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A Framework for Generating Counterfactual Explanations to Explain Black-Box Models

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A Framework for Generating Counterfactual Explanations to Explain Black-Box Models

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Abstract: Automated decision-making systems are becoming more prevalent across a range of fields. For example, they are used across the finance industry to decide whether customers are entitled to loans, and in medicine to support clinical decisions. With decisions that substantially impact individual lives, users will often want explanations of why these decisions were made. Indeed, current and in-progress legal frameworks have begun to require these. For example, GDPR entitles users to explanations about decisions made by these automated systems. Similarly, the Algorithmic Accountability Act would require companies to conduct impact assessments for bias, effectiveness and other factors. One way of producing such explanations for the decisions of machine learning models is to ask the question "What must I change in the input to change the output of a model". This is known as a counterfactual explanation. Our methodology begins by fitting simple models to the variation of the output caused by the change of one input feature. We then score each of these models using user-tuneable scoring functions. By selecting the best possible change and then repeating, we chain together these simple models into sequential counterfactuals. Our method is modular, which means that it is inherently extensible. Each component of out methodology can be easily modified to make it more useful for specific situations. We examine how well our methodology performs on multiple data formats: images and tabular data. We compare our framework to other methodologies. We demonstrate that our method can, in some cases, produce more interpretative counterfactuals that change fewer features than some existing methodologies. Finally, we make a Python implementation of our code available so that it can be used by the machine learning community.

Keywords: explainable AI; counterfactual reasoning; class-contrastive counterfactual explanations

1. Introduction

Automated artificially intelligent systems are increasingly intertwined with our everyday lives — from medical diagnosis to finance and image recognition. While some situations will use directly interpretable models — such as logistic regression [1] — others will be black-box [2]. For consumers to trust these black-box models, they often want some explanation as to what this automated system is doing — an answer to why it made the decision it did. Explainable AI (XAI) is a field of research that aims to develop tools and techniques to answer these questions. Many existing tools exist for generating these explanations for end users. Popular tools include SHAP [3] and LIME [4] XAI can also be used for debugging models by finding where the model has learnt spurious relationships in the training data and providing algorithmic accountability. Some proposed legislative frameworks have begun to demand this accountability from applied algorithms [5].

One way to provide these explanations is through counterfactuals. The classic example of a counterfactual explanation of a model involves a situation where we have trained a model to decide whether a bank should provide an individual with a loan. A helpful way to explain the predictions this model makes is to say what a user must modify to change the prediction made by a model. For example, "You were denied this loan, but if your income was £10,000 higher, you would have been granted this loan", or "You were granted this loan, but you would not have been granted a loan of a

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higher value". Similarly, we could say "This image was classified as a 1, but if we filled in these pixels, the image would be classified as a 0." This way of explaining the output of machine learning models has a number of benefits over existing models. In some sense, it is actionable to a user. Similarly, they may be easier to interpret - as this is an intuitive form of explanation that users will have encountered in their day-to-day lives.

Formally, given a data point x and a classification model f, we define a counterfactual as a different data point x' such that $f(x) \neq f(x')$. We want our counterfactual point to be, by some metric, close to the original point.

As with some existing research in this field [6], we aim to bring together ideas from program synthesis and explainable AI to develop a methodology for generating counterfactuals to explain the outputs of black-box systems. We chain together a series of individual changes. The selection of changes, which are themselves determined by local, simple surrogate models, are easily fine-tunable by an end user.

Overall, according to some quantitative and qualitative metrics, our novel methodology performs better than certain common existing methodologies on some data formats. Furthermore, our method can provide insights into how the model processes information, especially in the case of images.

1.1. Our Approach

We develop an approach that can produce counterfactual explanations (see Figure 1). We begin by varying the value of each input feature to generate hypothetical fake data-points. Once we have these we are able to apply our original model to this new local data-set ($\{\mathbf{x_k}, y_k := f(x_k)\}_k$ for our underlying model f) .

We then fit surrogate models (such as a Gaussian process) to the effect of varying each feature. These surrogate models estimate the high-level, local dependence of the underlying model on each feature. If any of these models predict that a possible feature value change is, in fact, a counterfactual x_j^{new}, we stop here - returning this to the end user. If not, we "score" each of these single variable explainer, and repeat the process from these new, fake data points.

