

# Counterfactual Shapley Additive Explanations

Emanuele Albini

J.P. Morgan AI Research  
London, UK

emanuele.albini@jpmorgan.com

Danial Dervovic

J.P. Morgan AI Research  
London, UK

danial.dervovic@jpmorgan.com

Jason Long

J.P. Morgan AI Research  
London, UK

jason.x.long@jpmorgan.com

Daniele Magazzeni

J.P. Morgan AI Research  
London, UK

daniele.magazzeni@jpmorgan.com

## ABSTRACT

Feature attributions are a common paradigm for model explanations due to their simplicity in assigning a single numeric score for each input feature to a model. In the actionable recourse setting, wherein the goal of the explanations is to improve outcomes for model consumers, it is often unclear how feature attributions should be correctly used. With this work, we aim to strengthen and clarify the link between actionable recourse and feature attributions. Concretely, we propose a variant of SHAP, *CoSHAP*, that uses counterfactual generation techniques to produce a *background dataset* for use within the marginal (a.k.a. interventional) Shapley value framework. We motivate the need within the actionable recourse setting for careful consideration of background datasets when using Shapley values for feature attributions, alongside the requirement for monotonicity, with numerous synthetic examples. Moreover, we demonstrate the efficacy of CoSHAP by proposing and justifying a quantitative score for feature attributions, *counterfactual-ability*, showing that as measured by this metric, CoSHAP is superior to existing methods when evaluated on public datasets using monotone tree ensembles.

## CCS CONCEPTS

• **Computing methodologies** → **Machine learning; Artificial intelligence**; *Classification and regression trees; Supervised learning by classification*; • **Human-centered computing** → **Human computer interaction (HCI)**; • **Theory of computation** → Algorithmic game theory and mechanism design.

## KEYWORDS

XAI, SHAP, actionable recourse, counterfactual explanations, feature attributions, explainability

## ACM Reference Format:

Emanuele Albini, Jason Long, Danial Dervovic, and Daniele Magazzeni. 2021. Counterfactual Shapley Additive Explanations. In *ACM ICAIF 2021*:

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XAI-FIN '21, November 03, 2021, Virtual

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ACM ISBN 978-x-xxxx-xxxx-x/YY/MM...\$15.00

<https://doi.org/10.1145/nnnnnnn.nnnnnnn>

*Workshop on Explainable AI in Finance, November 03, 2021, Virtual. ACM, New York, NY, USA, 9 pages. <https://doi.org/10.1145/nnnnnnn.nnnnnnn>*

## 1 INTRODUCTION

Government regulators are placing increasing emphasis on the fairness and discrimination issues in decision making processes using machine learning algorithms in high-stakes context as finance and healthcare. For example, U.S. credit regulations [47] put particular emphasis on the need to explain automatic decisions in terms of key factors that contributed to an adverse decision. Meanwhile, in the academic literature several techniques have been proposed in recent years to address this issue (see [1, 3, 13] for an overview).

In the context of *local explainability* many approaches on which researchers have focused in the last years are based on the notion of *feature attribution*, i.e., distributing the output of the model for a specific input to its features (e.g., LIME [38], SHAP [25], GIG [27]). In this paper in particular we will focus on SHAP, one of the most popular techniques to generate local explanations based on the notion of Shapley value [40] from game theory. Shapley value-based frameworks for Explainable AI (XAI) consider each feature as a player in a  $m$ -person game to fairly distribute the contribution of each feature to the output of the model. To do so they compare the output of the (same) model when a feature is present with that of when the same feature is missing. There are two main limitations with this approach that have been raised in the literature:

- It is not clear how to define the output of the model when a feature is missing. The most common approach is to estimate it as an expectation over a background distribution of the input features [26].
- There is no explicit guidance provided on how a user might alter one's behavior in a desirable way [21].

Another popular area of research has developed around *counterfactual explanations*, also known as *algorithmic recourse*, i.e., given a specific input one must find the “closest possible world (input)” [50] that gives rise to a different outcome. In practise, this means that these approaches aim to find one (or more) points that are (1) close to the one we want to explain; and (2) “plausible” (where plausibility can be defined in different ways in the literature, see [20] for more insights). Counterfactual explanations have two main limitations:

- Most of the approaches in the literature are limited at finding a single counterfactual point. While this may give the user a clear understanding of what they could do in order to reverse

an adverse outcome, it does not allow them to chose changes that are more suited for them.

- (b) While there has been some attempt at generating diverse sets of counterfactual points (e.g., [30, 39]), there is no consensus on how to limit the cognitive load for the user caused by the sheer amount of information that is provided, or – in other words – on how to provide a more amenable explanation (in terms of size), as advocated also from a social science perspective [28].

In this paper we present how these two general approaches for explainability can be combined in order to provide a *counterfactual feature attribution* grounded on the game-theoretic approach afforded by Shapley values that we call *Counterfactual SHAP (CoSHAP)*. We are motivated by the desire to retain the simple form of explanation provided by feature attributions, while introducing the actionability properties of counterfactual explanations.

In particular, our contributions are as follows.

- We enumerate the assumptions that are necessary to interpret Shapley values in a counterfactual sense and discuss what it means for a feature attribution method to demonstrate counterfactual behaviour.
- We introduce the notion of *counterfactual-ability* of a feature attribution as a way to quantitatively evaluate its ability to suggest to the user how to act upon the input in order to overcome an adverse prediction.
- We propose to use (a uniform distribution over) a set of counterfactual points as the background distribution for the computation of Shapley values in order to achieve higher counterfactual-ability, yielding the CoSHAP algorithm.
- We benchmark the CoSHAP algorithm using a number of different counterfactual generation techniques from the literature against baseline feature attribution techniques. CoSHAP (using 10-NN\* as the counterfactual generation technique) is shown to have the best counterfactual-ability on several public datasets taken from the financial domain.

