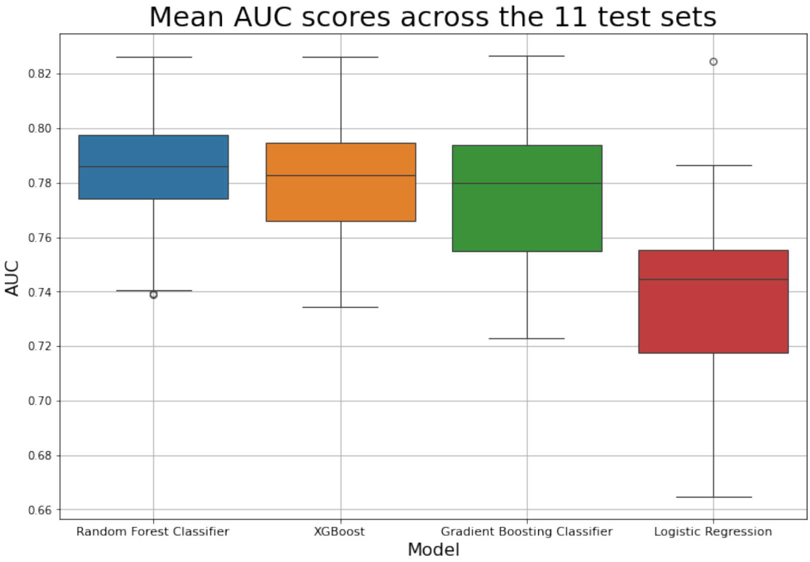
Ensemble models demonstrate higher robustness compared to the Logistic Regression baseline.

# Statistical Performance Comparison

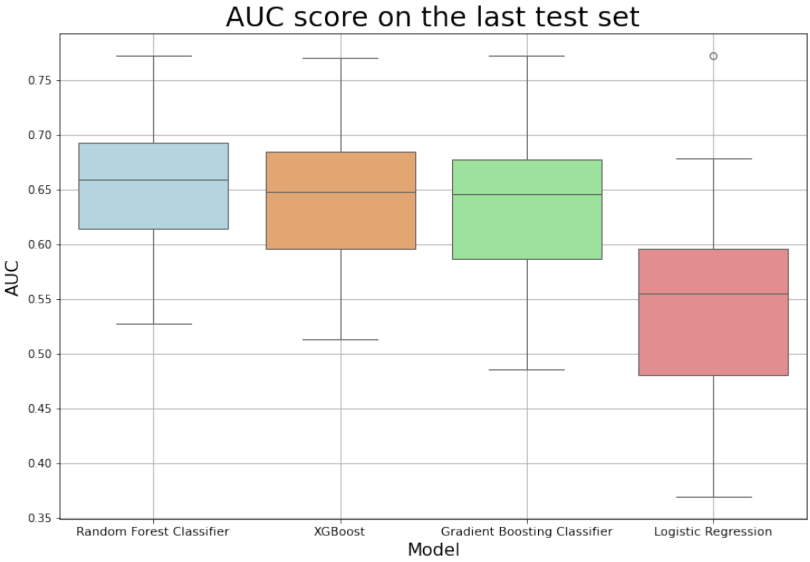
To give statistical support to our study we repeated this experiment $N = 50$ times. Keeping always the same training set (in order to not train the models several times), for each repetition we:

1. defined a new shifted ditribution $\mathcal{N}(\boldsymbol{\mu}_{\text{shift}}, \boldsymbol{\Sigma}_{\text{shift}})$
2. created 11 **testing** datasets $\mathcal{D}_\alpha$ with $\alpha \in \{0.0, 0.1, \ldots, 1.0\}$, where $\alpha$ 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

# 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:** $Data_{\text{train}}$, $Size$, $N$, $\varepsilon$.

$Data_{\%}$ ←random subset of N% of $\text{Data}_{train}$

**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**

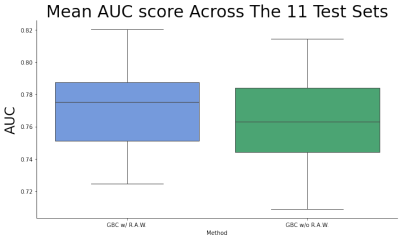
$Data_{\text{aug}} \leftarrow \text{Data}_{train} \cup Data_{\%}$

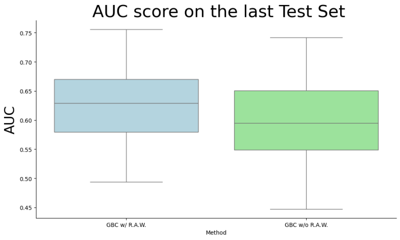
$Data_{\text{final}} \leftarrow \text{Downsample}(\text{Data}_{\text{aug}}, Size)$

**Return** $Data_{\text{final}}$

# Classify With Gradient Boosting Using R.A.W.

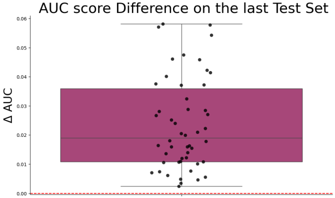
1. Apply the R.A.W. pre-processing method to the training data to address covariate shift.
2. Train a Gradient Boosting Classifier on the augmented dataset.
3. Evaluate the model's performance on shifted test sets.



# A Statistical Analysis Of The Results

- $H_0$:
  $\Delta_{AUC} = AUC_{\text{R.A.W.}} - AUC_{\text{base}} = 0$
- $H_1$:
  $\Delta_{AUC} = AUC_{\text{R.A.W.}} - AUC_{\text{base}} \neq 0$
- **Test:** Student's t-Test on 50 independent $\Delta_{AUC}$.




| | $\Delta_{AUC}$ | t-stat | p-value | 95% CI |
|---|---|---|---|---|
| $\Delta_{\overline{\text{AUC}}}$* | 0.0083 | 8.75 | $1.39 \times 10^{-11}$ | [0.006, 0.010] |
| $\Delta_{\text{AUC}_{\text{last}}}$** | 0.0235 | 10.59 | $2.86 \times 10^{-14}$ | [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!