This scoring phase allows for a domain expert to tune the explanation, through setting "changeability scores" for different variables, or by customising the scoring function itself.

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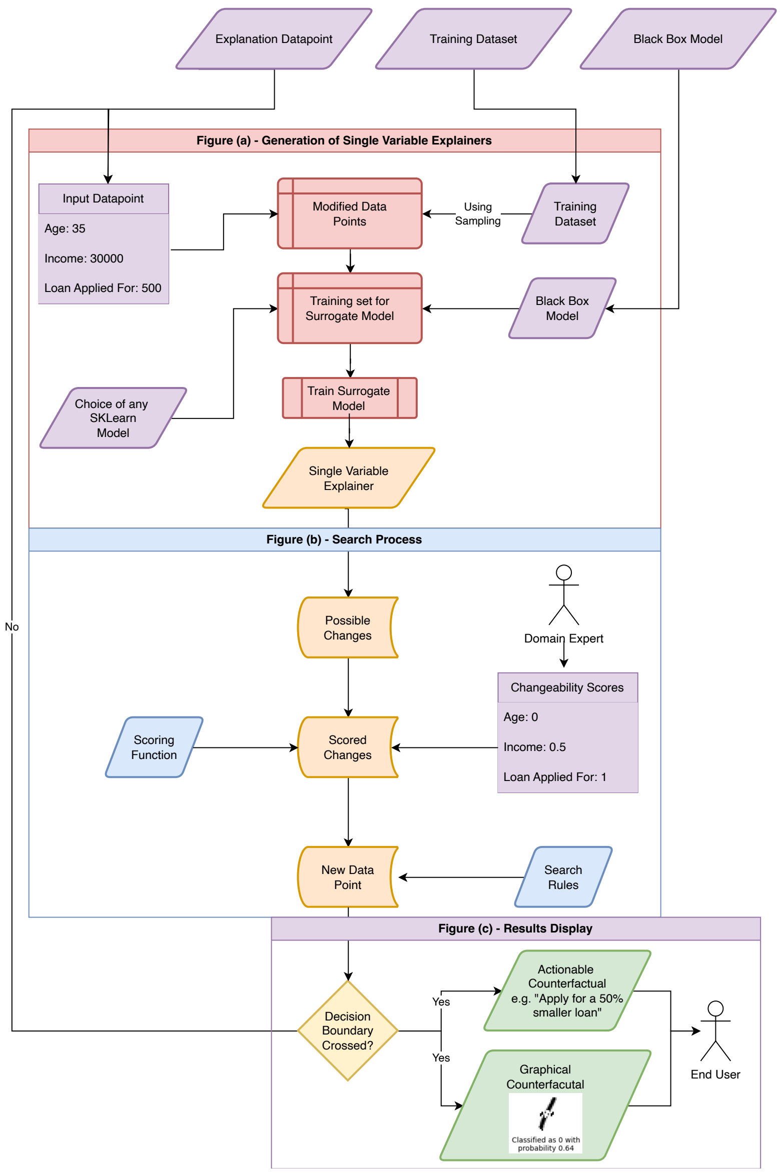

Figure 1. A visualization of our methodology. The required inputs (shown in the figure as parallelograms at the top of the image) are the data point to be explained, the training data set and the black box model. These go into the generation of single variable explainers. These "single-variable-explainers" are simple, surrogate models fit to the local variation of the underlying black-box model on one of it's input features. To generate these, we take our input data-point, and for each feature, replace that features values with other sampled values for that feature to generate "hypothetical" input datapoints. We then apply our underlying model to these data points and fit a simple surrogate model to these (sampled feature values, model prediction) pairs. This process is shown in Figure 1(a). We can then compute, given some scoring function on these surrogate models, possible changes that can be made to the input point. In a visual medium, this might mean changing a single pixel value. Using these scores we can the score these changes to select which is the most impactful on the underlying model's prediction. We make the change suggested by this and repeat the process from this new starting point. This is summarized in Figure 1(b) and is explained in more detail in Figure 3. Once the changes chosen are sufficient to change the model's classification, we can return this counterfactual to the user. This is shown in Figure 1(c).

2. Background

Automated systems driven by artificial intelligence are becoming integrated into our lives – from medical diagnoses to financial services and image analysis. While some employ interpretable models, such as logistic regression [1], others utilize black-box models [2]. To gain consumer trust in these black-box models, it is often necessary to provide some explanation of the system's operations – essentially, why a particular decision was reached.