We note that in this paper we concentrate on tree-based models for the following reasons: (1) in the context of classification and regression for tabular data, tree-based models as XGBoost, CatBoost and LightGBM are deemed as the state-of-the-art in terms of performance and therefore are widely adopted in many industries including finance [45]; (2) interventional Shapley values can be computed exactly for tree-based models using the algorithm proposed in [24]. We also note that in this paper we will put particular emphasis on models that are monotone, i.e., models in which their output is (positively or negatively) monotonic with respect to each of the input features. We do this for two reasons: (1) monotonicity is a key precondition for the interpretation of a feature attribution in counterfactual terms, as will be described in detail in Section 3.2; (2) high stakes models (that are usually the ones in most need of explanations) are usually constrained to be simpler at design-stage with the objective of making them more interpretable. One such common constraint is imposing some kind of monotonic relationship between the features and their output [45].

## 2 BACKGROUND

In the remainder of this paper we consider a binary classification model  $f : \mathcal{X} \rightarrow \mathcal{Y}$  where  $\mathcal{X} = \mathbb{R}^m$  and  $\mathcal{Y} = \mathbb{R}$ . We define the *decision function*  $F : \mathcal{X} \rightarrow \{0, 1\}$  as follows<sup>1</sup>.

$$F(\mathbf{x}) = \begin{cases} 1 & \text{if } f(\mathbf{x}) > 0 \\ 0 & \text{otherwise} \end{cases}$$

We refer to  $f(\mathbf{x})$  as the model *output* and to  $F(\mathbf{x})$  as the model *prediction* or *outcome*. Note that, as reported in the definition of  $F(\mathbf{x})$  and without loss of generality, we use 0 as decision threshold for the binary prediction. Moreover, without loss of generality, in the sequel we assume that an input  $\mathbf{x} \in \mathcal{X}$  such that  $F(\mathbf{x}) = 1$  is an adverse outcome for the user. We also note that all the results in this paper can be trivially generalized to multi-class models.

### 2.1 Shapley values

The Shapley values method is a technique used in classic game theory to fairly attribute the payoff to the players in an  $m$ -player cooperative game. Formally, given a set of players  $\mathcal{F} = \{1, \dots, m\}$  and the *characteristic function* of the game  $v : 2^{\mathcal{F}} \rightarrow \mathbb{R}$ , the Shapley value of player  $i$  is defined as:

$$\phi_i = \sum_{S \subseteq \mathcal{F} \setminus \{i\}} \binom{m-1}{|S|}^{-1} [v(S \cup \{i\}) - v(S)]$$

In the context of machine learning models the players are the features of the model and several ways have been proposed in order to simulate feature absence in the characteristic function (e.g., retraining the model without such feature [44], or using the conditional or marginal expectations over a background distribution [25]).

In this paper we use the approximation of the characteristic function proposed in [25] and [24] that simulates the absence of a feature using the marginal expectation over a background distribution  $\mathcal{D}$ .

$$v(S) = \mathbb{E}_{\mathbf{x}' \sim \mathcal{D}} [f(\mathbf{x}_S, \mathbf{x}'_{\mathcal{F} \setminus S})]$$

where with an abuse of notation  $f(\mathbf{x}_S, \mathbf{x}'_{\mathcal{F} \setminus S})$  indicates the output of the model with feature values  $\mathbf{x}$  for features in  $S$  and values  $\mathbf{x}'$  for feature values not in  $S$ . In the remainder of this paper we will refer to the space of Shapley values  $\mathbb{R}^m$  as  $\Phi$  and the Shapley values vector of  $\mathbf{x}$  as  $\phi$ .

### 2.2 Counterfactual Explanations

In its basic form, a (local) counterfactual explanation (CF) for an input  $\mathbf{x}$  is a point  $\mathbf{x}'$  such that (1)  $\mathbf{x}'$  gives rise to a different prediction, i.e.,  $F(\mathbf{x}) \neq F(\mathbf{x}')$ , (2)  $\mathbf{x}$  and  $\mathbf{x}'$  are close (under some distance metric) and (3)  $\mathbf{x}'$  is a “plausible” input. This last constraint has been interpreted in several ways in the literature, it may involve considerations about sparsity (e.g., [42]), closeness to the data manifold (e.g., [32]), causality (e.g., [19]), actionability (e.g., [34, 48]) or a combination thereof (e.g., [9]). A plethora of techniques for the generation of counterfactuals exist in the literature (we refer the reader to [18, 20, 43, 49] for recent surveys).

We note that, in the scope of this paper we will consider only counterfactual explanation methods that are (1) able to generate a

<sup>1</sup>We use lower-case bold symbols to indicate vectors.

diverse set of counterfactuals and (2) do not require the model to be differentiable since as described in Section 1 we focus on tree-based models. We note that few counterfactual explanation techniques that satisfying both of these requirements exist in the literature.

### 3 INTERPRETING SHAPLEY VALUES IN COUNTERFACTUAL TERMS

In general, Shapley values do not have an obvious interpretation in counterfactual terms, this means that they do not provide suggestions on how a user can change their features in order to change the prediction [2, 21]. We argue that this is due to 2 main reasons: (1) the “arbitrary” choice of background distribution for the computation of Shapley values and (2) the lack of monotonicity constraint of the model. We now discuss the details of these two reasons.

