Explanation Shift: How Did the Distribution Shift Impact the Model?

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Abstract

The performance of machine learning models on new data is critical for their success in real-world applications. However, the model's performance may deteriorate if the new data is sampled from a different distribution than the training data. Current methods to detect shifts in the input or output data distributions have limitations in identifying model behavior changes. In this paper, we define *explanation shift* as the statistical comparison between how predictions from training data are explained and how predictions on new data are explained. We propose explanation shift as a key indicator to investigate the interaction between distribution shifts and learned models. We introduce an Explanation Shift Detector that operates on the explanation distributions, providing more sensitive and explainable changes in interactions between distribution shifts and learned models. We compare explanation shifts with other methods that are based on distribution shifts, showing that monitoring for explanation shifts results in more sensitive indicators for varying model behavior. We provide theoretical and experimental evidence and demonstrate the effectiveness of our approach on synthetic and real data. Additionally, we release an open-source Python package, `skshift`, which implements our method and provides usage tutorials for further reproducibility.

1 Introduction

ML theory provides means to forecast the quality of ML models on unseen data, provided that this data is sampled from the same distribution as the data used to train and evaluate the model. If unseen data is sampled from a different distribution than the training data, model quality may deteriorate, making monitoring how the model's behavior changes crucial.

Recent research has highlighted the impossibility of reliably estimating the performance of machine learning models on unseen data sampled from a different distribution in the absence of further assumptions about the nature of the shift (Ben-David et al., 2010; Lipton et al., 2018; Garg et al., 2021b). State-of-the-art techniques attempt to model statistical distances between the distributions of the training and unseen data (Diethe et al., 2019; Labs, 2021) or the distributions of the model predictions (Garg et al., 2021b;a; Lu et al., 2023). However, these measures of *distribution shifts* only partially relate to changes of interaction between new data and trained models or they rely on the availability of a causal graph or types of shift assumptions, which limits their applicability. Thus, it is often necessary to go beyond detecting such changes and understand how the feature attribution changes (Kenthapadi et al., 2022; Haug et al., 2022; Mougan & Nielsen, 2023; Diethe et al., 2019).

The field of explainable AI has emerged as a way to understand model decisions (Barredo Arrieta et al., 2020; Molnar, 2019) and interpret the inner workings of ML models (Guidotti et al., 2018). The core idea of this paper is to go beyond the modeling of distribution shifts and monitor for *explanation shifts* to signal a change of interactions between learned models and dataset features in tabular data. We newly define explanation shift as the statistical comparison between how predictions from training data are explained and how predictions on new data are explained. In summary, our contributions are:

- We propose measures of explanation shifts as a key indicator for investigating the interaction between distribution shifts and learned models.
- We define an *Explanation Shift Detector* that operates on the explanation distributions allowing for more sensitive and explainable changes of interactions between distribution shifts and learned models.
- We compare our monitoring method that is based on explanation shifts with methods that are based on other kinds of distribution shifts. We find that monitoring for explanation shifts results in more sensitive indicators for varying model behavior.
- We release an open-source Python package `skshift`, which implements our "*Explanation Shift Detector*", along usage tutorials for reproducibility (cf. Statement 7).

2 Foundations and Related Work

2.1 Basic Notions

Supervised machine learning induces a function $f_\theta : \text{dom}(X) \to \text{dom}(Y)$, from training data $\mathcal{D}^{tr} = \{(x_0^{tr}, y_0^{tr}) \ldots, (x_n^{tr}, y_n^{tr})\}$. Thereby, f_θ is from a family of functions $f_\theta \in F$ and $\mathcal{D}^{tr}$ is sampled from the joint distribution $\mathbf{P}(X, Y)$ with predictor variables X and target variable Y. f_θ is expected to generalize well on new, previously unseen data $\mathcal{D}_X^{new} = \{x_0^{new}, \ldots, x_k^{new}\} \subseteq \text{dom}(X)$. We write $\mathcal{D}_X^{tr}$ to refer to $\{x_0^{tr}, \ldots, x_n^{tr}\}$ and $\mathcal{D}_Y^{tr}$ to refer to $\mathcal{D}_Y^{tr} = \{y_0^{tr} \ldots, y_n^{tr}\}$. For the purpose of formalizations and to define evaluation metrics, it is often convenient to assume that an oracle provides values $\mathcal{D}_Y^{new} = \{y_0^{new}, \ldots, y_k^{new}\}$ such that $\mathcal{D}^{new} = \{(x_0^{new}, y_0^{new}), \ldots, (x_k^{new}, y_k^{new})\} \subseteq \text{dom}(X) \times \text{dom}(Y)$.

The core machine learning assumption is that training data $\mathcal{D}^{tr}$ and novel data $\mathcal{D}^{new}$ are sampled from the same underlying distribution $\mathbf{P}(X, Y)$. The twin problems of *model monitoring* and recognizing that new data is *out-of-distribution* can now be described as predicting an absolute or relative performance drop between $\text{perf}(\mathcal{D}^{tr})$ and $\text{perf}(\mathcal{D}^{new})$, where $\text{perf}(\mathcal{D}) = \sum_{(x,y)\in\mathcal{D}} \ell_{\text{eval}}(f_\theta(x), y)$, ℓ_{eval} is a metric like 0-1-loss (accuracy), but $\mathcal{D}_Y^{new}$ is unknown and cannot be used for such judgment in an operating system.

Therefore related work analyses distribution shifts between training and newly occurring data. Let two datasets $\mathcal{D}, \mathcal{D}'$ define two empirical distributions $\mathbf{P}(\mathcal{D}), \mathbf{P}(\mathcal{D}')$, then we write $\mathbf{P}(\mathcal{D}) \not\sim \mathbf{P}(\mathcal{D}')$ to express that $\mathbf{P}(\mathcal{D})$ is sampled from a different underlying distribution than $\mathbf{P}(\mathcal{D}')$ with high probability $p > 1 - \epsilon$ allowing us to formalize various types of distribution shifts.

Definition 2.1 (Input Data Shift)**.** We say that data shift occurs from $\mathcal{D}^{tr}$ to $\mathcal{D}_X^{new}$, if $\mathbf{P}(\mathcal{D}_X^{tr}) \not\sim \mathbf{P}(\mathcal{D}_X^{new})$.

Specific kinds of data shift are:

Definition 2.2 (Univariate data shift)**.** There is a univariate data shift between $\mathbf{P}(\mathcal{D}_X^{tr}) = \mathbf{P}(\mathcal{D}_{X_1}^{tr}, \ldots, \mathcal{D}_{X_p}^{tr})$ and $\mathbf{P}(\mathcal{D}_X^{new}) = \mathbf{P}(\mathcal{D}_{X_1}^{new}, \ldots, \mathcal{D}_{X_p}^{new})$, if $\exists i \in \{1 \ldots p\} : \mathbf{P}(\mathcal{D}_{X_i}^{tr}) \not\sim \mathbf{P}(\mathcal{D}_{X_i}^{new})$.

Definition 2.3 (Covariate data shift)**.** There is a covariate data shift between $P(\mathcal{D}_X^{tr}) = \mathbf{P}(\mathcal{D}_{X_1}^{tr}, \ldots, \mathcal{D}_{X_p}^{tr})$ and $\mathbf{P}(\mathcal{D}_X^{new}) = \mathbf{P}(\mathcal{D}_{X_1}^{new}, \ldots, \mathcal{D}_{X_p}^{new})$ if $\mathbf{P}(\mathcal{D}_X^{tr}) \not\sim \mathbf{P}(\mathcal{D}_X^{new})$, which cannot only be caused by univariate shift.

The next two types of shift involve the interaction of data with the model f_θ, which approximates the conditional $\frac{P(\mathcal{D}_Y^{tr})}{P(\mathcal{D}_X^{tr})}$. Abusing notation, we write $f_\theta(\mathcal{D})$ to refer to the multiset $\{f_\theta(x) | x \in \mathcal{D}\}$.

Definition 2.4 (Predictions Shift)**.** There is a predictions shift between distributions $\mathbf{P}(\mathcal{D}_X^{tr})$ and $\mathbf{P}(\mathcal{D}_X^{new})$ related to model f_θ if $\mathbf{P}(f_\theta(\mathcal{D}_X^{tr})) \not\sim \mathbf{P}(f_\theta(\mathcal{D}_X^{new}))$.

Definition 2.5 (Concept Shift)**.** There is a concept shift between $\mathbf{P}(\mathcal{D}^{tr}) = \mathbf{P}(\mathcal{D}_X^{tr}, \mathcal{D}_Y^{tr})$ and $\mathbf{P}(\mathcal{D}^{new}) = \mathbf{P}(\mathcal{D}_X^{new}, \mathcal{D}_Y^{new})$ if conditional distributions change, i.e. $\frac{\mathbf{P}(\mathcal{D}_Y^{tr})}{\mathbf{P}(\mathcal{D}_X^{tr})} \not\sim \frac{\mathbf{P}(\mathcal{D}_Y^{new})}{\mathbf{P}(\mathcal{D}_X^{new})}$.

In practice, multiple types of shifts co-occur together and their disentangling may constitute a significant challenge that we do not address here.

2.2 Related Work on Tabular Data

We briefly review the related works below. See Appendix A for a more detailed related work.

Classifier two-sample test: Evaluating how two distributions differ has been a widely studied topic in the statistics and statistical learning literature (Hastie et al., 2001; Quiñonero-Candela et al., 2009; Liu et al., 2020a) and has advanced in recent years (Park et al., 2021a; Lee et al., 2018; Zhang et al., 2013). The use of supervised learning classifiers to measure statistical tests has been explored by Lopez-Paz & Oquab (2017) proposing a classifier-based approach that returns test statistics to interpret differences between two distributions. We adopt their power test analysis and interpretability approach but apply it to the explanation distributions instead of input data distributions.

Detecting distribution shift and its impact on model behaviour: A lot of related work has aimed at detecting that data is from out-of-distribution. To this end, they have created several benchmarks that measure whether data comes from in-distribution or not (Koh et al., 2021; Sagawa et al., 2021; Malinin et al., 2021a; 2022; 2021b). In contrast, our main aim is to evaluate the impact of the distribution shift on the model.

A typical example is two-sample testing on the latent space such as described by Rabanser et al. (2019). However, many of the methods developed for detecting out-of-distribution data are specific to neural networks processing image and text data and can not be applied to traditional machine learning techniques. These methods often assume that the relationships between predictor and response variables remain unchanged, i.e., no concept shift occurs. Our work is applied to tabular data where techniques such as gradient boosting decision trees achieve state-of-the-art model performance (Grinsztajn et al., 2022; Elsayed et al., 2021; Borisov et al., 2021).

Impossibility of model monitoring: Recent research findings have formalized the limitations of monitoring machine learning models in the absence of labelled data. Specifically (Garg et al., 2021b; Chen et al., 2022b) prove the impossibility of predicting model degradation or detecting out-of-distribution data with certainty (Fang et al., 2022; Zhang et al., 2021; Guerin et al., 2022). Although our approach does not overcome these limitations, it provides valuable insights for machine learning engineers to better understand changes in interactions between learned models and shifting data distributions.

Model monitoring and distribution shift under specific assumptions: Under specific types of assumptions, model monitoring and distribution shift become feasible tasks. One type of assumption often found in the literature is to leverage causal knowledge to identify the drivers of distribution changes (Budhathoki et al., 2021; Zhang et al., 2022; Schrouff et al., 2022). For example, Budhathoki et al. (2021) use graphical causal models and feature attributions based on Shapley values to detect changes in the distribution. Similarly, other works aim to detect specific distribution shifts, such as covariate or concept shifts. Our approach does not rely on additional information, such as a causal graph, labelled test data, or specific types of distribution shift. Still, by the nature of pure concept shifts, the model behaviour remains unaffected and new data need to come with labelled responses to be detected.

Explainability and distribution shift: Lundberg et al. (2020a) applied Shapley values to identify possible bugs in the pipeline by visualizing univariate SHAP contributions. Following this line of work, Nigenda et al. (2022) compare the order of the feature importance using the NDCG between training and unseen data. We go beyond their work and formalize the multivariate explanation distributions on which we perform a two-sample classifier test to detect how distribution shift impacts interaction with the model. Furthermore, we provide a mathematical analysis of how the SHAP values contribute to detecting distribution shift. In Appendix D we provide a formal comparison against Nigenda et al. (2022).