Explainable AI (XAI) is focused on creating tools and methodologies to address these questions. XAI can also aid in model debugging by identifying where the model has learned incorrect patterns from the training data and ensuring algorithmic accountability. AI models are very effective at solving a wide range of problems [7], they are often a black box [2] – i.e., characterised by their inputs and outputs but whose inner workings cannot be directly interpreted by a user or programmer.

Due to the growing popularity of AI in high-stakes decision-making [8], there has been a vast body of research into techniques to explain the decisions of these models [9]. Some state-of-the-art techniques include feature attribution models such as SHAP [10] and LIME [4]. Other methods rely on gradients – such as GRAD-CAM [11], or concept-based explainability, such as through concept bottleneck models [12] – often with automated concept extraction [13,14].

We use some ideas from the LIME paper – such as fitting simple surrogate models to perturbations around our sample of interest - alongside ideas from the SHAP paper - such as working on a feature-by-feature basis.

2.1. Counterfactuals

One way to provide these explanations is through counterfactuals [15]. The classic example of a counterfactual explanation of a model involves a situation where we have trained a model to decide whether a bank should provide an individual with a loan. A helpful way to explain the predictions this model makes is to say what a user must modify to change the prediction made by a model. For example, "You were denied this loan, but if your income was £10,000 higher, you would have been granted this loan", or "You were granted this loan, but you would not have been granted a loan of a higher value". Similarly, we could say "This image was classified as a 1, but if we filled in these pixels, the image would be classified as a 0."

Formally, given a data point x and a classification model f, we define a counterfactual as a different data point x' such that $f(x) \neq f(x')$.

The problem of finding counterfactuals (sometimes referred to as the inverse classification problem [16]) is an active area of research. In the next section, we will review some of these methods; however, this is not meant to be an exhaustive review, but instead just to give an overview of the range of existing methods.

2.2. SHAP Values

[10] introduce a technique for assigning importance to different features by (using ideas from game theory) taking the difference between models trained with and without the feature present.

$$\phi_i = \underbrace{\sum_{S \subseteq F \setminus \{i\}}}_{\text{Sets of features}} \underbrace{\frac{|S|!(|F|-|S|-1)!}{|F|!}}_{\text{Weighting Factor}} \times \underbrace{\left(\underbrace{f_{S\cup\{i\}}\left(x_{S\cup\{i\}}\right)}_{\text{Model with features } S \text{ and } i} - \underbrace{f_S(x_S)}_{\text{Model without feature } i} \right)}_{\text{Difference in Output}} \tag{1}$$

However, this computation is incredibly expensive, but for most models, we can approximate this using Monte Carlo methods.

$$\hat{\phi}_j = \frac{1}{M} \sum_{m=1}^{M} \left(\hat{f}(x^m_{+j}) - \hat{f}(x^m_{-j}) \right) \tag{2}$$

The authors also developed a Python library [3] implementing this.

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2.3. LIME

Local Interpretable Model-agnostic Explanations (LIME), introduced by [4], works by fitting simple, explainable models to the local behaviour of the model. They choose the explainer model $\xi(\boldsymbol{x})$ as follows:

$$\xi(\boldsymbol{x}) = \arg\min_{g \in G} \mathcal{L}(f, g, \Pi_x) + \Omega(g) \tag{3}$$

Where $\mathcal{L}$ measures how unfaithful g is in approximating f in the locality defined by Π_x, G is the class of simple models being considered and $\Omega(g)$ guides towards simpler explainer models. In effect, this finds the best simple, interpretable model in the neighbourhood of the relevant point and uses this to explain the model's decisions. They focus on the case where G is the class of linear models and use the locally weighted square loss as $\mathcal{L}$. They show that this works well for text and image classification.

2.3.1. Existing Methodologies for Generating Counterfactuals

[17] is considered one of the first papers to introduce counterfactuals [18]. They treat this as an optimisation problem on the loss function $\mathcal{L} = \lambda(b(x') - y')^2 + d(x, x')$ for some distance function d. Researchers can use various strategies to complete the optimisation – some of which, such as Adam [19], require gradient-level access to the model, whereas others, such as Nelder-Mead [20], do not.