#### 3.1 Choice of the background distribution

As described in Section 2.1 Shapley values describe the contributions of the players (features) to the game payoff (model output). In the context of machine learning model explainability an important assumption is made: the simulation of each player’s (feature) absence in the cooperative game using a background distribution  $\mathcal{D}$ . As pointed out in [26], this means that Shapley values explain a prediction of an input *in contrast to a distribution of background points*. In practise, the background distribution is taken as a uniform distribution over unit point masses at a finite number of points, called the *background dataset*.

Therefore, the background dataset should be chosen according to the contrastive question that we aim to answer. We list some of the most common distributions that have been proposed/used.

- *Training Set* ( $\mathcal{D}_{\text{TRAIN}}$ ) [25]. The whole training set, including the samples that are labelled and/or predicted of being of the same class of the input.
- *Differently-Labelled Samples* ( $\mathcal{D}_{\text{DIFF-LAB}}$ ). The samples in the training set labelled (in the data) differently than the input.
- *Differently-Predicted Samples* ( $\mathcal{D}_{\text{DIFF-PRED}}$ ). The samples in the training set predicted (by the model) with a different class.
- *Differently-Predicted Samples Median* ( $\mathcal{D}_{\text{DIFF-MEDIAN}}$ ). A single point obtained as the feature-wise median of the points predicted with a different class.

These choices of background dataset have in common the fact that they are defined a priori, i.e., they are equal for all the inputs. This means that we are contrasting an input  $\mathbf{x}$  with a (input-invariant) distribution  $\mathcal{D}$  that may potentially be very different from  $\mathbf{x}$ . This can give rise to explanations that are sometimes misleading for a user who is typically interested in understanding which features led to the adverse outcome (in order to reverse it). In other words the contrastive question that we are answering with the Shapley values is not tailored to the specific input (user) and therefore instead of answering the question of “Why was a user rejected when compared to similar users that were accepted?” we will be answering the question of “Which features are most important in making my outcome different from that of other (accepted) users?” (potentially very different from  $\mathbf{x}$ ).

If we consider the example in Figure 1.i that shows an explanation where the training set is used as background dataset, we note that

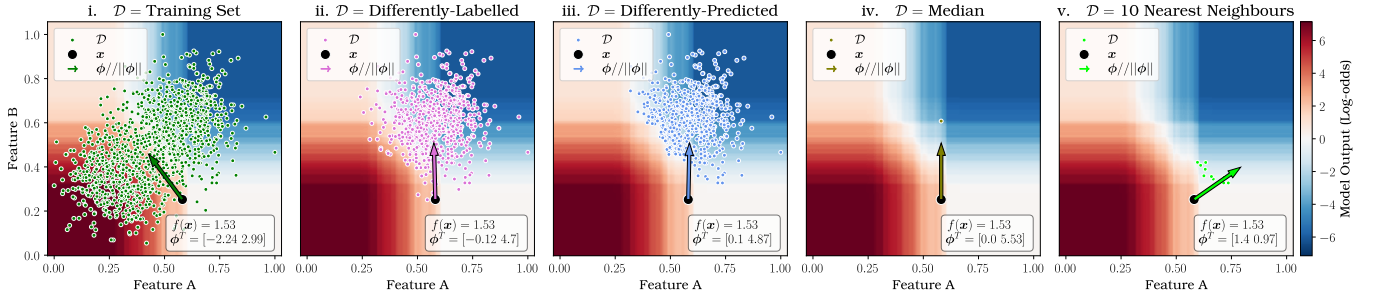
the Shapley values suggest that *Feature A* negatively contributed to the model output; this means that the current value of *Feature A* is “protective” against rejection when *put in contrast* with the expected output of the model obtained when using the background distribution  $\mathcal{D}_{\text{TRAIN}}$ . This may be useful information for the model developers **but it does not allow one to gain any (actionable) insight** unless we assume access to the underlying distribution  $\mathcal{D}_{\text{TRAIN}}$ . In fact, this explanation only informs a potential user that its *Feature A* is better than the one of an average customer but it does not either (a) advise them on how they can change their features in order to overcome the (adverse) outcome; or (b) inform them on which features were most important in rejecting their application.

Figures 1.ii, 1.iii and 1.iv show how alternative (but still input-invariant) background distributions ( $\mathcal{D}_{\text{DIFF-LAB}}$ ,  $\mathcal{D}_{\text{DIFF-PRED}}$  and  $\mathcal{D}_{\text{MEDIAN}}$ , respectively) may improve the explanations in terms of informing the user on which features were most important in rejecting their application when compared to other rejected samples, but they still lack the ability of giving useful insight on which features were the most important and therefore should be acted upon in order to reverse the adverse decision  $F(\mathbf{x}) = 1$ . This is due to the contrastive question being posed with respect to (a) samples that have much better (lower) model outputs and (b) samples that have similar model output but that are very different from  $\mathbf{x}$ .