2.3 Explainable AI: Local Feature Attributions

Attribution by Shapley values explains machine learning models by determining the relevance of features used by the model (Lundberg et al., 2020a; Lundberg & Lee, 2017b). The Shapley value is a concept from coalition game theory that aims to allocate the surplus generated by the grand coalition in a game to each of its players (Shapley, 1953). The Shapley value $\mathcal{S}_j$ for the j'th player is defined via a value function $\mathrm{val}: 2^N \to \mathbb{R}$ of players in T:

$$\mathcal{S}_j(\mathrm{val}) = \sum_{T \subseteq N \setminus \{j\}} \frac{|T|!(p-|T|-1)!}{p!}(\mathrm{val}(T \cup \{j\}) - \mathrm{val}(T)) \tag{1}$$

$$\text{where} \quad \mathrm{val}_{f,x}(T) = E_{X|X_T=x_T}[f(X)] - E_X[f(X)] \tag{2}$$

In machine learning, $N = \{1, \ldots, p\}$ is the set of features occurring in the training data. Given that x is the feature vector of the instance to be explained, and the term $\mathrm{val}_{f,x}(T)$ represents the prediction for the feature values in T that are marginalized over features that are not included in T. The Shapley value framework satisfies several theoretical properties (Molnar, 2019; Shapley, 1953; Winter, 2002; Aumann & Dreze, 1974). Our approach is based on the efficiency and uninformative properties:

Efficiency Property. Feature contributions add up to the difference of prediction from $x^\star$ and the expected value,$\sum_{j \in N} \mathcal{S}_j(f, x^\star) = f(x^\star) - E[f(X)])$

Uninformativeness Property. A feature j that does not change the predicted value has a Shapley value of zero.$\forall x, x_j, x'_j : f(\{x_{N\setminus\{j\}}, x_j\}) = f(\{x_{N\setminus\{j\}}, x'_j\}) \Rightarrow \forall x : \mathcal{S}_j(f, x) = 0$.

Our approach works with explanation techniques that fulfill efficiency and uninformative properties, and we use Shapley values as an example. It is essential to distinguish between the theoretical Shapley values and the different implementations that approximate them, in Appendix H we provide an experimental comparison of different aproaches.

LIME is another explanation method candidate for our approach (Ribeiro et al., 2016b;a) that can potentially satisfy efficiency and uninformative properties, even thought several research has highlighted unstability and difficulties with the definition of neighborhoods. In Appendix G, we analyze LIME's relationship with Shapley values for the purpose of describing explanation shifts.

3 A Model for Explanation Shift Detection

Our model for explanation shift detection is sketched in Fig. 1. We define it as follows:

Definition 3.1 (Explanation distribution)**.** An explanation function $\mathcal{S} : F \times \mathrm{dom}(X) \to \mathbb{R}^p$ maps a model $f_\theta \in F$ and data $x \in \mathbb{R}^p$ to a vector of attributions $\mathcal{S}(f_\theta, x) \in \mathbb{R}^p$. We call $\mathcal{S}(f_\theta, x)$ an explanation. We write $\mathcal{S}(f_\theta, \mathcal{D})$ to refer to the empirical *explanation distribution* generated by $\{\mathcal{S}(f_\theta, x) | x \in \mathcal{D}\}$.

We use local feature attribution methods SHAP and LIME as explanation functions $\mathcal{S}$.

Definition 3.2 (Explanation shift)**.** Given a model f_θ learned from $\mathcal{D}^{tr}$, explanation shift with respect to the model f_θ occurs if $\mathcal{S}(f_\theta, \mathcal{D}_X^{new}) \not\sim \mathcal{S}(f_\theta, \mathcal{D}_X^{tr})$.

Definition 3.3 (Explanation shift metrics)**.** Given a measure of statistical distances d, explanation shift is measured as the distance between two explanations of the model f_θ by $d(\mathcal{S}(f_\theta, \mathcal{D}_X^{tr}), \mathcal{S}(f_\theta, \mathcal{D}_X^{new}))$.

We follow Lopez et al. (Lopez-Paz & Oquab, 2017) to define an explanation shift metrics based on a two-sample test classifier. We proceed as depicted in Figure 1. To counter overfitting, given the model f_θ trained on $\mathcal{D}^{\mathrm{tr}}$, we compute explanations $\{\mathcal{S}(f_\theta, x) | x \in \mathcal{D}_X^{\mathrm{val}}\}$ on an in-distribution validation data set $\mathcal{D}_X^{\mathrm{val}}$. Given a dataset $\mathcal{D}_X^{new}$, for which the status of in- or out-of-distribution is unknown, we compute its explanations $\{\mathcal{S}(f_\theta, x) | x \in \mathcal{D}_X^{\mathrm{new}}\}$. Then, we construct a two-samples dataset $E = \{(S(f_\theta, x), a_x) | x \in \mathcal{D}_X^{\mathrm{val}}, a_x = 0\} \cup \{(S(f_\theta, x), a_x) | x \in \mathcal{D}_X^{\mathrm{new}}, a_x = 1\}$ and we train a discrimination model $g_\psi : R^p \to \{0, 1\}$ on E, to predict if an explanation should be classified as in-distribution (ID) or out-of-distribution (OOD):

$$\psi = \arg\min_{\tilde{\psi}} \sum_{x \in \mathcal{D}_X^{\mathrm{val}} \cup \mathcal{D}_X^{\mathrm{new}}} \ell(g_{\tilde{\psi}}(\mathcal{S}(f_\theta, x)), a_x), \tag{3}$$

where ℓ is a classification loss function (e.g. cross-entropy). g_ψ is our two-sample test classifier, based on which AUC yields a test statistic that measures the distance between the D_X^{tr} explanations and the explanations of new data D_X^{new}.

Explanation shift detection allows us to detect *that* a novel dataset D^{new} changes the model's behavior. Beyond recognizing explanation shift, using feature attributions for the model g_ψ, we can interpret *how* the features of the novel dataset D_X^{new} interact differently with model f_θ than the features of the validation dataset D_X^{val}. These features are to be considered for model monitoring and for classifying new data as out-of-distribution.

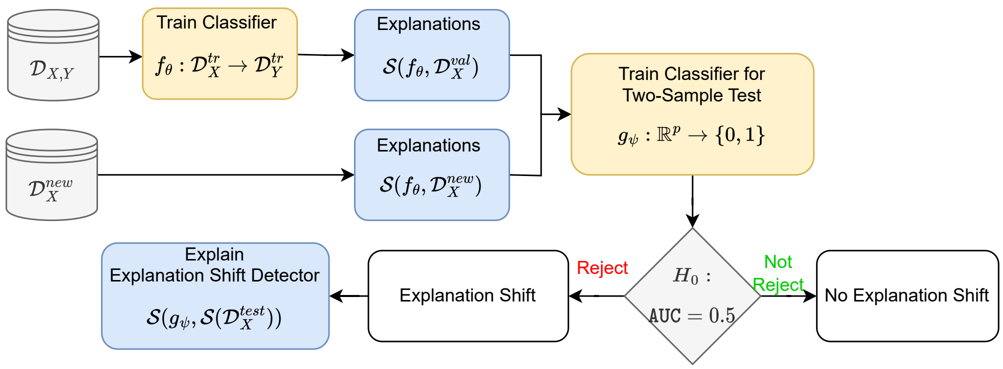

Figure 1: Our model for explanation shift detection. The model f_θ is trained on $\mathcal{D}^{tr}$ implying explanations for distributions $\mathcal{D}_X^{val}, \mathcal{D}_X^{new}$. The AUC of the two-sample test classifier g_ψ decides for or against explanation shift. If an explanation shift occurred, it could be explained which features of the $\mathcal{D}_X^{new}$ deviated in f_θ compared to $\mathcal{D}_X^{val}$.

4 Relationships between Common Distribution Shifts and Explanation Shifts

This section analyses and compares data shifts and prediction shifts with explanation shifts. Appendix B extends this into a detailed analysis, and Appendix C draws from these analyses to derive experiments with synthetic data.

4.1 Explanation Shift vs Data Shift

One type of distribution shift that is challenging to detect comprises cases where the univariate distributions for each feature j are equal between the source $\mathcal{D}_X^{tr}$ and the unseen dataset $\mathcal{D}_X^{new}$, but where interdependencies among different features change. Multi-covariance statistical testing is a hard taks with high sensitivity that can lead to false positives. The following example demonstrates that Shapley values account for co-variate interaction changes while a univariate statistical test will provide false negatives.

Example 4.1. ***(Covariate Shift)*** *Let* $D^{tr} \sim N\left(\begin{bmatrix}\mu_1\\ \mu_2\end{bmatrix}, \begin{bmatrix}\sigma^2_{X_1} & 0\\ 0 & \sigma^2_{X_2}\end{bmatrix}\right) \times Y$. *We fit a linear model* $f_\theta(x_1, x_2) = \gamma + a \cdot x_1 + b \cdot x_2$. *If* $\mathcal{D}_X^{new} \sim N\left(\begin{bmatrix}\mu_1\\ \mu_2\end{bmatrix}, \begin{bmatrix}\sigma^2_{X_1} & \rho\sigma_{X_1}\sigma_{X_2}\\ \rho\sigma_{X_1}\sigma_{X_2} & \sigma^2_{X_2}\end{bmatrix}\right)$, *then* $\mathbf{P}(\mathcal{D}_{X_1}^{tr})$ *and* $\mathbf{P}(\mathcal{D}_{X_2}^{tr})$ *are identically distributed with* $\mathbf{P}(\mathcal{D}_{X_1}^{new})$ *and* $\mathbf{P}(\mathcal{D}_{X_2}^{new})$, *respectively, while this does not hold for the corresponding* $\mathcal{S}_j(f_\theta, \mathcal{D}_X^{tr})$ *and* $\mathcal{S}_j(f_\theta, \mathcal{D}_X^{new})$.

False positives frequently occur in out-of-distribution data detection when a statistical test recognizes differences between a source distribution and a new distribution, though the differences do not affect the model behavior (Grinsztajn et al., 2022; Huyen, 2022). Shapley values satisfy the *Uninformativeness* property, where a feature j that does not change the predicted value has a Shapley value of 0 (equation 2.3).

Example 4.2. ***Shifts on Uninformative Features.*** *Let the random variables* X_1, X_2 *be normally distributed with* $N(0;1)$. *Let dataset* $\mathcal{D}^{tr} \sim X_1 \times X_2 \times Y^{tr}$, *with* $Y^{tr} = X_1$.

Thus $Y^{tr} \perp X_2$. Let $\mathcal{D}_X^{new} \sim X_1 \times X_2^{new}$ and X_2^{new} be normally distributed with $N(\mu;\sigma^2)$ and $\mu, \sigma \in \mathbb{R}$. When f_θ is trained optimally on $\mathcal{D}^{tr}$ then $f_\theta(x) = x_1$. $\mathbf{P}(\mathcal{D}_{X_2}^{tr})$ can be different from $\mathbf{P}(\mathcal{D}_{X_2}^{new})$ but $\mathcal{S}_2(f_\theta, \mathcal{D}_X^{tr}) = 0 = \mathcal{S}_2(f_\theta, \mathcal{D}_X^{new})$.

4.2 Explanation Shift vs Prediction Shift

Analyses of the explanations detect distribution shifts that interact with the model. In particular, if a prediction shift occurs, the explanations produced are also shifted.

Proposition 1. Given a model $f_\theta : \mathcal{D}_X \to \mathcal{D}_Y$. If $f_\theta(x') \neq f_\theta(x)$, then $\mathcal{S}(f_\theta, x') \neq \mathcal{S}(f_\theta, x)$.

By efficiency property of the Shapley values (Aas et al., 2021) (equation ((2.3))), if the prediction between two instances is different, then they differ in at least one component of their explanation vectors.

The opposite direction does not always hold: Thus, an explanation shift does not always imply a prediction shift.