[18,21] perform large-scale reviews of the existing research on finding counterfactuals. Guidotti begins by highlighting several beneficial properties – such as validity (that it is genuinely counterfactual), similarity (that the distance between the original data point and the counterfactual data point is sufficiently small), actionability and others that we do not have space to list in this report.

Model Specific Explanations

While many proposed methods are model-agnostic, others are designed to work with specific models. For example, [22–24] focus on tree-based models, [25,26] focus on Linear Classifiers. Similarly, [27] focus on Random Forests [28] while [29] focus on Boosted Trees [30,31].

Counterfactuals as an Optimisation Problem

Generally, the problem of finding counterfactuals can be considered an optimisation problem [21]. Various researchers investigate different algorithms for solving this optimisation problem — for example, [32] utilise a "Growing Spheres" algorithm, while [33,34] utilise FISTA (Fast Iterative Shrinkage-Thresholding Algorithm) [35]. Other researchers, such as [36], fit simpler, interpretable models to the output of the more complex model within a neighbourhood of the data point. We build on this by fitting simpler models to the effect of varying each feature.

Similarly, [37] treat this as a "Multi-Objective" Optimisation problem – including distance from the original point, number of changed features and how well the counterfactual point fits the original distribution. Using the multi-objective optimisation framework, they return a "Pareto set" of counterfactuals representing different trade-offs between their proposed objectives. [38] expand on this by also including a "causality" objective.

Van Looveren et al. [39] improve on optimisation-based strategies by using Auto-encoders [40] to build "Class Prototypes" and including this as a term in the optimisation problem. Similarly, [41] use the Mahalanobis' distance [42] and the local outlier factor [43] to create distribution-aware counterfactuals. Additionally, [44] expand on such strategies by building in causal constraints, while [45] use variational auto-Encoders [46].

Sequential Counterfactuals

Sequential counterfactuals differ from traditional counterfactuals in the sense that they provide not just examples of nearby points that have the opposite classification but that they also provide a sequence of steps. [21] note that sequential counterfactuals are an active area of research. [47]

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demonstrate, through a user study, that end-users generally strongly prefer such directive explanations. However, they note that social factors can affect these preferences.

Similar Work

Similar to our proposal, [6] chain together instances of possible changes to find counterfactuals. In their proposed methodology, a domain expert would curate a list of plausible changes and Boolean pre-conditions for when these changes could be made. An optimisation algorithm using the model's gradient is then used to find the best (by some scoring metric) counterfactual for that instance. A range of papers build on this work. For example, [48] expand on this, allowing it to work on non-differentiable models, provide multiple solutions, and improve efficiency through pruning. They also build on the Boolean pre-condition model of when changes can be made by introducing a notion of consequences (e.g. age increases as a consequence of obtaining a higher degree).

Our project differs from existing research in a few critical aspects. Firstly, both Ramakrishnan et al.'s [6] and Naumann & Ntoutsi's [48] methodologies use a pre-defined series of actions that can be taken. This approach has numerous advantages; it can model the relations between different variables well – for example, in a financial application, doubling the income would also reduce the debt-to-income ratio. However, this would require a significant time investment for a domain expert to collate. Our approach (explained in the next section), through fitting simple surrogate models, can choose the most effective changes to make without this. We design our scoring mechanism to be easily interpreted by a domain expert – meaning results can be efficiently personalised.

2.3.2. Other Methodologies We Evaluate Our Methodology Against

To examine the effectiveness and utility of our novel methodology, we compare it with some existing methodologies to generate counterfactuals. We chose these options as there are publicly available Python packages [49,50] implementing these. As we also make a Python implementation of our methodology publicly available [51], these are reasonable points of comparison — although it is not exhaustive.

AlibiExplain, developed by Klaise et al. [50] implements the method described by Wachter et al. [17]. This methodology works by performing the following minimization, where x' is the counterfactual data-point:

$$\arg\min_{x'} \left(\max_{\lambda} \left(\lambda \left(f_w(x') - y_i \right)^2 + d(x_i, x') \right) \right) \tag{4}$$

In this case, (x_i, y_i) represents the point we are trying to find a counterfactual for, f_w is the model and d is some distance metric. Wachter et al. propose using the ADAM distance metric [19].