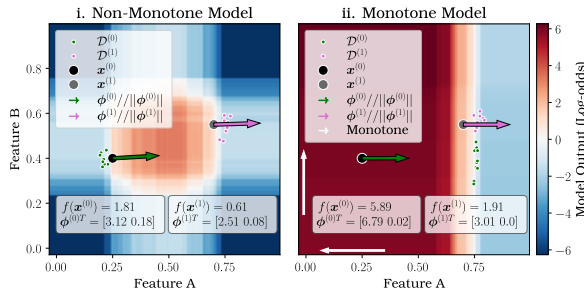
Using a set of counterfactual points as the background dataset solves the issues mentioned in the preceding example. In particular, using counterfactuals as the background dataset allows one to answer a contrastive question that is (a) of interest for the user because it is comparing  $\mathbf{x}$  to samples that are similar to them (and implicitly more “reachable”) and (b) more amenable in terms of access to the underlying distributions. In fact, as mentioned earlier, a useful interpretation of Shapley values-based explanations requires access to the background distribution. Arguably, a user can relate to a set of similar customers more easily than the training set (that may contain very different users). For example, imagine a fraud-prone millionaire being rejected for a consumer trading account who is given an explanation that contrasts them with the average customer (who is very likely neither fraud-prone nor a millionaire).

For example, if we consider Figure 1.v that shows the direction of the Shapley values calculated using the 10 nearest neighbors of the input that were accepted, we note how both features are deemed as contributing to the rejection when compared to similar customers that were instead accepted. And in fact, *Feature A* has a higher importance than *Feature B* since the model is locally more sensitive to *Feature A* than *Feature B* as shown by the sharper color gradient in the horizontal direction.

As noted earlier, using a set of diverse counterfactual points as a background distribution (contrary to “classic” input-invariant background distributions) means that the background distribution depends on the input  $\mathbf{x}$ . Therefore, in the sequel we will denote such distributions as  $\mathcal{D}_C(\mathbf{x})$  where  $C$  is the name of the counterfactual technique used to generate the background dataset. For simplicity of exposition, from now on we refer to explanations using a diverse set of counterfactual points as the background distribution for the computation of Shapley values as *Counterfactual SHAP* or, for short, *CoSHAP*.



**Figure 1: Effect of different choices of background dataset on the Shapley values of the same input with the same model. Red regions correspond to areas of the feature space where the decision is adverse, i.e.  $F(x) = 1$ , with blue regions representing the opposite, i.e. those  $x \in \mathcal{X}$  for which  $F(x) = 0$ .**



**Figure 2: Effect of the lack of monotonicity constraint on the Shapley values of two same inputs.**

### 3.2 Monotonicity of the model

As remarked in [2], feature attributions do not clearly provide guidance on how to alter the features in order to change the prediction of a model, and sometimes they can be even misleading in that respect because they make the assumption that the model is monotone.

For instance, if we consider Figure 2.i showing the Shapley values of two points,  $\mathbf{x}^{(0)}$  and  $\mathbf{x}^{(1)}$ , for a monotonic model, we note how both explanations have a positive Shapley value for *Feature A* but in order to overcome the adverse outcome *Feature A* must be increased for  $\mathbf{x}^{(0)}$  while it must be decreased for  $\mathbf{x}^{(1)}$ . This means that a user (that has no access to the model) is unable to move the feature in the most sensible direction. In contrast, we observe in Figure 2.ii – where the model is monotone in both features A and B – that the Shapley values for  $\mathbf{x}^{(0)}$  and  $\mathbf{x}^{(1)}$  both again have similar Shapley values. Changing feature A in the same direction as the sign of its Shapley value will decrease the value of the model output for both of the points  $\mathbf{x}^{(0)}$  and  $\mathbf{x}^{(1)}$ , thereby yielding a better outcome for both points. In fact, if the model is monotone then moving a feature with a positive (negative) monotone trend in one direction will give rise to a predictable change in the model output in the same (opposite) direction.

Having described how the background distribution used for the computation of Shapley values and the monotonic behaviour of the model play a key role in giving a counterfactual interpretation to Shapley values, we now turn to the open question on how we can numerically measure this “counterfactual-ability” of a feature attribution. We will tackle this problem in Section 4.

## 4 COUNTERFACTUAL-ABILITY

We seek to formalise the notion that certain feature attributions will be more useful for a model user in changing features to reverse an adverse outcome. It is important to emphasise that predicting how users might engage with explanations is a very challenging problem, and behaviour may vary dramatically depending on the context. We do not claim to resolve this problem. However, we aim to set up a flexible framework to measure the ability of an explanation to help a user reverse an adverse decision, before specialising this framework under certain plausible assumptions about how a user could act on the explanations that they receive.

**Counterfactual-ability.** To define the *counterfactual-ability* of a feature attribution  $\phi$  we will measure the cost that a user will incur when changing the input  $\mathbf{x}$  into a new input  $\mathbf{x}'$  based on the information provided by the feature attribution  $\phi$ .

We will measure the cost of changing an input  $\mathbf{x}$  into another input  $\mathbf{x}'$  via a *cost function*. Formally, a *cost function* is a function  $c : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}^+$  where  $c(\mathbf{x}, \mathbf{x}')$  is the cost for the user of moving from  $\mathbf{x}$  to  $\mathbf{x}'$ . A very simple example of cost function could be the Euclidean distance defined in the input space.

In order to describe how a user acts upon the input  $\mathbf{x}$  based on the information provided by the feature attribution  $\phi$  we use an *action function*. Formally, an *action function* is a function  $A : \mathcal{X} \times \Phi \rightarrow 2^{\mathcal{X}}$  where  $A(\mathbf{x}, \phi) \subset \mathcal{X}$  is a subset of the input space describing plausible changes the user may enact upon  $\mathbf{x}$  when provided with an explanation  $\phi$ . We will refer to  $A(\mathbf{x}, \phi)$  as the *action subset*. Note that we do not constraint the action subset to be finite.