Example 4.3. ***(Explanation shift not affecting prediction distribution)*** *Given $\mathcal{D}^{tr}$ is generated from $(X_1 \times X_2 \times Y), X_1 \sim U(0,1), X_2 \sim U(1,2), Y = X_1 + X_2 + \epsilon$ and thus the optimal model is $f(x) = x_1 + x_2$. If $\mathcal{D}^{new}$ is generated from $X_1^{new} \sim U(1,2), X_2^{new} \sim U(0,1), \quad Y^{new} = X_1^{new} + X_2^{new} + \epsilon$, the prediction distributions are identical $f_\theta(\mathcal{D}_X^{tr}), f_\theta(\mathcal{D}_X^{new}) \sim U(1,3)$, but explanation distributions are different $S(f_\theta, \mathcal{D}_X^{tr}) \not\sim S(f_\theta, \mathcal{D}_X^{new})$, because $\mathcal{S}_i(f_\theta, x) = \alpha_i \cdot x_i$.*

4.3 Explanation Shift vs Concept Shift

Concept shift comprises cases where the covariates retain a given distribution, but their relationship with the target variable changes (cf. Section 2.1). This example shows the negative result that concept shift cannot be indicated by the detection of explanation shift.

Example 4.4. ***Concept Shift*** *Let $\mathcal{D}^{tr} \sim X_1 \times X_2 \times Y$, and create a synthetic target $y_i^{tr} = a_0 + a_1 \cdot x_{i,1} + a_2 \cdot x_{i,2} + \epsilon$. As new data we have $\mathcal{D}_X^{new} \sim X_1^{new} \times X_2^{new} \times Y$, with $y_i^{new} = b_0 + b_1 \cdot x_{i,1} + b_2 \cdot x_{i,2} + \epsilon$ whose coefficients are unknown at prediction stage. With coefficients $a_0 \neq b_0, a_1 \neq b_1, a_2 \neq b_2$. We train a linear regression $f_\theta : \mathcal{D}_X^{tr} \to \mathcal{D}_Y^{tr}$. Then explanations have the same distribution, $\mathbf{P}(\mathcal{S}(f_\theta, \mathcal{D}_X^{tr})) = \mathbf{P}(\mathcal{S}(f_\theta, \mathcal{D}_X^{new}))$, input data distribution $\mathbf{P}(\mathcal{D}_X^{tr}) = \mathbf{P}(\mathcal{D}_X^{new})$ and predictions $\mathbf{P}(f_\theta(\mathcal{D}_X^{tr})) = \mathbf{P}(f_\theta(\mathcal{D}_X^{new}))$. But there is no guarantee on the performance of f_θ on $\mathcal{D}_X^{new}$ (Garg et al., 2021b)*

In general, concept shift cannot be detected because $\mathcal{D}_Y^{new}$ is unknown (Garg et al., 2021b). Some research studies have made specific assumptions about the conditional $\frac{P(\mathcal{D}_Y^{new})}{P(\mathcal{D}_X^{new})}$ in order to monitor models and detect distribution shift (Lu et al., 2023; Alvarez et al., 2023). In Appendix B.2.2, we analyze a situation in which an oracle — hypothetically — provides $\mathcal{D}_Y^{new}$.

5 Empirical Evaluation

We evaluate the effectiveness of explanation shift detection on tabular data by comparing it against methods from the literature, which are all based on discovering distribution shifts. For this comparison, we systematically vary models f, model parametrizations θ, and input data distributions $\mathcal{D}_X$. We complement core experiments described in this section by adding further experimental results in the appendix that (i) add details on experiments with synthetic data (Appendix C), (ii) add experiments on further natural datasets (Appendix E), (iii) exhibit a larger range of modeling choices (Appendix F),and (iv) contrast our SHAP-based method against the use of LIME, an alternative explanation approach (Appendix G). Core observations made in this section will only be confirmed and refined but not countered in the appendix.

5.1 Baseline Methods and Datasets

Baseline Methods. We compare our method of explanation shift detection (Section 3) with several methods that aim to detect that input data is out-of-distribution: *(B1)* statistical Kolmogorov Smirnov test on input data (Rabanser et al., 2019), *(B2)* prediction shift detection by Wasserstein distance (Lu et al., 2023), *(B3)* NDCG-based test of feature importance between the two distributions (Nigenda et al., 2022), *(B4)* prediction shift detection by Kolmogorov-Smirnov test (Diethe et al., 2019), and *(B5)* model agnostic uncertainty estimation (Mougan & Nielsen, 2023; Kim et al., 2020). All Distribution Shift Metrics are scaled between 0 and 1. We also compare against Classifier Two-Sample Test (Lopez-Paz & Oquab, 2017) on different distributions as discussed in Section 4, viz. *(B6)* classifier two-sample test on input distributions (g_ϕ) and *(B7)* classifier two-sample test on the predictions distributions (g_Υ):

$$\phi = \arg\min_{\tilde{\phi}} \sum_{x \in \mathcal{D}_X^{val} \cup \mathcal{D}_X^{new}} \ell(g_{\tilde{\phi}}(x)), a_x) \qquad \Upsilon = \arg\min_{\tilde{\Upsilon}} \sum_{x \in \mathcal{D}_X^{val} \cup \mathcal{D}_X^{new}} \ell(g_{\tilde{\Upsilon}}(f_\theta(x)), a_x) \tag{4}$$

Datasets. In the main body of the paper we base our comparisons on the UCI Adult Income dataset Dua & Graff (2017) and on synthetic data. In the Appendix, we extend experiments to several other datasets, which confirm our findings: ACS Travel Time (Ding et al., 2021b), ACS Employment, Stackoverflow dataset (Stackoverflow, 2019).

5.2 Experiments on Synthetic Data

Our first experiment on synthetic data showcases the two main contributions of our method: (i) being more sensitive than prediction shift and input shift to changes in the model and (ii) accounting for its drivers. We first generate a synthetic dataset $\mathcal{D}^\rho$, with a parametrized multivariate shift between (X_1, X_2), where ρ is the correlation coefficient, and an extra variable $X_3 = N(0,1)$ and generate our target $Y = X_1 \cdot X_2 + X_3$. We train the f_θ on $\mathcal{D}^{tr,\rho=0}$ using a gradient boosting decision tree, while for $g_\psi : \mathcal{S}(f_\theta, \mathcal{D}_X^{val,\rho}) \rightarrow \{0,1\}$, we train on different datasests with different values of ρ. For g_ψ we use a logistic regression. In Appendix F, we benchmark other models f_θ and detectors g_ψ.

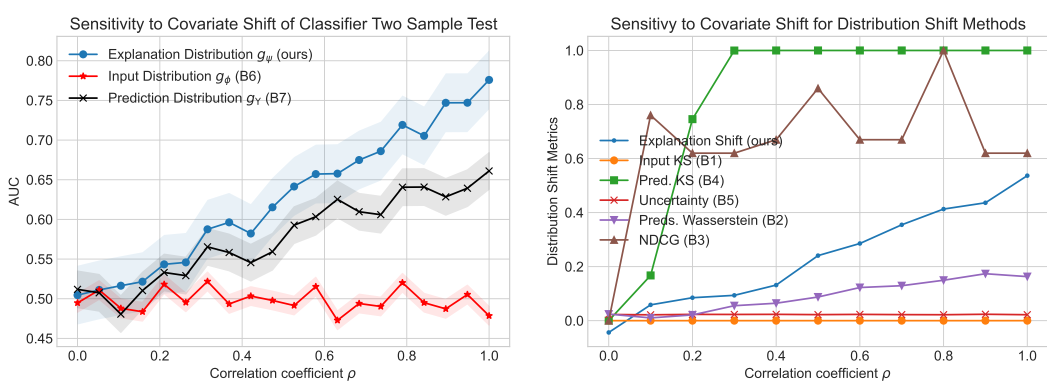

Figure 2: In the left figure, we compare the Classifier Two-Sample Test on explanation distribution (ours) versus input distribution *(B6)* and prediction distribution *(B6)*. Explanation distribution shows the highest sensitivity. The right figure, related work comparison of distribution shift methods*(B1-B5)*, as the experimental setup has a gradual distribution shift, good indicators should follow a progressive steady positive slope, following the correlation coefficient, as our method does.

The left image in Figure 2 compares our approach against C2ST on input data distribution *(B6)* and on the predictions distribution *(vii)* different data distributions, for detecting multi-covariate shifts on different distributions. In our covariate experiment, we observed that using the explanation shift led to higher sensitivity towards detecting distribution shift. We interpret the results with the efficiency property of the Shapley values, which decomposes the vector $f_\theta(\mathcal{D}_X)$ into the matrix $\mathcal{S}(f_\theta, \mathcal{D}_X)$. Moreover, we can identify the features that cause the drift by extracting the coefficients of g_ψ, providing global and local explainability.

The right image features the same setup comparing against the other out-of-distribution detection methods previously discused. We can see how our method behaves favorably compared to the others.

5.2.1 Novel Group Shift

The distribution shift in this experimental setup is constituted by the appearance of a hitherto unseen group at prediction time (the group information is not present in the training features). We vary the ratio of presence of this unseen group in $\mathcal{D}_X^{new}$ data. As f_θ we use a gradient-boosting decision tree (f_θ) and a logistic regression(g_ϕ). We compare the performance of different algorithms for f_θ and g_ψ in Appendix F.1, vary hyperparameters in Appendix F.2 and extend experiments in Appendix D.

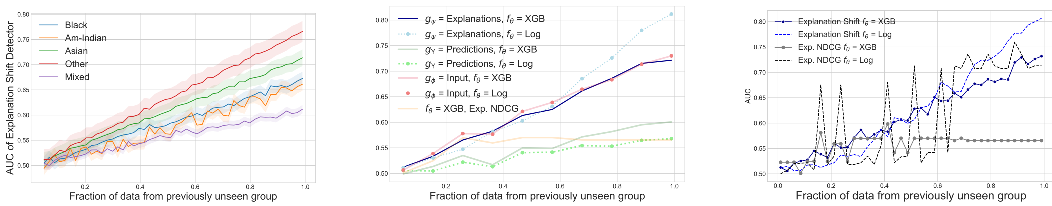

Figure 3: Novel group shift experiment on the US Income dataset. Sensitivity (AUC) increases with the growing fraction of previously unseen social groups. *Left figure*: The explanation shift indicates that different social groups exhibit varying deviations from the distribution on which the model was trained. *Middle Figure*: We vary the model f_θ by training it using both `XGBoost` (solid lines) and Logistic Regression (dots), excluding the black ethnicity group, and compare it with models trained on different distributions (comparison against *(B5)* and *(B6)*). *Right figure*: Comparison against Exp. NDCG *(B4)* we see how this monitoring methods is more unstable with a linear model and with an `xgboost` it erroneously finds a horizontal asymptote.

5.2.2 Geopolitical and Temporal Shift

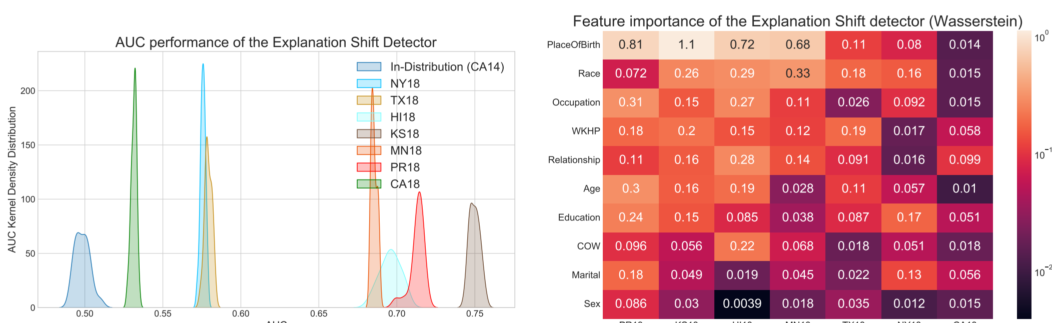

Figure 4: In the left figure, comparison of the performance of *Explanation Shift Detector* in different states. In the right figure, strength analysis of features driving the change in the model, in the y-axis the features and on the x-axis the different states. Explanation shifts allow us to identify how the distribution shift of different features impacted the model.