Klaise et al. also implement a more complex methodology that utilizes prototypes, as introduced by Van Looveren et al. [52]. This methodology also minimizes a loss function $\mathcal{L}$ over some D-dimensional feature space. The loss function they use is

$$\mathcal{L} = c \cdot L_{pred} + \beta \cdot L_1 + L_2 + L_{AE}^{\gamma} + L_{proto}^{\theta} \tag{5}$$

$$\Delta\text{Class} = \underbrace{[f(x_0 + \delta)]_i}_{\text{Original class}} - \underbrace{\max_{t \neq i}([f(x_0 + \delta)]_i)}_{\text{New class}} \tag{6}$$

$$L_{pred} = \max(\Delta\text{Class}, -\kappa) \tag{7}$$

L_{pred} encourages the class to change, L_{AE}^{γ} penalizes (by a factor of γ) out of distribution counterfactual instances (by using the L_2 reconstruction error from an auto-encoder and, L_{proto} acts by a factor of θ to both speed up the search process and guide the perturbation towards an interpretable counterfactual, and L_1 and L_2 correspond to the usual norms.

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2.3.3. Practical Uses of Counterfactual Explanations

As with all forms of explanation for automated systems, they can increase a user's trust in an automated system [53]. By attempting to approximate the reasoning that these automated systems have employed, users can assess whether they agree with this reasoning. These counterfactual explanations can also be tuned to be actionable — this means that an end-user can take actions based on their received explanations. For example, if an explainer suggests that an applicant was denied for a loan but would have been accepted for a smaller loan, the applicant can respond by applying for this smaller loan. Similarly, in a medical situation, if the explainer suggests that a patient who exercised more would be less likely to have severe complications from a disease, the patient could respond by doing this. Of course, not all changes are possible for all situations, so a tuneable, human-in-the-loop methodology is beneficial.

Similarly, users of an automated system are entitled to an explanation of why such a system made the decision it did [54]. Counterfactual explanations can be one part of meeting this legal requirement [55]. Counterfactuals can also help data scientists understand the model's internal structure better and correct for unintentional biases in the training data. For example, suppose that counterfactuals generated for a financial model suggest that "protected characteristics" should be changed to change the output of the model. In that case, it is likely that the model has learnt unintended biases and that further work is needed to de-bias the training data before deploying the model in practice.

When domain experts are presented with such counterintuitive explanations, they can be prompted to examine the training data set for these biases, leading to fairer, more accurate models. Ultimately, this also can be a part of legal requirements to conduct impact assessments for model bias and effectiveness [5].

2.4. Relation to Adversarial Machine Learning

Adversarial Machine Learning is closely related to Counterfactual Explanations. As discussed by [56], many families of machine learning models are vulnerable to adversarial examples: inputs specifically designed to cause the target model to produce erroneous outputs. This problem of modifying an input to "trick" the model into giving a different output is, at a high level, similar to that of finding counterfactuals. While there is a difference in focus - instead of trying to trick the model, counterfactual explanations focus on providing useful explanations to users - this similarity has been exploited to develop strategies for generating counterfactuals, for example, by [52]. Similarly, [57] utilise Generative Adversarial Networks [58].

3. Methods

3.1. Methodology for Generating Counterfactuals

Our approach is summarized in Figure 1.

We can summarize our general methodology as follows:

1. Fit simple, surrogate models to the effect of changing each input feature in the underling model, keeping all other features the same.
    - We might for example, fit linear models to the local effect of changing each pixel of an image, or the effect of each input feature to a system that makes decisions about whether applicants are entitled to loans.
    - Consider the example where we have an individual with an income of £30k, applying for a loan of £1k. We will imagine this individual has a debt-to-income ratio of 10% and they are denied a loan by the hypothetical system (with a class probability of 0.9).
2. For each of these models,
    (a) Select the 'feature value' that they predict will maximise the "score".
        - This may, for example, be reducing the size of the loan they are applying for by £250.