Intuitively the output of an action function can be interpreted as a subset of the possible options that a user may consider when changing the input based on the information provided by the feature attribution. For instance, a user may consider as possible options only changes to the most important feature according to the feature attribution. In the most extreme scenario a user may ignore the information provided by  $\phi$  and therefore consider any change as a possible option; this would correspond to a constant action function always returning the whole input space as the action subset. In a more realistic scenario though, we expect the user to use the information provided by the feature attribution and therefore we expect the action subset to be a restricted subset of the input space, e.g., allowing only changes to the most top-3 features according to

$\phi$ . Later in this section we will formally describe the action function that we use in the scope of this paper.

The counterfactual-ability of a feature attribution  $\phi$  is defined as the negation of the infimum cost to act upon  $x$  given the action subset for  $\phi$ . Intuitively, the higher the cost the lower the counterfactual-ability. We formally define the counterfactual-ability of a feature attribution  $\phi$  given an input  $x$  and an action function  $A$  as follows.

$$CA(x, \phi, A, c) = - \inf_{\substack{x' \in A(x, \phi) \\ F(x') \neq F(x)}} c(x, x')$$

Note that the action function is fixed for a given user; the goal in fact is to compare how different feature attributions perform under a (given) action function rather than optimising the action function for a specific user. We note that, in the degenerate case in which the action function is a constant function always returning the whole input space, solving this optimisation problem is equivalent to finding the (possibly synthetic) counterfactual point  $x'$  with minimum cost from the input  $x$ .

Note that the larger the action subset, the smaller the counterfactual cost and therefore the larger the counterfactual-ability. However, if the action subset has multiple dimensions then the user must solve a difficult optimisation problem to realise the full potential of the counterfactual-ability - in many cases this will be unrealistic to expect. The assumptions we include below will be used to make the optimisation tractable for the user by restricting the action subset to a single line.

**Choice of action function.** After defining the general concepts of action and cost functions we now define a concrete instance that we use in this paper. To do so, we start with a number of assumptions. These assumptions are designed to create a sensible metric for the counterfactual-ability of an explanation in the context of algorithmic recourse. Intuitively, the assumptions aim to cast the feature attribution as a suggested direction for a user to move in feature space, and the counterfactual-ability of the a feature will therefore measure the distance (under a sensible metric) to the decision boundary along this line.

**Action Function.** In the scope of this paper, we use the following set of assumptions:

- **Monotonic recourse.** When changing a feature a user will move its value in the *opposite direction of the monotonic trend*, e.g., to reduce the risk of default a user will try to increase their income (as opposed to reducing it).
- **Adverse factors recourse.** A user will change the features with *positive* Shapley values, i.e, the features contributing to the adverse prediction (as opposed to also improving features that are already good).
- **Proportional recourse.** A user will change the features with the *highest* (positive) Shapley values changing them proportionally to their Shapley values.
- **Recourse cost.** When moving feature proportionally to their Shapley values we use the *quantile shift* as metric to compare the cost of the recourse.

We will call the action function satisfying this assumptions  $\tilde{A}_k$  where  $k$  is the number of top features that a user is considering.

We formally define it as follows<sup>2</sup>.

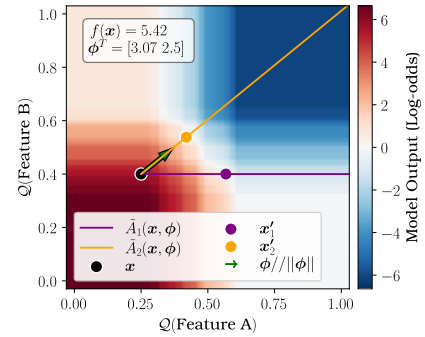
$$\tilde{A}_k(x, \phi) = \{x' : Q(x') - Q(x) = -\lambda \phi \odot \mathbb{T} \odot \mathbb{I}_k(\phi), \forall \lambda > 0, x' \in \mathcal{X}\}$$

where  $\mathbb{T} \in \{-1, +1\}^m$  is the trend vector, satisfying  $\mathbb{T}_k = 1$  if the trend is positive and  $\mathbb{T}_k = -1$  if the trend is negative;  $Q : \mathcal{X} \rightarrow [0, 1]^m$  is a function computing the quantile (inverse cdf) of each of the features with respect to the distribution induced by the training data; and  $\mathbb{I}_k(\phi) \in \{0, 1\}^m$  is an indicator vector for the top- $k$  features in  $\phi$ . Formally:

$$\mathbb{I}_i^k(\phi) = \begin{cases} 1 & \text{if } i \in \arg \max_{S \subseteq \{1, \dots, m\}, |S| \leq k} \sum_{i \in S} \phi_i \\ 0 & \text{otherwise} \end{cases}$$

The intuition behind this choice of action function is that the feature attribution should provide a suggested direction to the user that takes them towards the decision boundary. However, realistic actions will not involve changes to every feature; rather, a user may focus on making changes to only the top- $k$  most important features, and we reflect this in our choice of action function. We use the quantile shift as a normalised metric for recourse cost, so that the action subset induced by our action function is a semi-infinite line in the normalized quantile input space in the direction of the Shapley vector with its sign adjusted to match the monotonic trend. To better understand this concept we can consider Figure 3, showing an example of the action subset induced for an input  $x$  and an attribution  $\phi$ .

We note that our choice of action function is just one instantiation of the framework that we propose. We argue that casting the explanation as a direction in which an input point may move is a natural choice that allows for concrete comparisons between methods, but we acknowledge that there is no clear answer to the question of how different users may act upon  $x$  given  $\phi$  in full generality. We believe that this topic represents an interesting future research direction, and we discuss this further in Section 7.