In this section, we tackle a geopolitical and temporal distribution shift; for this, the training data $\mathcal{D}^{tr}$ for the model f_θ is composed of data from California in 2014 and $\mathcal{D}^{new}$ from rest of the states in 2018. The model g_ψ is trained each time on each state using only the $\mathcal{D}_X^{new}$ in the absence of the label, and a 50/50 random train-test split evaluates its performance. As models, we use `xgboost` as f_θ and logistic regression for the *Explanation Shift Detector* (g_ψ).

We hypothesize that the AUC of the Explanation Shift Detector on new data will be distinct from that on in-distribution data, primarily owing to the distinctive nature of out-of-distribution model explanations. Figure 4 illustrates the performance of our method on different data distributions, where the baseline is a ID hold-out set of CA14. The AUC for CA18, where there is only a temporal shift, is the closest to the baseline, and the OOD detection performance is better in the rest of the states. The most disparate state is Puerto Rico (PR18).

Our next objective is to identify the features where the explanations differ between $\mathcal{D}_X^{tr}$ and $\mathcal{D}_X^{new}$ data. To achieve this, we compare the distribution of linear coefficients of the detector between both distributions. We use the Wasserstein distance as a distance measure, generating 1000 in-distribution bootstraps using a 63.2% sampling fraction from California-14 and 1000 bootstraps from other states in 2018. In the right image of Figure 4, we observe that for PR18, the most crucial feature is the Place of Birth.

Furthermore, we conduct an across-task evaluation by comparing the performance of the "Explanation Shift Detector" on another prediction task in the Appendix E. Although some features are present in both prediction tasks, the weights and importance order assigned by the "Explanation Shift Detector" differ. One of this method's advantages is that it identifies differences in distributions and how they relate to the model.

6 Discussion

In this study, we conducted a comprehensive evaluation of explanation shift by systematically varying models (f), model parametrizations (θ), feature attribution explanations ($\mathcal{S}$), and input data distributions ($\mathcal{D}_X$). Our objective was to investigate the impact of distribution shift on the model by explanation shift and gain insights into its characteristics and implications.

Our approach cannot detect concept shifts, as concept shift requires understanding the interaction between prediction and response variables. By the nature of pure concept shifts, such changes do not affect the model. To be understood, new data need to come with labelled responses. We work under the assumption that such labels are not available for new data, nor do we make other assumptions; therefore, our method is not able to predict the degradation of prediction performance under distribution shifts. All papers such as (Garg et al., 2021b; Baek et al., 2022; Chen et al., 2022b; Fang et al., 2022; Miller et al., 2021; Lu et al., 2023) that address the monitoring of prediction performance have the same limitation. Only under specific assumptions, e.g., no occurrence of concept shift or causal graph availability, can performance degradation be predicted with reasonable reliability.

The potential utility of explanation shifts as distribution shift indicators that affect the model in computer vision or natural language processing tasks remains an open question. We have used feature attribution explanations to derive indications of explanation shifts, but other AI explanation techniques may be applicable and come with their advantages.

7 Conclusions

Commonly, the problem of detecting the impact of the distribution shift on the model has relied on measurements for detecting shifts in the input or output data distributions or relied on assumptions either on the type of distribution shift or causal graphs availability. In this paper, we have provided evidence that explanation shifts can be a more suitable indicator for detecting and identifying distribution shifts' impact on machine learning models. We provide software, mathematical analysis examples, synthetic data, and real-data experimental evaluation. We found that measures of explanation shift can provide more insights than input distribution and prediction shift measures when monitoring machine learning models.

Reproducibility Statement

To ensure reproducibility, we make the data, code repositories, and experiments publicly available https://anonymous.4open.science/r/ExplanationShift-COCO/README.md. Also, an open-source Python package `skshift` https://anonymous.4open.science/r/skshift-65A5/README.md is attached with methods routines and tutorials. For our experiments, we used default `scikit-learn` parameters Pedregosa et al. (2011). We describe the system requirements and software dependencies of our experiments. Experiments were run on a 4 vCPU server with 32 GB RAM.

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Contents

A Extended Related Work

This section provides an in-depth review of the related theoretical works that inform our research.

A.1 Out-Of-Distribution Detection

Evaluating how two distributions differ has been a widely studied topic in the statistics and statistical learning literature Hastie et al. (2001); Quiñonero-Candela et al. (2009); Liu et al. (2020a), that have advanced recently in last years Park et al. (2021a); Lee et al. (2018); Zhang et al. (2013). Rabanser et al. (2019) provides a comprehensive empirical investigation, examining how dimensionality reduction and two-sample testing might be combined to produce a practical pipeline for detecting distribution shifts in real-life machine learning systems. Other methods to detect if new data is OOD have relied on neural networks based on the prediction distributions Fort et al. (2021); Garg et al. (2020). They use the maximum softmax probabilities/likelihood as a confidence score Hendrycks & Gimpel (2017), temperature or energy-based scores Ren et al. (2019); Liu et al. (2020b); Wang et al. (2021), they extract information from the gradient space Huang et al. (2021), relying on the latent space Crabbé et al. (2021), they fit a Gaussian distribution to the embedding, or they use the Mahalanobis distance for out-of-distribution detection Lee et al. (2018); Park et al. (2021b).

Many of these methods are explicitly developed for neural networks that operate on image and text data, and often, they can not be directly applied to traditional ML techniques. For image and text data, one may build on the assumption that the relationships between relevant predictor variables (X) and response variables (Y) remain unchanged, i.e., that no *concept shift* occurs. For instance, the essence of how a dog looks remains unchanged over different data sets, even if contexts may change. Thus, one can define invariances on the latent spaces of deep neural models, which do not apply to tabular data in a similar manner. For example, predicting buying behaviour before, during, and after the COVID-19 pandemic constitutes a conceptual shift that is not amenable to such methods. We focus on such tabular data where techniques such as gradient boosting decision trees achieve state-of-the-art model performance Grinsztajn et al. (2022); Elsayed et al. (2021); Borisov et al. (2021).

A.2 Explainability and Distribution Shift

An approach using Shapley values by Balestra et al. (2022) allows for tracking distributional shifts and their impact among for categorical time series using slidSHAP, a novel method for unlabelled data streams. This approach is particularly useful for unlabelled data streams, offering insights into the changing data distribution dynamics. In contrast, our work focuses on defining explanation distributions and leveraging their theoretical properties in the context of distribution shift detection, employing a two-sample classifier test for detection.

Another perspective in the field of explainability is explored by Adebayo et al. (2020; 2018), who investigate the effectiveness of post-hoc model explanations for diagnosing model errors. They categorize these errors based on their source. While their work is geared towards model debugging, our research takes a distinct path by aiming to quantify the influence of distribution shifts on the model.

Hinder et al. (2022) proposes to explain concept drift by contrasting explanations describing characteristic changes of spatial features. Haug & Kasneci (2021) track changes in the distribution of model parameter values that are directly related to the input features to identify concept drift early on in data streams. In a more recent paper, Haug et al. (2022) also exploits the idea that local changes to feature attributions and distribution shifts are strongly intertwined and uses this idea to update the local feature attributions efficiently. Their work focuses on model retraining and concept shift, in our work, the original model f_θ remains unaltered, and since we are in an unsupervised monitoring scenario, we can't detect concept shifts see discussion in Section 6

B Extended Analytical Examples

This appendix provides more details about the analytical examples presented in Section 4.1.

B.1 Explanation Shift vs Prediction Shift

Proposition 2. Given a model $f_\theta : \mathcal{D}_X \to \mathcal{D}_Y$. If $f_\theta(x') \neq f_\theta(x)$, then $\mathcal{S}(f_\theta, x') \neq \mathcal{S}(f_\theta, x)$.

$$\texttt{Given} \quad f_\theta(x) \neq f_\theta(x') \tag{5}$$

$$\sum_{j=1}^{p} \mathcal{S}_j(f_\theta, x) = f_\theta(x) - E_X[f_\theta(\mathcal{D}_X)] \tag{6}$$

$$\texttt{then} \quad \mathcal{S}(f, x) \ \neq \mathcal{S}(f, x') \tag{7}$$

Example B.1. ***Explanation shift that does not affect the prediction distribution*** *Given $\mathcal{D}^{tr}$ is generated from $(X_1, X_2, Y), X_1 \sim U(0,1), X_2 \sim U(1,2), Y = X_1 + X_2 + \epsilon$ and thus the model is $f(x) = x_1 + x_2$. If $\mathcal{D}^{new}$ is generated from $X_1^{new} \sim U(1,2), X_2^{new} \sim U(0,1)$, the prediction distributions are identical $f_\theta(\mathcal{D}_X^{tr}), f_\theta(\mathcal{D}_X^{new})$, but explanation distributions are different $S(f_\theta, \mathcal{D}_X^{tr}) \neq S(f_\theta, \mathcal{D}_X^{new})$*

$$\forall i \in \{1,2\} \quad \mathcal{S}_i(f_\theta, x) = \alpha_i \cdot x_i \tag{8}$$

$$\forall i \in \{1,2\} \Rightarrow \mathcal{S}_i(f_\theta, \mathcal{D}_X)) \neq \mathcal{S}_i(f_\theta, \mathcal{D}_X^{new}) \tag{9}$$

$$\Rightarrow f_\theta(\mathcal{D}_X) = f_\theta(\mathcal{D}_X^{new}) \tag{10}$$

B.2 Explanation Shifts vs Input Data Distribution Shifts

B.2.1 Multivariate Shift

Example B.2. ***Multivariate Shift*** *Let* $D_X^{tr} = (\mathcal{D}_{X_1}^{new}, \mathcal{D}_{X_2}^{new}) \sim N\left(\begin{bmatrix}\mu_1\\ \mu_2\end{bmatrix}, \begin{bmatrix}\sigma_{x_1}^2 & 0\\ 0 & \sigma_{x_2}^2\end{bmatrix}\right)$,$\mathcal{D}_X^{new} = (\mathcal{D}_{X_1}^{new}, \mathcal{D}_{X_2}^{new}) \sim N\left(\begin{bmatrix}\mu_1\\ \mu_2\end{bmatrix}, \begin{bmatrix}\sigma_{x_1}^2 & \rho\sigma_{x_1}\sigma_{x_2}\\ \rho\sigma_{x_1}\sigma_{x_2} & \sigma_{x_2}^2\end{bmatrix}\right)$. *We fit a linear model* $f_\theta(X_1, X_2) = \gamma + a \cdot X_1 + b \cdot X_2$. $\mathcal{D}_{X_1}$ *and* $\mathcal{D}_{X_2}$ *are identically distributed with* $\mathcal{D}_{X_1}^{new}$ *and* $\mathcal{D}_{X_2}^{new}$*, respectively, while this does not hold for the corresponding SHAP values* $\mathcal{S}_j(f_\theta, \mathcal{D}_X^{tr})$ *and* $\mathcal{S}_j(f_\theta, \mathcal{D}_X^{val})$*.*

$$\mathcal{S}_1(f_\theta, x) = a(x_1 - \mu_1) \tag{11}$$

$$\mathcal{S}_1(f_\theta, x^{new}) = \tag{12}$$

$$= \frac{1}{2}[\text{val}(\{1,2\}) - \text{val}(\{2\})] + \frac{1}{2}[\text{val}(\{1\}) - \text{val}(\emptyset)] \tag{13}$$

$$\text{val}(\{1,2\}) = E[f_\theta | X_1 = x_1, X_2 = x_2] = ax_1 + bx_2 \tag{14}$$

$$\text{val}(\emptyset) = E[f_\theta] = a\mu_1 + b\mu_2 \tag{15}$$

$$\text{val}(\{1\}) = E[f_\theta(x) | X_1 = x_1] + b\mu_2 \tag{16}$$

$$\text{val}(\{1\}) = \mu_1 + \rho\frac{\rho_{x_1}}{\sigma_{x_2}}(x_1 - \sigma_1) + b\mu_2 \tag{17}$$

$$\text{val}(\{2\}) = \mu_2 + \rho\frac{\sigma_{x_2}}{\sigma_{x_1}}(x_2 - \mu_2) + a\mu_1 \tag{18}$$

$$\Rightarrow \mathcal{S}_1(f_\theta, x^{new}) \neq a(x_1 - \mu_1) \tag{19}$$

B.2.2 Concept Shift

One of the most challenging types of distribution shift to detect are cases where distributions are equal between source and unseen data-set $\mathbf{P}(\mathcal{D}_X^{tr}) = \mathbf{P}(\mathcal{D}_X^{new})$ and the target variable $\mathbf{P}(\mathcal{D}_Y^{tr}) = \mathbf{P}(\mathcal{D}_Y^{new})$ and what changes are the relationships that features have with the target $\mathbf{P}(\mathcal{D}_Y^{tr} | \mathcal{D}_X^{tr}) \neq \mathbf{P}(\mathcal{D}_Y^{new} | \mathcal{D}_X^{new})$, this kind of distribution shift is also known as concept drift or posterior shift (Huyen, 2022) and is especially difficult to notice, as it requires labeled data to detect. The following example compares how the explanations change for two models fed with the same input data and different target relations.