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(b) In the initial data-point, replace this feature with this new value.
   - We now have a new data-point - an applicant with an income £30k, applying for a loan of £750k with a debt-to-income ratio of 10%

3. If any of these new data-points change the model prediction (possibly plus some additional threshold), this is the counterfactual.
   - Suppose running this original classifier now accepted the applicant the loan, with a class probability of 0.6. We can take this new data-point as counterfactual and return it, in a human-readable-format to the user.
4. Otherwise, select the best scoring one of these new data-points and repeat the process from here.
   - If instead, the system still denied the use the loan, but this time with a class probability of 0.6, we take this new hypothetical point and repeat the process from here.
   - Note: we would in fact do this for all allowed input data-points and pick the one which maximised some score.
5. If we have run out of variables to change - or reached the maximum search depth - then return to previous unexplored branches and search from there.
   We can think of the change to single variable as being a node on a graph, connected to points it shares "all but one feature value" with. In this sense, our search process is akin to a depth-first-search on this graph. This is visualised in Figure 3
6. Repeat the previous step until either a counterfactual has been found, or all notes of the graph have been searched.

We note that we have built our system such that it is modular, so that we can easily change the search process. For example, we can change the order in which we change the features. We can also change the stopping criteria — i.e. when we stop changing features and decide there does not exist a counterfactual subject to the given criteria.

By some metrics, our method can be considered to be generating local counterfactuals. Since it starts from the initial data-point and aims to make small changes until it shifts the model's prediction, it inherently tries to make as few changes as possible. However, through our tunable changeability scores and scoring functions we made it possibly to change how "local" these counterfactuals truly are.

3.1.1. Surrogate Models

These surrogate models, which we will often refer to as single variable explainers (SVEs), attempt to explain the dependence of the model's output on the variation of one parameter locally.

For a particular variable, we generate a set of input data points by replacing that variable with other values that the variable takes in the training data set. Either we do this through Monte-Carlo like sampling — i.e. replacing with randomly chosen other values in the data set — or by selecting uniformly placed points across some interval, such as $[\mu \pm \sigma]$ (where μ is the variable's mean value in the training data and σ is the standard deviation) or defined quantiles of the values of that feature in the training data. We then apply the (black-box) model to these to get a series of sampling variables and class probabilities pairs.

We then fit a simple explainable model to this new data set. We use either a Gaussian process or a linear model.

Our framework is sufficiently general to allow for any SciKit-Learn [59] regression model to be used. The existing tools built in Keras [60] also make our tool compatible with TensorFlow/Keras models. We discuss our technical implementation in more detail in Section 3.2.

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3.1.2. Scoring Rules

A range of rules can be used to score these models; by default, we consider the following, where $S(x)$ represents the score when the feature is changed from its original value to a new value x.

$$S_{\text{basic}}(x_i^{\text{new}}) = \left|\text{Model}\left(\mathbf{x}^{\text{original}}\right) - \text{SVE}(x_i^{\text{new}})\right| \tag{8}$$

This, measures the change in class probability caused by a given change in an input feature.

There may be situations, where there is a "cost" to changing a feature too much, so we implement a "scorer" that allows for smaller changes. To encourage smaller feature changes we can apply the following mask:

$$\text{Mask}(x_i) = \exp\left(-\frac{1}{2}\left(\frac{x_i^{\text{new}} - x_i^{\text{original}}}{\sigma_i^{\text{train}} \times f(w_i)}\right)^2\right) \tag{9}$$

$$S_{\text{masked}}(x_i^{\text{new}}) = \text{Mask}(x_i^{\text{new}}) \times S_{\text{basic}}(x_i^{\text{new}}) \tag{10}$$

Finally, each score is weighted by a user-provided "feature changeability score" that quantifies the ease with which a feature can be changed. $S_{\text{Final}}\left(x_i^{\text{new}}\right) = w_i \cdot S\left(x_i^{\text{new}}\right)$.

Borrowing ideas from the field of human-computer interaction, this allows the user to tune the methodology to their use case. This is visualized in Figure 2.

As mentioned above, a user could choose a "masked" scoring function with a small standard deviation to guide the methodology for selecting small changes.