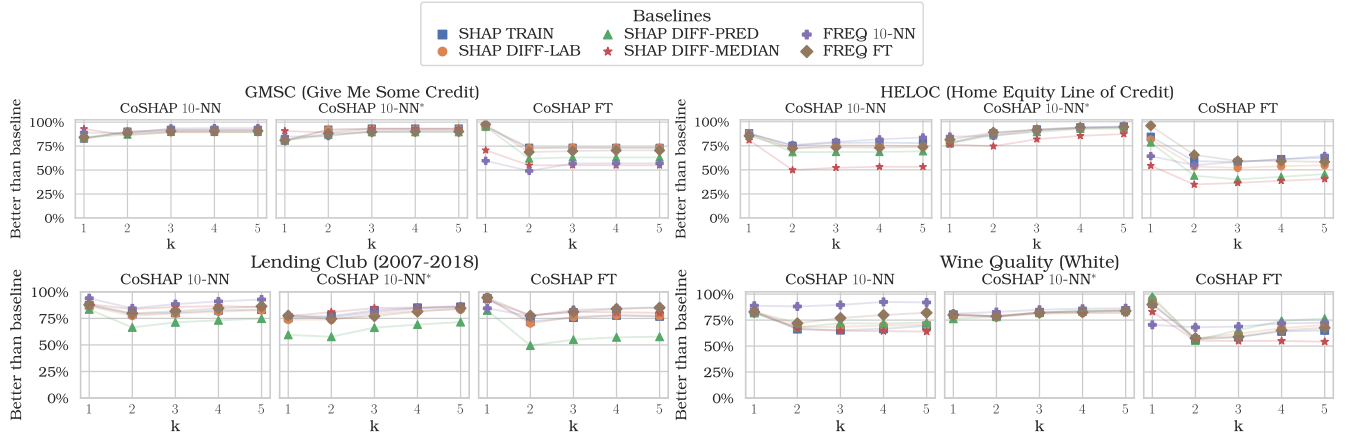
**Figure 3: Algorithmic intuition of the action function. Note that the feature axes are in the quantile space.**

**Cost Function.** We measured the cost using the quantile shift under L1 and L2-norm, common metrics in the actionable recourse literature [48]. Formally:

$$c_{L1}(x, x') = \|Q(x') - Q(x)\|_1, \quad c_{L2}(x, x') = \|Q(x') - Q(x)\|_2.$$

<sup>2</sup>We use  $\cdot$  and  $\odot$  to indicate the dot and element-wise product, respectively.





**Figure 4: Percentage of times in which the counterfactual-ability  $CA(\mathbf{x}, \phi, \tilde{A}_k, c_{L1})$  of different versions of CoSHAP (CoSHAP 10-NN, CoSHAP 10-NN\* and CoSHAP FT) is higher (better) than the counterfactual-ability of the baseline feature attributions (one line for each baseline). The plots show how the counterfactual-ability changes when varying the number of top- $k$  features considered in the action function.**

Method Name	Type <sup>†</sup>	Distribution <sup>‡</sup>
COUNTERFACTUAL SHAP		
CoSHAP FT	Shapley	$\mathcal{D}_{FT}(\mathbf{x})$
CoSHAP 10-NN	Shapley	$\mathcal{D}_{10-NN}(\mathbf{x})$
CoSHAP 10-NN*	Shapley	$\mathcal{D}_{10-NN}^*(\mathbf{x})$
BASELINES		
SHAP TRAIN	Shapley	$\mathcal{D}_{TRAIN}$
SHAP DIFF-LAB	Shapley	$\mathcal{D}_{DIFF-LAB}$
SHAP DIFF-PRED	Shapley	$\mathcal{D}_{DIFF-PRED}$
SHAP DIFF-MEDIAN	Shapley	$\mathcal{D}_{DIFF-MEDIAN}$
FREQ 10-NN	Frequency	$\mathcal{D}_{10-NN}(\mathbf{x})$
FREQ FT	Frequency	$\mathcal{D}_{FT}(\mathbf{x})$

**Table 1: Explanation methods used in the experiments divided among Counterfactual SHAP variants and baselines. (\*) Variant of the distribution where points are projected on the decision boundary (see Section 5); (†) type of feature attribution, i.e., Shapley values or Frequency-based feature attribution; (‡) distribution used as background (for Shapley values) or to generate a (diverse) set of counterfactual points (for frequency-based feature attribution), refer to Section 3.1 for details.**

## 5 EXPERIMENTS

In order to understand how different variants of CoSHAP perform in terms of counterfactual-ability we compared them against existing feature attribution techniques. Table 1 describes in detail the feature attributions that we considered in our experiments.

In particular, we considered 3 variants of Counterfactual SHAP that differs from each others for the technique used to generate counterfactual points that are as follows.