Example B.3. ***Concept shift*** *Let* $\mathcal{D}_X = (X_1, X_2) \sim N(\mu, I)$*, and* $\mathcal{D}_X^{new} = (X_1^{new}, X_2^{new}) \sim N(\mu, I)$*, where* I *is an identity matrix of order two and* $\mu = (\mu_1, \mu_2)$*. We now create two synthetic targets* $Y = a + \alpha \cdot X_1 + \beta \cdot X_2 + \epsilon$ *and* $Y^{new} = a + \beta \cdot X_1 + \alpha \cdot X_2 + \epsilon$*. Let* f_θ *be a linear regression model trained on* $f_\theta : \mathcal{D}_X \to \mathcal{D}_Y$*) and* h_ϕ *another linear model trained on* $h_\phi : \mathcal{D}_X^{new} \to \mathcal{D}_Y^{new}$*). Then* $\mathbf{P}(f_\theta(X)) = \mathbf{P}(h_\phi(X^{new}))$*,* $P(X) = \mathbf{P}(X^{new})$ *but* $\mathcal{S}(f_\theta, X) \neq \mathcal{S}(h_\phi, X)$*.*

$$X \sim N(\mu, \sigma^2 \cdot I), X^{new} \sim N(\mu, \sigma^2 \cdot I) \tag{20}$$

$$\to P(\mathcal{D}_X) = P(\mathcal{D}_X^{new}) \tag{21}$$

$$Y \sim a + \alpha N(\mu, \sigma^2) + \beta N(\mu, \sigma^2) + N(0, \sigma^{'2}) \tag{22}$$

$$Y^{new} \sim a + \beta N(\mu, \sigma^2) + \alpha N(\mu, \sigma^2) + N(0, \sigma^{'2}) \tag{23}$$

$$\to P(\mathcal{D}_Y) = P(\mathcal{D}_Y^{new}) \tag{24}$$

$$\mathcal{S}(f_\theta, \mathcal{D}_X) = \begin{pmatrix}\alpha(X_1 - \mu_1)\\ \beta(X_2 - \mu_2)\end{pmatrix} \sim \begin{pmatrix}N(\mu_1, \alpha^2\sigma^2)\\ N(\mu_2, \beta^2\sigma^2)\end{pmatrix} \tag{25}$$

$$\mathcal{S}(h_\phi, \mathcal{D}_X) = \begin{pmatrix}\beta(X_1 - \mu_1)\\ \alpha(X_2 - \mu_2)\end{pmatrix} \sim \begin{pmatrix}N(\mu_1, \beta^2\sigma^2)\\ N(\mu_2, \alpha^2\sigma^2)\end{pmatrix} \tag{26}$$

$$\text{If} \quad \alpha \neq \beta \to \mathcal{S}(f_\theta, \mathcal{D}_X) \neq \mathcal{S}(h_\phi, \mathcal{D}_X) \tag{27}$$

C Further Experiments on Synthetic Data

This experimental section explores the detection of distribution shifts in the previous synthetic examples.

C.1 Detecting multivariate shift

Given two bivariate normal distributions $\mathcal{D}_X = (X_1, X_2) \sim N\left(0, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\right)$ and $\mathcal{D}_X^{new} = (X_1^{new}, X_2^{new}) \sim N\left(0, \begin{bmatrix} 1 & 0.2 \\ 0.2 & 1 \end{bmatrix}\right)$, then, for each feature j the underlying distribution is equally distributed between $\mathcal{D}_X$ and $\mathcal{D}_X^{new}$, $\forall j \in \{1, 2\} : P(\mathcal{D}_{X_j}) = P(\mathcal{D}_{X_j}^{new})$, and what is different are the interaction terms between them. We now create a synthetic target $Y = X_1 \cdot X_2 + \epsilon$ with $\epsilon \sim N(0, 0.1)$ and fit a gradient boosting decision tree $f_\theta(\mathcal{D}_X)$. Then we compute the SHAP explanation values for $\mathcal{S}(f_\theta, \mathcal{D}_X)$ and $\mathcal{S}(f_\theta, \mathcal{D}_X^{new})$

Table 1: Displayed results are the one-tailed p-values of the Kolmogorov-Smirnov test comparison between two underlying distributions. Small p-values indicate that compared distributions would be very unlikely to be equally distributed. SHAP values correctly indicate the interaction changes that individual distribution comparisons cannot detect

Comparison	**p-value**	**Conclusions**
$\mathbf{P}(\mathcal{D}_{X_1})$, $\mathbf{P}(\mathcal{D}_{X_1}^{new})$	0.33	Not Distinct
$\mathbf{P}(\mathcal{D}_{X_2})$, $\mathbf{P}(\mathcal{D}_{X_2}^{new})$	0.60	Not Distinct
$\mathcal{S}_1(f_\theta, \mathcal{D}_X)$, $\mathcal{S}_1(f_\theta, \mathcal{D}_X^{new})$	3.9e−153	Distinct
$\mathcal{S}_2(f_\theta, \mathcal{D}_X)$, $\mathcal{S}_2(f_\theta, \mathcal{D}_X^{new})$	2.9e−148	Distinct

Having drawn 50,000 samples from both $\mathcal{D}_X$ and $\mathcal{D}_X^{new}$, in Table 1, we evaluate whether changes in the input data distribution or in the explanations are able to detect changes in covariate distribution. For this, we compare the one-tailed p-values of the Kolmogorov-Smirnov test between the input data distribution and the explanations distribution. Explanation shift correctly detects the multivariate distribution change that univariate statistical testing can not detect.

C.2 Detecting concept shift

As mentioned before, concept shift cannot be detected if new data comes without target labels. If new data is labelled, the explanation shift can still be a useful technique for detecting concept shifts.

Given a bivariate normal distribution $\mathcal{D}_X = (X_1, X_2) \sim N(1, I)$ where I is an identity matrix of order two. We now create two synthetic targets $Y = X_1^2 \cdot X_2 + \epsilon$ and $Y^{new} = X_1 \cdot X_2^2 + \epsilon$ and fit two machine learning models $f_\theta : \mathcal{D}_X \to \mathcal{D}_Y)$ and $h_\Upsilon : \mathcal{D}_X \to \mathcal{D}_Y^{new})$. Now we compute the SHAP values for $\mathcal{S}(f_\theta, \mathcal{D}_X)$ and $\mathcal{S}(h_\Upsilon, \mathcal{D}_X)$

Table 2: Distribution comparison for synthetic concept shift. Displayed results are the one-tailed p-values of the Kolmogorov-Smirnov test comparison between two underlying distributions

Comparison	**Conclusions**
$\mathbf{P}(\mathcal{D}_X)$, $\mathbf{P}(\mathcal{D}_X^{new})$	Not Distinct
$\mathbf{P}(\mathcal{D}_Y)$, $\mathbf{P}(\mathcal{D}_Y^{new})$	Not Distinct
$\mathbf{P}(f_\theta(\mathcal{D}_X))$, $\mathbf{P}(h_\Upsilon(\mathcal{D}_X^{new}))$	Not Distinct
$\mathbf{P}(\mathcal{S}(f_\theta, \mathcal{D}_X))$, $\mathbf{P}(\mathcal{S}(h_\Upsilon, \mathcal{D}_X))$	Distinct

In Table 2, we see how the distribution shifts are not able to capture the change in the model behavior while the SHAP values are different. The "Distinct/Not distinct" conclusion is based on the one-tailed p-value of the Kolmogorov-Smirnov test with a 0.05 threshold drawn out of 50,000 samples for both distributions. As in the synthetic example, in table 2

SHAP values can detect a relational change between $\mathcal{D}_X$ and $\mathcal{D}_Y$, even if both distributions remain equivalent.

C.3 Uninformative features on synthetic data

To have an applied use case of the synthetic example from the methodology section, we create a three-variate normal distribution $\mathcal{D}_X = (X_1, X_2, X_3) \sim N(0, I_3)$, where I_3 is an identity matrix of order three. The target variable is generated $Y = X_1 \cdot X_2 + \epsilon$ being independent of X_3. For both, training and test data, $50,000$ samples are drawn. Then out-of-distribution data is created by shifting X_3, which is independent of the target, on test data $\mathcal{D}^{new}_{X_3} = \mathcal{D}^{te}_{X_3} + 1$.

Table 3: Distribution comparison when modifying a random noise variable on test data. The input data shifts while explanations and predictions do not.

Comparison	**Conclusions**
$\mathbf{P}(\mathcal{D}^{te}_{X_3})$, $\mathbf{P}(\mathcal{D}^{new}_{X_3})$	Distinct
$f_\theta(\mathcal{D}^{te}_X)$, $f_\theta(\mathcal{D}^{new}_X)$	Not Distinct
$\mathcal{S}(f_\theta, \mathcal{D}^{te}_X)$, $\mathcal{S}(f_\theta, \mathcal{D}^{new}_X)$	Not Distinct

In Table 3, we see how an unused feature has changed the input distribution, but the explanation distributions and performance evaluation metrics remain the same. The "Distinct/Not Distinct" conclusion is based on the one-tailed p-value of the Kolmogorov-Smirnov test drawn out of $50,000$ samples for both distributions.

C.4 Explanation shift that does not affect the prediction

In this case we provide a situation when we have changes in the input data distributions that affect the model explanations but do not affect the model predictions due to positive and negative associations between the model predictions and the distributions cancel out producing a vanishing correlation in the mixture of the distribution (Yule's effect 4.2).

We create a train and test data by drawing $50,000$ samples from a bi-uniform distribution $X_1 \sim U(0,1), \quad X_2 \sim U(1,2)$ the target variable is generated by $Y = X_1 + X_2$ where we train our model f_θ. Then if out-of-distribution data is sampled from $X_1^{new} \sim U(1,2)$, $X_2^{new} \sim U(0,1)$

Table 4: Distribution comparison over how the change on the contributions of each feature can cancel out to produce an equal prediction (cf. Section 4.2), while explanation shift will detect this behaviour changes on the predictions will not.

Comparison	**Conclusions**
$f(\mathcal{D}^{te}_X)$, $f(\mathcal{D}^{new}_X)$	Not Distinct
$\mathcal{S}(f_\theta, \mathcal{D}^{te}_{X_2})$, $\mathcal{S}(f_\theta, \mathcal{D}^{new}_{X_2})$	Distinct
$\mathcal{S}(f_\theta, \mathcal{D}^{te}_{X_1})$, $\mathcal{S}(f_\theta, \mathcal{D}^{new}_{X_1})$	Distinct

In Table 4, we see how an unused feature has changed the input distribution, but the explanation distributions and performance evaluation metrics remain the same. The "Distinct/Not Distinct" conclusion is based on the one-tailed p-value of the Kolmogorov-Smirnov test drawn out of $50,000$ samples for both distributions.

D Experimental Comparison against Specific Related Work

In this section, we expand upon our comparison with related work by providing a summary table that encompasses all the methods examined under synthetic shift scenarios.

D.1 Summary Comparison on Synthetic data

To assess the effectiveness of different detection methods in identifying and accounting for synthetic shifts, we present a conceptual comparison in Table 5. We evaluate these methods based on their capacity to capture synthetic shifts, following the methodology detailed in the main body of the paper (cf. Section 5.2). We illustrate this comparison by considering two scenarios: a multicovariate shift (cf. Example 4.1) and a shift involving uninformative features (cf. Example 4.2).

This comparison focuses on their ability to detect synthetic distribution shifs using the examples of covariate shift and uninformative shifts, and provides valuable insights while ensuring accountability.