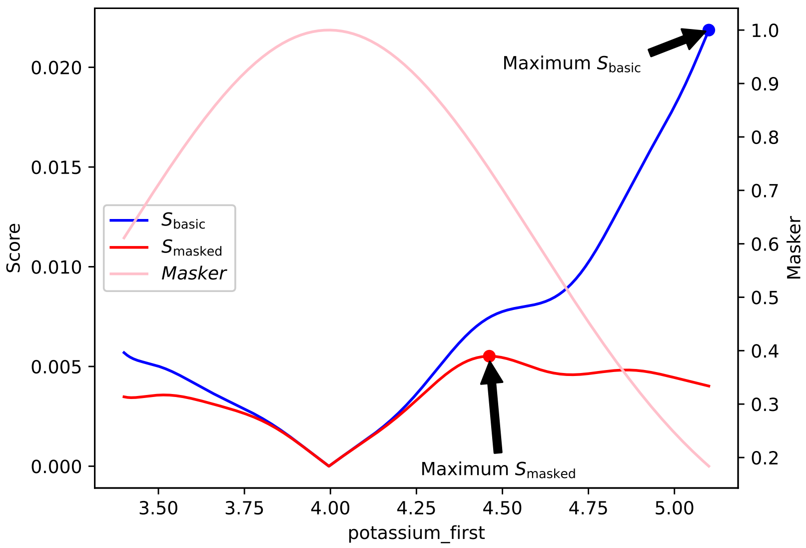

Figure 2. Example of how scoring rules work. Here we have have trained a surrogate model on the effect of changing the "potassium_first" feature (the level of potassium in the blood when the patient was admitted), and plotted the scores of each possible feature value. The basic scoring rule (Equation 8) is shown in blue, while the masked scoring rule (Equation 10) is shown in red. The masked scoring rule is masked by a bell curve, shown in pink. The initial value of the feature value is $x_i = 4.0$, while the blue and red circles demonstrate the locations of the maxima of the scoring function. Given that our method selects the feature value that maximises the score, this represents an example of a situation where the two scoring functions would lead to two different suggested changes.

3.1.3. Benefits

There are several benefits to counterfactuals as a method for explaining the output of machine learning models. Indeed, through a user study, [61] demonstrate, that counterfactual explanations elicit greater satisfaction and trust than causal explanations.

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Similarly, these counterfactual explanations can be considered more actionable to an end user - especially sequential counterfactuals, which can act as a series of steps for a user to take. This is confirmed by [47].

Our method also has a number of specific benefits. Firstly, it's modularity makes it easy to specialise to specific situations. We explain how we achieved this modular structure in our "Technical Implementation" section. Similarity, our "scorer" builds in ideas of a "changability score" which makes our method tunable by a domain expert or end user.

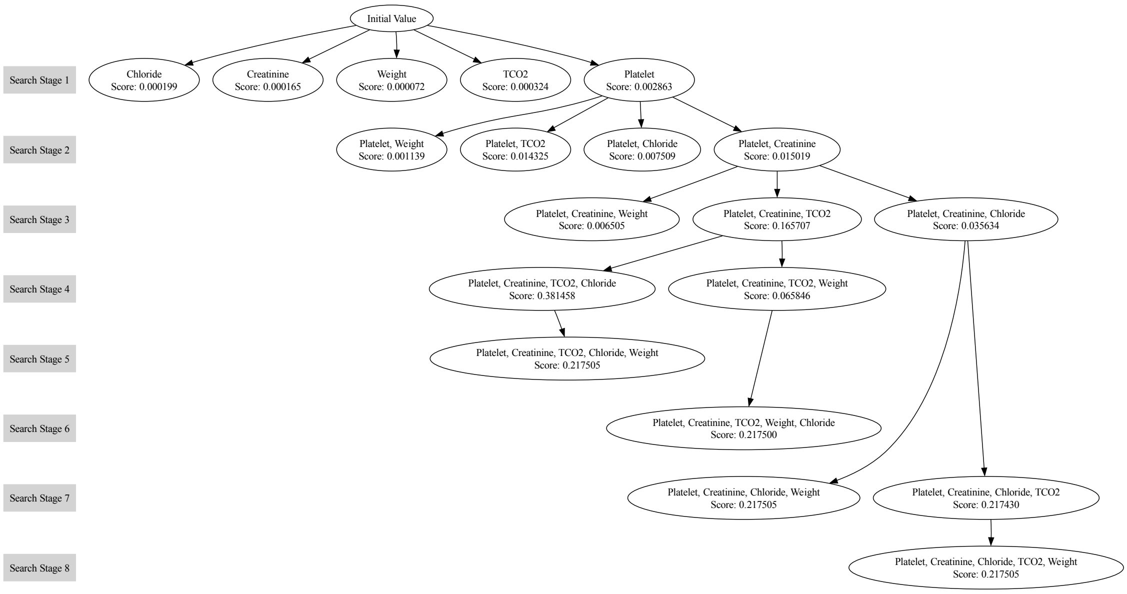

Figure 3. This figures shows our search process. Here, we used our method to explain the output of a medical model. Each node represents a single variable explainer trained on the specified feature around the maximum scoring data point of the node's parent. Each layer of the graph represents a set of single variable explainers that are evaluated together. This graph demonstrates the depth first nature of our process.