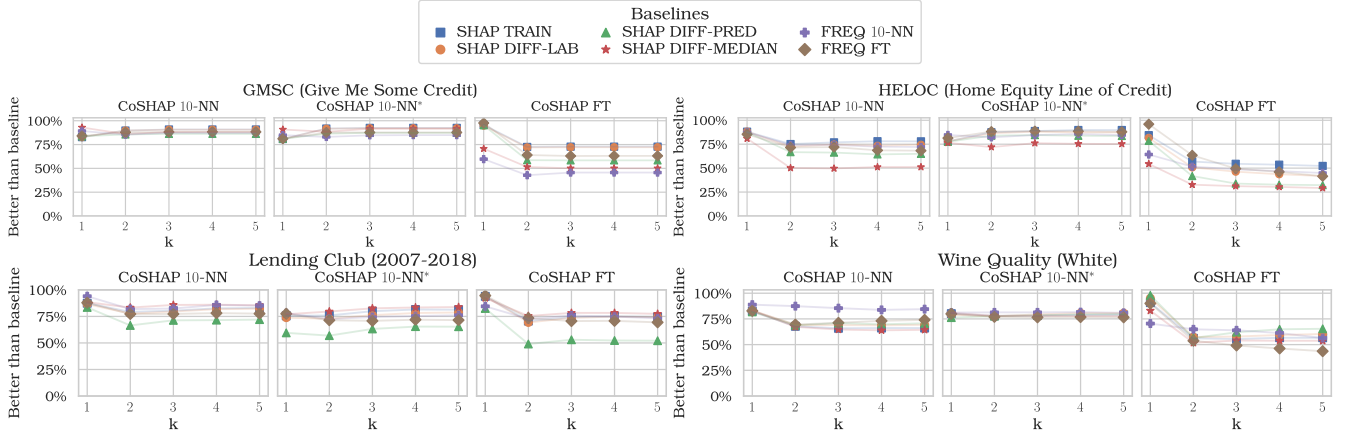
- *Feature Tweaking (FT)* [46]. We take all the  $\epsilon$ -perturbations of the input that lead to a different prediction. In our experiments we used  $\epsilon = 10^{-6}$ .

- *K-Nearest Neighbours (K-NN)* [31]. We take the  $K$  nearest points to  $\mathbf{x}$  in the training set, referred to as  $\mathcal{D}_{KNN}^K$ , such that their predictions are different from  $\mathbf{x}$ 's. In our experiments we used  $K = 10$  and the euclidean distance over the quantile space as distance metric.
- *Decision Boundary K-Nearest Neighbours (K-NN\*)*. Since the counterfactual points generated using K-NN are samples extracted from the training set they tend to be at a greater distance from the decision boundary (DB) than artificially generated counterfactual points (for instance those generated using FT). For this reason we generated a variant of K-NN obtained by intersecting the DB with the lines connecting  $\mathbf{x}$  with the  $K$  nearest points<sup>3</sup>.

For comparison with CoSHAP, we considered baselines belonging to two broad families of feature attribution methods from the literature. On the one hand, we compared CoSHAP with Shapley values obtained using common input-invariant background distributions:  $\mathcal{D}_{TRAIN}$ ,  $\mathcal{D}_{DIFF-PRED}$ ,  $\mathcal{D}_{DIFF-LAB}$  and  $\mathcal{D}_{DIFF-MEDIAN}$ . We refer to Section 3.1 for more details about these distributions. On the other hand, we compared CoSHAP with existing feature attribution techniques (non-Shapley values-based) that have a counterfactual intent. In particular we considered the frequency-based approach proposed in [29], that for each feature generates the attribution score as the fraction of counterfactual points possessing a modified value of the feature with respect to the input  $\mathbf{x}$ . In order to generate a (diverse) set of counterfactual points we used the same techniques that we used to generate the background datasets for CoSHAP described earlier in this section, i.e., FT, K-NN, K-NN\*.

**Setup.** To run the experiments we used 4 publicly available datasets: **GMSC** (Give Me Some Credit) [15], **HELOC** (Home Equity Line Of Credit) [11], **LC** (Lending Club Loan Data) [16] and

<sup>3</sup> $X_{K-NN^*} = \{\mathbf{x}_C^* : \mathbf{x}_C^* = (\mathbf{x}_C \perp \mathbf{x}) \cap DB, \forall \mathbf{x}_C \in X_{K-NN}\}$  where  $\mathbf{x}_C \perp \mathbf{x}$  denotes the line segment between  $\mathbf{x}$  and  $\mathbf{x}_C$  and  $X_{K-NN}$  and  $X_{K-NN^*}$  are the CoSHAP K-NN and CoSHAP K-NN\* background datasets, respectively. In practise, we obtained  $X_{K-NN^*}$  by simply applying the bisection method in order to find the intersections.



**Figure 5: Percentage of times in which the counterfactual-ability  $CA(x, \phi, \tilde{A}_k, c_{L2})$  of different versions of CoSHAP (CoSHAP 10-NN, CoSHAP 10-NN\* and CoSHAP FT) is higher (better) than the counterfactual-ability of the baseline feature attributions (one line for each baseline). The plots show how the counterfactual-ability changes when varying the number of top- $k$  features considered in the action function.**

**WINE** (UCI Wine Quality) [8]. For each dataset we used a 70/30 split. We trained a monotonic XGBoost model [7], using the Spearman’s Rho (with respect to the target variable) to determine the monotonic trend of the features. We hyper-trained the parameters maximizing the average ROC-AUC under a 5-fold cross validation. As described in Section 2, we used 0 as decision threshold for the binary prediction.

**Results.** We measured the percentage of times in which CoSHAP performs better in terms of counterfactual-ability than baselines over 1000 rejected (i.e. with  $F(x) = 1$ ) random samples close to the decision boundary (for which<sup>4</sup>  $\sigma(f(x)) \leq 0.6$ ) for each of the 4 datasets. Figure 4 and Figure 5 show the results using the cost functions  $c_{L1}$  and  $c_{L2}$ , respectively. We report the main findings.