Table 5: Conceptual comparison of different detection methods over the examples discussed in the mathematical analsyis of the main body of the paper(cf. Section 4): a multicovariate shift(cf. Example 4.1)and a uninformative features shift(cf. Example 4.2) . Learning a Classifier Two-Sample test g over the explanation distributions is the only method that achieves the desired results (✓) and is accountable. We evaluate accountability by checking if the feature attributions of the detection method correspond to the synthetic shift generated in both scenarios

Detection Method	**Covariate**	**Uninformative**	**Accountability**
Input distribution(g_ϕ)	✓	✗	✗
Prediction distribution(g_Υ)	✓	✓	✗
Input KS	✗	✗	✗
Classifier Drift	✓	✗	✗
Output KS	✓	✓	✗
Output Wasserstein	✓	✓	✗
Uncertainty	$\sim$	✓	✓
NDCG	✗	✓	✗
Explanation distribution (g_ψ) Explanation Shift Detector	✓	✓	✓

D.2 Comparison Against Changes on Feature Attribution Relevance

In this section, we present a comparative analysis against the work of (Nigenda et al., 2022),

which involves assessing the disparity in feature importance orders between training data and out-of-distribution data. To quantify this disparity, we employ the normalized discount cumulative gain (NDCG) metric. This method is versatile, accommodating both individual sample analysis and distribution-level assessments. In cases involving distributions, we aggregate the average feature importance.

D.2.1 Novel Group Shift

Experimental Set-Up: This experiment extends the core experiment detailed in Section 5, where distribution shifts arise due to the emergence of previously unseen groups during the prediction phase.

Datasets: We use ACS Income, ASC Employment, ACS Mobility and ACS Travel time (Ding et al., 2021b). The group that is not present on the features is the *black* ethnicity.

Baseline: We compare against the method proposed by Nigenda et al. (2022), *(B6)* of the experimental comparison of the main body, that compares the order of the feature importance using the NDCG between train and unseen data. We vary f_θ to be a `xgboost` and a Logistic regression. For the "Explanation Shift Detector", g_ψ , we use a logistic regression in both

Metrics: To facilitate a direct comparison with the Area Under the Curve (AUC) metric, we adapt the NDCG metric, to have the same interval range as follows: $(1 - NDCG) + 0.5$, ensuring a consistent metric range.

This extended experiment aims to further validate the effectiveness of the "Explanation Shift Detector" under novel group shifts in real-world datasets. It demonstrates how the approach

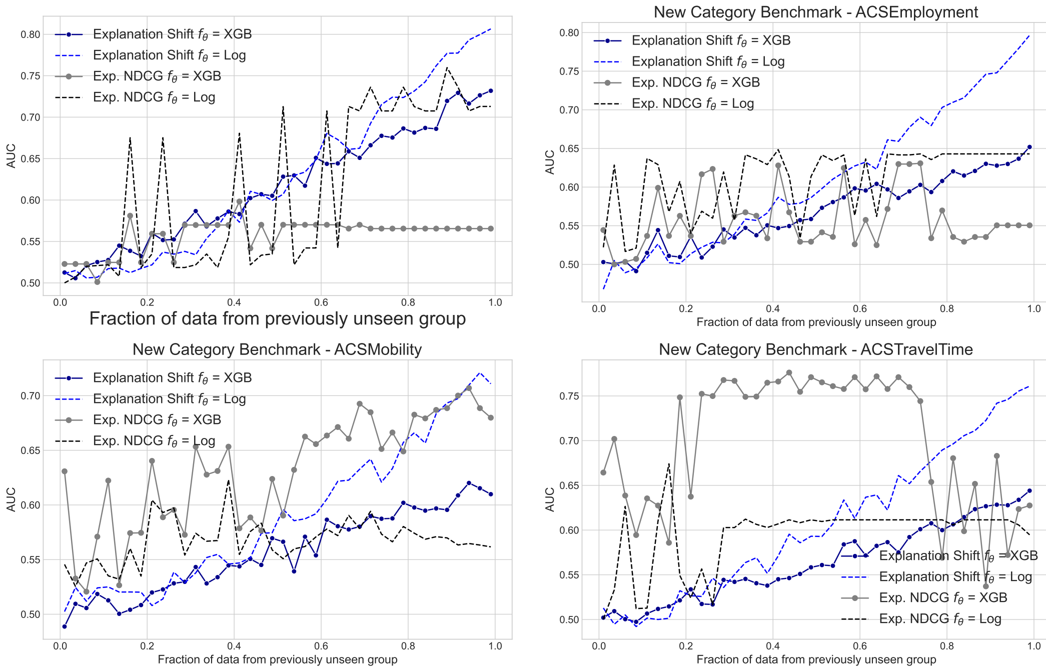

Figure 5: Novel group shift experiment conducted on the 4 Datasets. Sensitivity (AUC) increases as the proportion of previously unseen social groups grows. As the experimental setup has a gradual distribution shift, ideal indicators should exhibit a steadily increasing slope. However, in all figures, NDCG exhibits saturation and instability. These observations align with the analysis presented in the synthetic experiment section, as discussed in Section 5.2 of the main paper

performs consistently across multiple datasets and provides insights into the sensitivity of model behavior as previously unseen social groups become a larger part of the prediction data. The results are presented in Figure 5, where our proposed method is compared against Exp. NDCG *(B6)* across the four datasets. We can see how Exp. NDCG *(B6)* is more unstable and finds often an horizontal asymptot, in all the situations, this is due to changes on the feature importance order do not have information about the value, where our approach of performing a Classifier Two Sample Test on the distributions of explanations do.

D.2.2 Synthetic Data Comparison

In this section, we evaluate changes in the distribution of explanations and the order of feature importance when faced with a synthetic data shift scenario. We begin with a bivariate normal distribution $\mathcal{D}_X^{tr} = (X_1, X_2) \sim N(1, I)$, where I represents the identity matrix of order two. We create a synthetic target variable $Y = X_1^2 \cdot X_2 + \epsilon$, and develop a machine learning model $f_\theta : \mathcal{D}_X \to \mathcal{D}_Y$ using a non-linear model, specifically an `xgboost` model. Subsequently, we generate new data from $\mathcal{D}_X^{new} = (X_1, X_2) \sim N(2, I)$, which constitutes a shift of $D_X^{new} = D^{tr}X + 1$. We then compute SHAP values for $\mathcal{S}(f\theta, \mathcal{D}_X)$ and compare the average contributions' orders.

Having sampled 50,000 instances from both $\mathcal{D}_X^{tr}$ and $\mathcal{D}_X^{new}$, we analyze whether alterations in explanation distributions and explanation importance orders can detect these changes. To achieve this, we compare one-tailed p-values from the Kolmogorov-Smirnov test for explanation shifts and the order of average SHAP values between the distributions.

D.2.3 Analytical Comparison under Monotonous Uniform Shift

In this section, we conduct an analytical comparison between changes in explanation distributions and changes in the order of feature importance.

Table 6: Comparison between distribution shifts in explanations and shifts in feature attribution importance orders(previous work of (Nigenda et al., 2022)). Explanation distributions exhibit differences, while the importance order remains consistent

Comparison	**Conclusions**
$\mathbf{P}(\mathcal{D}^{te}_X)$, $\mathbf{P}(\mathcal{D}^{new}_X)$	Distinct
$\mathbf{P}(\mathcal{S}(f_\theta, \mathcal{D}^{te}_X))$, $\mathbf{P}(\mathcal{S}(f_\theta, \mathcal{D}^{new}_X))$	Distinct
$\mathbf{P}(\mathcal{S}_1(f_\theta, \mathcal{D}^{te}_X) > \mathcal{S}_2(f_\theta, \mathcal{D}^{te}_X))$, $\mathbf{P}(\mathcal{S}_1(f_\theta, \mathcal{D}^{new}_X) > \mathcal{S}_2(f_\theta, \mathcal{D}^{new}_X))$	Not Distinct

Example D.1. ***Comparison against NDCG*** Let $\mathcal{D}^{tr}_X = (\mathcal{D}^{tr}_{X_1}, \mathcal{D}^{tr}_{X_2}) \sim N([\mu_1, \mu_1], I)$ and $\mathcal{D}^{new}_X = (\mathcal{D}^{new}_{X_1}, \mathcal{D}^{new}_{X_2}) \sim N([\mu_2, \mu_2], I)$ where the relationship between μ_1 and μ_2 is monotonous uniform shift characterized by $\mu_2 = \mu_1 + N$ where N is a real number. We fit a linear model $f_\theta(X_1, X_2) = \gamma + a_1 \cdot X_1 + a_2 \cdot X_2$, where $a_1 > a_2$. Then even if the distribution of SHAP values are distinct between $\mathcal{S}(f_\theta, \mathcal{D}^{tr}_X)$ and $\mathcal{S}(f_\theta, \mathcal{D}^{new}_X)$, the order of importance between the distributions is not distinct. If $\mathcal{S}_1(f_\theta, \mathcal{D}^{tr}_X) > \mathcal{S}_2(f_\theta, \mathcal{D}^{tr}_X)$ then $\mathcal{S}_1(f_\theta, \mathcal{D}^{new}_X) > \mathcal{S}_2(f_\theta, \mathcal{D}^{new}_X)$. But the distributions are distinct $\mathcal{S}_1(f_\theta, \mathcal{D}^{tr}_X) \neq \mathcal{S}_1(f_\theta, \mathcal{D}^{new}_X)$ and $\mathcal{S}_2(f_\theta, \mathcal{D}^{tr}_X) \neq \mathcal{S}_2(f_\theta, \mathcal{D}^{new}_X)$

$$\mathcal{S}_j(f_\theta, \mathcal{D}_X) = a_j \cdot (\mathcal{D}_{X_j} - \mu_1), \mathcal{S}_j(f_\theta, \mathcal{D}^{new}_X) = a_j \cdot (\mathcal{D}^{new}_{X_j} - \mu_2) \tag{28}$$

$$\mu_2 = \mu_1 + N \tag{29}$$

$$\text{Then} \quad \mathcal{S}_j(f_\theta, \mathcal{D}_X) \neq \mathcal{S}_j(f_\theta, \mathcal{D}^{new}_X) \tag{30}$$

$$\text{But} \quad \mathcal{S}_1(f_\theta, \mathcal{D}_X) > \mathcal{S}_2(f_\theta, \mathcal{D}_X) \quad \Leftrightarrow \quad \mathcal{S}_1(f_\theta, \mathcal{D}^{new}_X) > \mathcal{S}_2(f_\theta, \mathcal{D}^{new}_X) \tag{31}$$

Conclusion of the comparison to Nigenda et al. (2022) In the context of natural data, when confronted with a novel covariate shift, our findings indicate that NDCG demonstrates limited sensitivity and fails to detect shifts when the fraction of data from previously unseen groups exceeds ratios 0.2 to 0.4 threshold.

Furthermore, in our analyses both synthetic and natural data, we observe that NDCG struggles to provide accurate and consistent estimates when faced with multicovariate shifts.

Both analytically and in our experiments with synthetic data, it becomes evident that NDCG lacks robustness and sensitivity when confronted with even a basic, uniform, and monotonous shift.

E Further Experiments on Real Data

In this section, we extend the prediction task of the main body of the paper. The methodology used follows the same structure. We start by creating a distribution shift by training the model f_θ in California in 2014 and evaluating it in the rest of the states in 2018, creating a geopolitical and temporal shift. The model g_θ is trained each time on each state using only the X^{New} in the absence of the label, and its performance is evaluated by a 50/50 random train-test split. As models, we use a gradient boosting decision tree(Chen & Guestrin, 2016; Prokhorenkova et al., 2018) for f_θ, approximating the Shapley values by TreeExplainer (Lundberg et al., 2020a), and using logistic regression for the *Explanation Shift Detector*.

For further understanding of the meaning of the features the ACS PUMS data dictionary contains a comprehensive list of available variables `https://www.census.gov/programs-surveys/acs/microdata/documentation.html`.

E.1 ACS Employment

The objective of this task is to determine whether an individual aged between 16 and 90 years is employed or not. The model's performance was evaluated using the AUC metric in different states, except PR18, where the model showed an explanation shift. The explanation shift was observed to be influenced by features such as Citizenship and Military Service. The performance of the model was found to be consistent across most of the states, with an AUC below 0.60. The impact of features such as difficulties in hearing or seeing was negligible in the distribution shift impact on the model. The left figure in Figure 6 compares the performance of the Explanation Shift Detector in different states for the ACS Employment dataset.

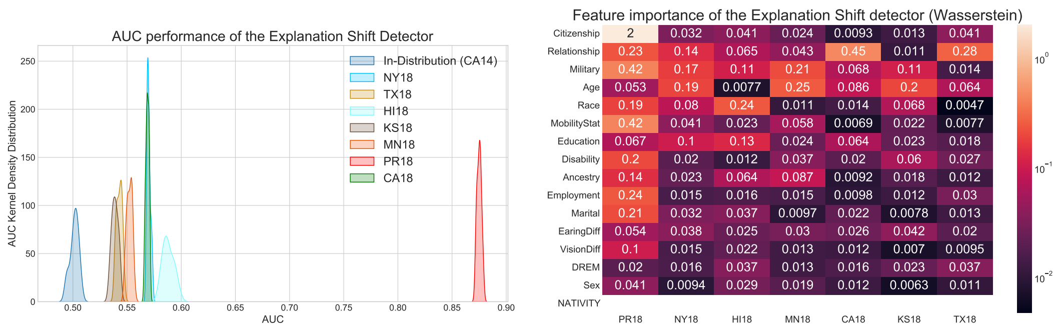

Figure 6: The left figure shows a comparison of the performance of the Explanation Shift Detector in different states for the ACS Employment dataset. The right figure shows the feature importance analysis for the same dataset.

Additionally, the feature importance analysis for the same dataset is presented in the right figure in Figure 6.

E.2 ACS Travel Time

The goal of this task is to predict whether an individual has a commute to work that is longer than +20 minutes. For this prediction task, the results are different from the previous two cases; the state with the highest OOD score is $KS18$, with the "Explanation Shift Detector" highlighting features as Place of Birth, Race or Working Hours Per Week. The closest state to ID is CA18, where there is only a temporal shift without any geospatial distribution shift.

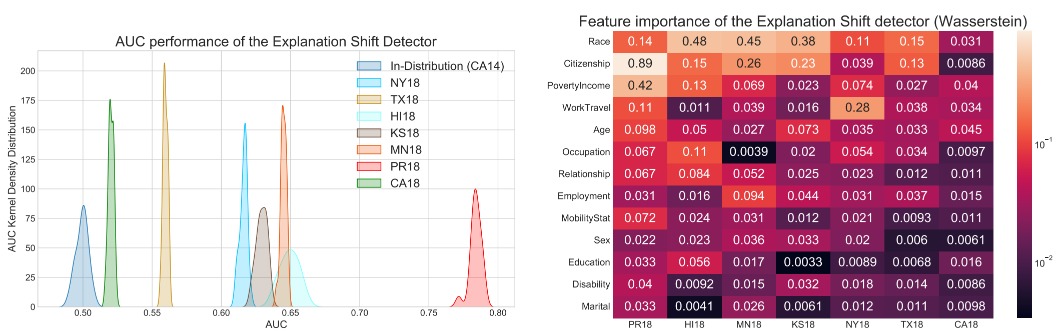

Figure 7: In the left figure, comparison of the performance of *Explanation Shift Detector*, in different states for the ACS TravelTime prediction task. In the left figure, we can see how the state with the highest OOD AUC detection is KS18 and not PR18 as in other prediction tasks; this difference with respect to the other prediction task can be attributed to "Place of Birth", whose feature attributions the model finds to be more different than in CA14.

E.3 ACS Mobility

The objective of this task is to predict whether an individual between the ages of 18 and 35 had the same residential address as a year ago. This filtering is intended to increase the difficulty of the prediction task, as the base rate for staying at the same address is above 90% for the population (Ding et al., 2021b).

The experiment shows a similar pattern to the ACS Income prediction task (cf. Section 4), where the inland US states have an AUC range of $0.55 - 0.70$, while the state of PR18 achieves a higher AUC. For PR18, the model has shifted due to features such as Citizenship, while for the other states, it is Ancestry (Census record of your ancestors' lives with details like where they lived, who they lived with, and what they did for a living) that drives the change in the model.

As depicted in Figure 8, all states, except for PR18, fall below an AUC of explanation shift detection of 0.70. Protected social attributes, such as Race or Marital status, play an essential role for these states, whereas for PR18, Citizenship is a key feature driving the impact of distribution shift in model.

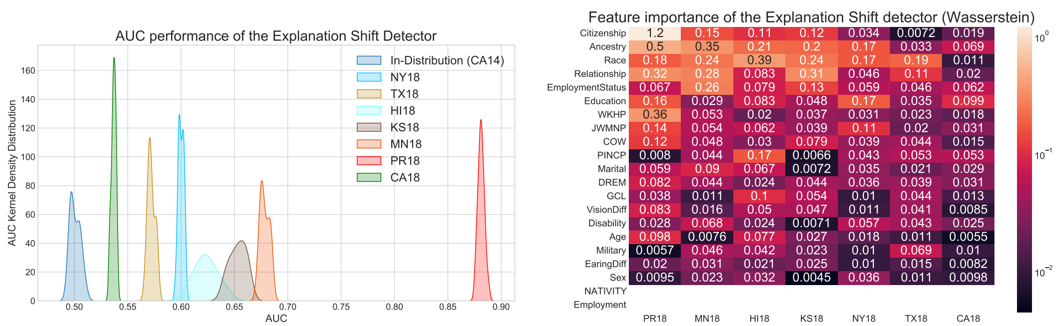

Figure 8: Left figure shows a comparison of the *Explanation Shift Detector*'s performance in different states for the ACS Mobility dataset. Except for PR18, all other states fall below an AUC of explanation shift detection of 0.70. The features driving this difference are Citizenship and Ancestry relationships. For the other states, protected social attributes, such as Race or Marital status, play an important role.

E.4 StackOverflow Survey Data: Novel Covariate Group

This experimental section evaluates the proposed Explanation Shift Detector approach on real-world data under novel group distribution shifts. In this scenario, a new unseen group appears at the prediction stage, and the ratio of the presence of this unseen group in the new data is varied. The model $f_\theta$used is a gradient-boosting decision tree or logistic regression, and a logistic regression is used for the detector. The results show that the AUC of the Explanation Shift Detector varies depending on the quantification of OOD explanations, and it show more sensitivity w.r.t. to model variations than other state-of-the-art techniques.

The dataset used is the StackOverflow annual developer survey has over 70,000 responses from over 180 countries examining aspects of the developer experience (Stackoverflow, 2019). The data has high dimensionality, leaving it with +100 features after data cleansing and feature engineering. The goal of this task is to predict the total annual compensation.

F Experiments with Modeling Methods and Hyperparameters

In the next sections, we are going to show the sensitivity or our method to variations of the model f, the detector g, and the parameters of the estimator f_θ.

As an experimental setup, In the main body of the paper, we have focused on the UCI Adult Income dataset. The experimental setup has been using Gradient Boosting Decision Tree as the model f_θ and then as "Explanation Shift Detector" g_ψ a logistic regression. In this section, we extend the experimental setup by providing experiments by varying the types of algorithms for a given experimental set-up: the UCI Adult Income dataset using the Novel Covariate Group Shift for the "Asian" group with a fraction ratio of 0.5 (cf. Section 5).

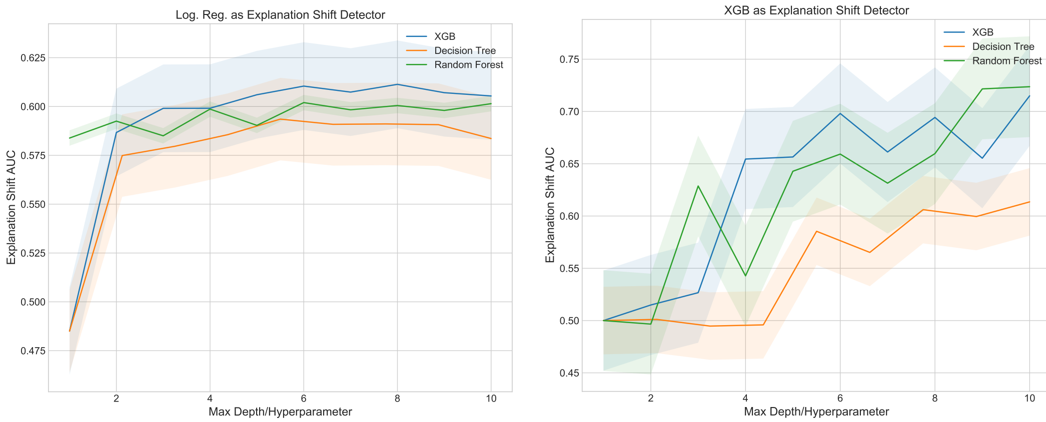

Figure 9: Both images represent the AUC of the *Explanation Shift Detector* for different countries on the StackOverflow survey dataset under novel group shift. In the left image, the detector is a logistic regression, and in the right image, a gradient-boosting decision tree classifier. By changing the model, we can see that low-complexity models are unaffected by the distribution shift, while when increasing the model complexity, the out-of-distribution model behaviour starts to be tangible

F.1 Varying Models and Explanation Shift Detectors

OOD data detection methods based on input data distributions only depend on the type of detector used, being independent of the model f_θ. OOD Explanation methods rely on both the model and the data. Using explanations shifts as indicators for measuring distribution shifts impact on the model enables us to account for the influencing factors of the explanation shift. Therefore, in this section, we compare the performance of different types of algorithms for explanation shift detection using the same experimental setup. The results of our experiments show that using Explanation Shift enables us to see differences in the choice of the original model f_θ and the Explanation Shift Detector g_ϕ

	Estimator f_θ						
Detector g_ϕ	**XGB**	**Log.Reg**	**Lasso**	**Ridge**	**Rand.Forest**	**Dec.Tree**	**MLP**
XGB	0.583	0.619	0.596	0.586	0.558	0.522	0.597
LogisticReg.	0.605	0.609	0.583	0.625	0.578	0.551	0.605
Lasso	0.599	0.572	0.551	0.595	0.557	0.541	0.596
Ridge	0.606	0.61	0.588	0.624	0.564	0.549	0.616
RandomForest	0.586	0.607	0.574	0.612	0.566	0.537	0.611
DecisionTree	0.546	0.56	0.559	0.569	0.543	0.52	0.569

Table 7: Comparison of explanation shift detection performance, measured by AUC, for different combinations of explanation shift detectors and estimators on the UCI Adult Income dataset using the Novel Covariate Group Shift for the "Asian" group with a fraction ratio of 0.5 (cf. Section 5). The table shows that the algorithmic choice for f_θ and g_ψ can impact the OOD explanation performance. We can see how, for the same detector, different f_θ models flag different OOD explanations performance. On the other side, for the same f_θ model, different detectors achieve different results.

F.2 Hyperparameters Sensitivity Evaluation

This section presents an extension to our experimental setup where we vary the model complexity by varying the model hyperparameters $\mathcal{S}(f_\theta, X)$. Specifically, we use the UCI Adult Income dataset with the Novel Covariate Group Shift for the "Asian" group with a fraction ratio of 0.5 as described in Section 5.

In this experiment, we changed the hyperparameters of the original model: for the decision tree, we varied the depth of the tree, while for the gradient-boosting decision, we changed the number of estimators, and for the random forest, both hyperparameters. We calculated the Shapley values using TreeExplainer (Lundberg et al., 2020a). For the Detector choice of model, we compare Logistic Regression and XGBoost models.