- CoSHAP 10-NN and CoSHAP 10-NN\* consistently beat (i.e.,  $> 50\%$ ) all of the baselines, performing between 51.2% and 96.4% of the cases better than the baselines. We note that further investigation is necessary to fully understand the effects of the hyper-parameters of  $K$ -NN ( $K$ ) on the resulting CoSHAP explanation and how they related with the size and dimensionality of the training data.
- For several datasets, CoSHAP FT does not perform well against the baselines (i.e., in more than 50% of the considered samples the counterfactual-ability is lower than that of the baselines). In particular, CoSHAP FT fails to beat the performance of the (baseline) SHAP DIFF-PRED that uses the full set of samples predicted as belonging to a different class as background dataset. This is due to the sparsity of the counterfactual points generated by FT.
- The results are robust with respect to the norm (L1 or L2) used to aggregate the cost of different features.

<sup>4</sup> $\sigma$  denotes the sigmoid function.

## 6 RELATED WORK

There has been recently an increasing interest in exploring the relationship between feature attribution techniques and counterfactual explanations.

A recent work [51] has proposed a Bayesian decision theory-based approach to the computation of the Shapley values. In particular the idea of [51] is to optimize the choice of the background distribution for the computation of Shapley values maximizing the expected reward for the user, i.e.,  $\mathcal{D}^* = \arg \max_{\mathcal{D}^* \subseteq \mathcal{D}} E_{x \sim \mathcal{D}^*}[r(x)]$ , under a certain reward function  $r$ . The work provides a theoretical framework for modelling user preference and beliefs but lacks (by design) concrete (1) guidance on how to select  $\mathcal{D}^*$ , (2) how to update the reward function  $r$  based on the observed Shapley values and (3) how to interpret the feature attribution  $\phi$  into practical actions on the input  $x$  in order to (automatically) solve the optimisation problem without resorting to an update in human-in-the-loop fashion.

Other works have proposed to fill the gap between feature attributions and counterfactual explanations by different means than Shapley values. In particular, [29] and [41] propose techniques to generate feature attributions from a set of diverse counterfactual points but (contrary to us) they use frequency-based approaches, i.e., they give higher attribution to features that are more often changed in counterfactual points. This implies that also features potentially ignored by the model may receive a high feature importance because they are correlated with other features that are really used by the model. As remarked in [6] this behaviour may be desirable in some context as medical sciences but not in others, as in the credit scoring scenario in which users are ultimately interested in understanding why they have been rejected *by the model* rather than which features correlate with rejection *in the data*. We used [29] as a baseline in the experiments in Section 5. In [5] feature attributions are generated by approximating the minimal adversarial perturbation using an adversarially trained neural network

on a (differentiable) neural network-based surrogate model. This approach tends to follow the most strictest interpretation of the “true to the model” paradigm [6] enforcing only the class change but does not directly allow for the enforcement of other constraints, e.g., regarding the plausibility of such changes, as we do by providing a background distribution that is based on counterfactuals.

Other works such as [10, 35, 36] analyze the complementary problem to that we analyze in this paper: they show how feature attributions can guide the search of counterfactual points (while we investigate how different techniques for the generation of counterfactual examples can empower better feature attribution).

In general, many works have explored how to evaluate counterfactual explanations (e.g., [23, 37, 48]) and feature attributions (e.g., [12, 22, 33]) but few proposed a quantitative metric to evaluate feature attributions in counterfactual terms. In [52] the authors propose to evaluate feature attributions with a *fidelity error* for each of the features that (differently from counterfactual-ability) is computed changing only a single feature at a time. We also note that in this paper, our definition of counterfactual-ability is inspired by the notion of *quantile shift cost* proposed in [48], originally designed to evaluate counterfactual explanations (while counterfactual-ability is a metric for feature attributions).

## 7 CONCLUSION AND FUTURE WORK

Towards the more general goal of unifying feature attribution techniques and counterfactual explanations, we have shown how using counterfactual points as the background distribution for the computation of Shapley values (CoSHAP) allows one to obtain feature attributions that can better advise towards useful changes of the input in order to overcome an adverse outcome. We proposed a new quantitative framework to evaluate such an effect that we called counterfactual-ability, and remarked on the role that monotonicity of the model plays in the generation of feature attributions with a counterfactual intent. We evaluated CoSHAP on 4 publicly available datasets and highlighted that using simpler counterfactual techniques such as those based on nearest-neighbours within CoSHAP performs better than existing feature attribution methods.

Our proposal can be extended in several directions. Firstly, it would be interesting to explore alternative notions of action and cost function, grounding their definition with findings in psychology and the social sciences concerning how users interpret feature attributions and how they consequently change their behaviour. For example, one possibility would be to expand the definition of action function to take into account user preferences for certain actions – this could be achieved by coupling each “possible action” returned by the action function with a probability. Secondly, investigating additional metrics for the evaluation of a feature attribution in counterfactual terms would also be of interest. For instance, one could include considerations about the sparsity and/or the plausibility of the feature attributions, as well as other metrics drawn from the counterfactual explanations literature. Lastly, testing our approach on different models (e.g., neural networks) and using a wider variety of (potentially model-agnostic) counterfactual explanation techniques as [9, 14, 17–19, 37] represents another interesting future direction.

From a wider perspective, our work draws attention to some gaps in the literature that we believe are worthy of further investigation. On the one hand, the importance of techniques for the generation of a diverse set of counterfactuals advocated by many practitioners [30, 39, 42]. On the other hand, it highlights how few techniques have the capabilities of generating diverse counterfactual explanations in the context of non-differentiable models, such as ensembles of decision trees that are among the most widely adopted in industry.

## ACKNOWLEDGMENTS

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