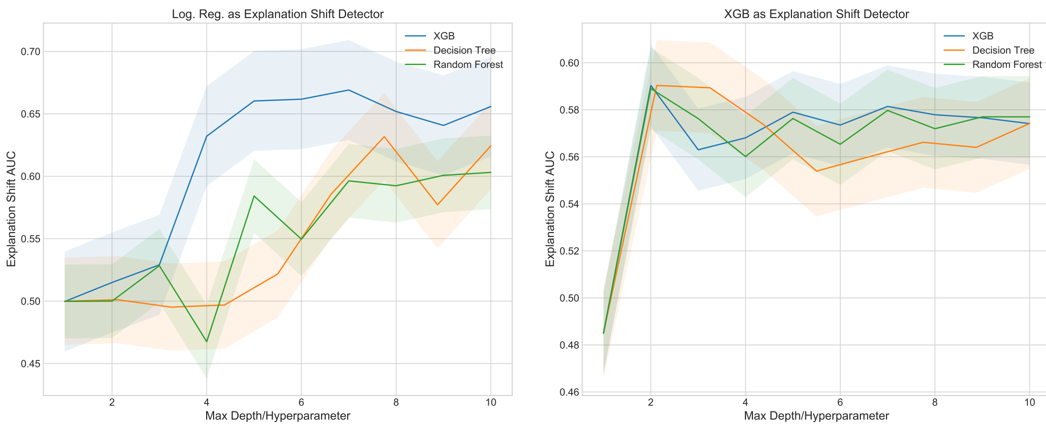

Figure 10: Both images represent the AUC of the *Explanation Shift Detector*, in different states for the ACS Income dataset under novel group shift. In the left image, the detector is a logistic regression, and in the right image, a gradient-boosting decision tree classifier. By changing the model, we can see that vanilla models (decision tree with depth 1 or 2) are unaffected by the distribution shift, while when increasing the model complexity, the out-of-distribution impact of the data in the model starts to be tangible

The results presented in Figure 10 show the AUC of the *Explanation Shift Detector* for the ACS Income dataset under novel group shift. We observe that the distribution shift does not affect very simplistic models, such as decision trees with depths 1 or 2. However, as we increase the model complexity, the out-of-distribution data impact on the model becomes more pronounced. Furthermore, when we compare the performance of the *Explanation Shift Detector* across different models, such as Logistic Regression and Gradient Boosting Decision Tree, we observe distinct differences(note that the y-axis takes different values).

In conclusion, the explanation distributions serve as a projection of the data and model sensitive to what the model has learned. The results demonstrate the importance of considering model complexity under distribution shifts.

G LIME as an Alternative Explanation Method

Another feature attribution technique that satisfies the aforementioned properties (efficiency and uninformative features Section 2) and can be used to create the explanation distributions is LIME (Local Interpretable Model-Agnostic Explanations). The intuition behind LIME is to create a local interpretable model that approximates the behavior of the original model in a small neighbourhood of the desired data to explain (Ribeiro et al., 2016b;a) whose mathematical intuition is very similar to the Taylor series. In this work, we have proposed explanation shifts as a key indicator for investigating the impact of distribution shifts on ML models. In this section, we compare the explanation distributions composed by SHAP and LIME methods. LIME can potentially suffers several drawbacks:

- **Computationally Expensive:** Its currently implementation is more computationally expensive than current SHAP implementations such as TreeSHAP (Lundberg et al., 2020a), Data SHAP (Kwon et al., 2021; Ghorbani & Zou, 2019) or Local and Connected SHAP (Chen et al., 2019), the problem increases when we produce explanations of distributions. Even though implementations might be improved, LIME requires sampling data and fitting a linear model which is a computationally more expensive approach than the aforementioned model-specific approaches to SHAP.
- **Local Neighborhood:** The definition of a local "neighborhood", which can lead to instability of the explanations. Slight variations of this explanation hyperparameter

lead to different local explanations. In (Slack et al., 2020) the authors showed that the explanations of two very close points can vary greatly.

- **Dimensionality:** LIME requires as a hyperparameter the number of features to use for the local linear approximation. This creates a dimensionality problem as for our method to work, the explanation distributions have to be from the exact same dimensions as the input data. Reducing the number of features to be explained might improve the computational burden.

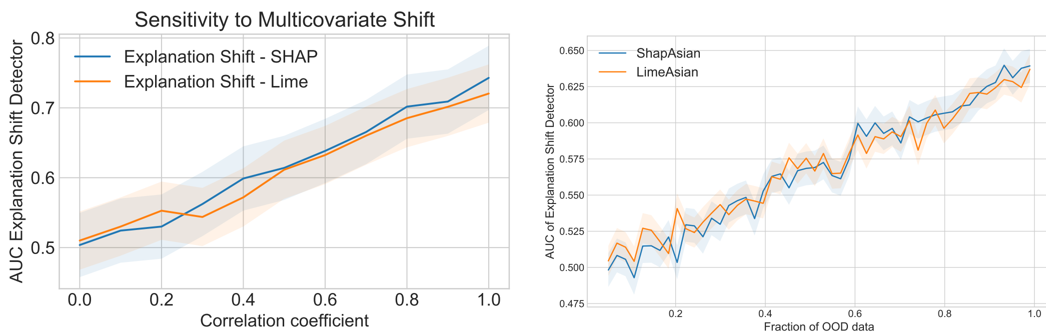

Figure 11: Comparison of the explanation distribution generated by LIME and SHAP. The left plot shows the sensitivity of the predicted probabilities to multicovariate changes using the synthetic data experimental setup of 2 on the main body of the paper. The right plot shows the distribution of explanation shifts for a New Covariate Category shift (Asian) in the ASC Income dataset.

Figure 11 compares the explanation distributions generated by LIME and SHAP. The left plot shows the sensitivity of the predicted probabilities to multicovariate changes using the synthetic data experimental setup from Figure 2 in the main body of the paper. The right plot shows the distribution of explanation shifts for a New Covariate Category shift (Asian) in the ASC Income dataset. The performance of OOD explanations detection is similar between the two methods, but LIME suffers from two drawbacks: its theoretical properties rely on the definition of a local neighborhood, which can lead to unstable explanations (false positives or false negatives on explanation shift detection), and its computational runtime required is much higher than that of SHAP (see experiments below).

G.1 Runtime

We conducted an analysis of the runtimes of generating the explanation distributions using the two proposed methods. The experiments were run on a server with 4 vCPUs and 32 GB of RAM. We used `shap` version 0.41.0 and `lime` version 0.2.0.1 as software packages. In order to define the local neighborhood for both methods in this example we use all the data provided as background data. As an f_θ model, we use an `xgboost` and compare the results of TreeShap against LIME. When varying the number of samples we use 5 features and while varying the number of features we use 1000 samples.

Figure 12, shows the wall time required for generating explanation distributions using SHAP and LIME with varying numbers of samples and columns. The runtime required of generating an explanation distributions using LIME is much higher than using SHAP, especially when producing explanations for distributions. This is due to the fact that LIME requires training a local model for each instance of the input data to be explained, which can be computationally expensive. In contrast, SHAP relies on heuristic approximations to estimate the feature attribution with no need to train a model for each instance. The results illustrate that this difference in computational runtime becomes more pronounced as the number of samples and columns increases.

We note that the computational burden of generating the explanation distributions can be further reduced by limiting the number of features to be explained, as this reduces the dimensionality of the explanation distributions, but this will inhibit the quality of the

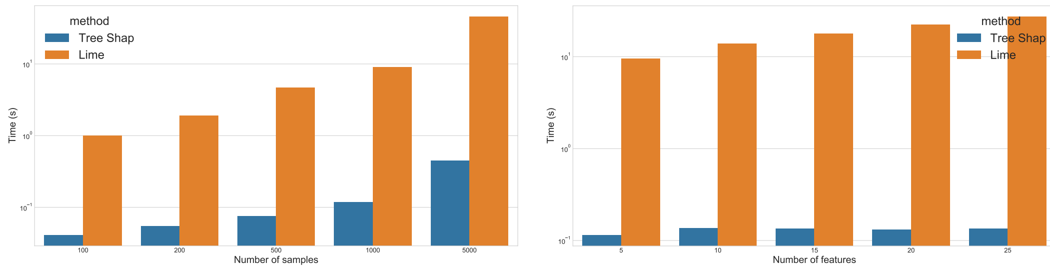

Figure 12: Wall time for generating explanation distributions using SHAP and LIME with different numbers of samples (left) and different numbers of columns (right). Note that the y-scale is logarithmic. The experiments were run on a server with 4 vCPUs and 32 GB of RAM. The runtime required to create an explanation distributions with LIME is far greater than SHAP for a gradient-boosting decision tree

explanation shift detection as it won't be able to detect changes on the distribution shift that impact model on those features.

Given the current state-of-the-art of software packages we have used SHAP values due to lower runtime required and that theoretical guarantees hold with the implementations. In the experiments performed in this paper, we are dealing with a medium-scaled dataset with around $\sim 1,000,000$ samples and $20-25$ features. Further work can be envisioned on developing novel mathematical analysis and software that study under which conditions which method is more suitable.

H True to the Model or True to the Data?

The "Explanation Shift Detector" proposed in this work relies on the explanation distributions that satisfy efficiency and uninformative theoretical properties. We have used the Shapley values as an explainable AI method that satisfies these properties. A variety of (current) papers discusses the application of Shapley values for feature attribution in machine learning models (Strumbelj & Kononenko, 2014; Lundberg et al., 2020b; Lundberg & Lee, 2017a; Lundberg et al., 2018). However, the correct way to connect a model to a coalitional game, which is the central concept of Shapley values, is a source of controversy, with two main approaches (i) an interventional (Aas et al., 2021; Frye et al., 2020; Zern et al., 2023) or (ii) an observational formulation of the conditional expectation(Sundararajan & Najmi, 2020; Datta et al., 2016; Mase et al., 2019).

In the following experiment, we compare what are the differences between estimating the Shapley values using one or the other approach. We benchmark this experiment on the four prediction tasks based on the US census data (Ding et al., 2021a) and using the "Explanation Shift Detector", where both the model $f_\theta(X)$ and $g_\psi(\mathcal{S}(f_\theta, X))$ are linear models. We will calculate the Shapley values using the SHAP linear explainer. [1]

The comparison depends on a feature perturbation hyperparameter: whether the approach to compute the SHAP values is either *interventional* or *correlation dependent*. The interventional SHAP values break the dependence structure between features in the model to uncover how the model would behave if the inputs were changed (as it was an intervention). This option is said to stay "true to the model", meaning it will only give allocation credit to the features that the model actually uses (Aas et al., 2021).

On the other hand, the full conditional approximation of the SHAP values respects the correlations of the input features. If the model depends on one input that is correlated with another input, then both get some credit for the model's behaviour. This option is said to say "true to the data", meaning that it only considers how the model would behave when respecting the correlations in the input data (Chen et al., 2020b; 2022a; Frye et al., 2020; Chen et al., 2020a).

[1] https://shap.readthedocs.io/en/latest/generated/shap.explainers.Linear.html

In our case, we will measure the difference between the two approaches by looking at the linear coefficients of the model g_ψ and comparing the performance using the geo-political and temporal experiment of the previous section 5, for this case between California 2014 and Puerto Rico 2018.

Table 8: AUC comparison of the "Explanation Shift Detector" between estimating the Shapley values between the interventional and the correlation-dependent approaches for the four prediction tasks based on the US census dataset (Ding et al., 2021a). The % character represents the relative difference. The performance differences are negligible.

	Interventional	Correlation	%
Income	0.736438	0.736439	1.1e-06
Employment	0.747923	0.747923	4.44e-07
Mobility	0.690734	0.690735	8.2e-07
Travel Time	0.790512	0.790512	3.0e-07

Table 9: Linear regression coefficients comparison of the "Explanation Shift Detector" between estimating the Shapley values between the interventional and the correlation-dependent approaches for one of the US census-based prediction tasks (ACS Income). The % character represents the relative difference. The coefficients show negligible differences between the calculation methods

	Interventional	Correlation	%
Marital	0.348170	0.348190	2.0e-05
Worked Hours	0.103258	-0.103254	3.5e-06
Class of worker	0.579126	0.579119	6.6e-06
Sex	0.003494	0.003497	3.4e-06
Occupation	0.195736	0.195744	8.2e-06
Age	-0.018958	-0.018954	4.2e-06
Education	-0.006840	-0.006840	5.9e-07
Relationship	0.034209	0.034212	2.5e-06

In Table 8 and Table 9, we can see the comparison of the effects of using the aforementioned approaches to learn our proposed method, the "Explanation Shift Detector". Even though the two approaches differ theoretically, the differences become negligible when explaining the protected characteristic, i.e. when providing the linear regression coefficients.