3.2. Technical Implementation

We have made our tool open-source and available on GitHub, with full documentation included in this repository.

https://github.com/JoshanParmar/TuneableCounterfactuals

We also make it available as a python package for easy installation.

```
pip install tuneable-counterfactuals-explainer
```

Our method, implemented in Python, can wrap around any black-box model with a `predict_proba` method that can take in a Pandas [62] DataFrame and return a list of tuples of class probabilities. This is the case for SciKit-Learn [59] models.

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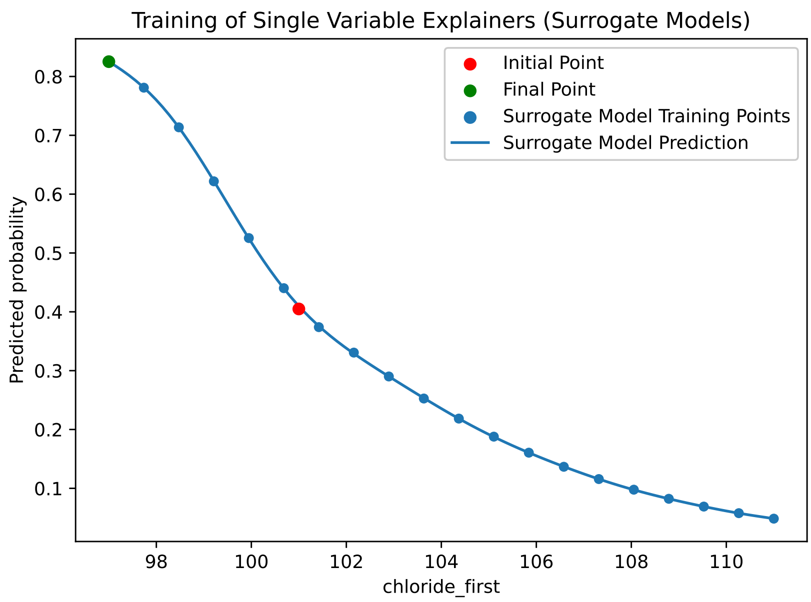

Figure 4. This graph shows the process of training the "SingleVariableExplainer" objects. The red point shows the initial value of the chloride_first feature against the initial class probability for the classification. The blue points represent hypothetical new patients, with a changed chloride_first value (initial amount of chloride measured at admission time), but with all other features remaining the same. We plotted the new feature values against the class probability for these new hypothetical patients. It can be seen that we have used uniform sampling for these points. The blue line represents the Single Variable Explainer (SVE) itself, in this case a Gaussian Process surrogate model. The green point, represents the selected best change to the feature, according to the S_{basic} scoring function.

Table 1. This table lists all the possible optional parameters that the user can set when creating the Explainer object alongside what their effects in guiding the search process are.

Parameter Name	Description
`variables`	A list of variables to be "searched over". If this is not specified, it will be assumed from the training data.
`sampling_method`	The method used the sample the points used to train the surrogate models. By default this is "uniform", such that the training points shown in Figure 4 are evenly spaced. Alternatively, "random" will sample values at random from the training dataset.

`bounding_method`
`override_variable_bounds`
`std_dev`
`quantiles`
	If uniform sampling is used, the user is able to define the "bounds" for the sampling. While the user can provide the bounds manually (in override_variable_bounds), either in the form of a Python Dictionary containing "min, max" tuples or as a single such tuple; they can also instruct the use of a method to calculate the bounds based on the training data. The methods available are "minmax", which takes the minimum and maximum values of the feature in the training data; "quantile", which will take the specified upper and lower quantiles; and "meanstd", which takes the mean plus/minus a specified number of standard deviations.

`number_of_samples`	The number of samples to be used to train each surrogate model. This is the number of points shown in Figure 4.
`regressor`	The SKLearn Regressor used for each surrogate model. Any SciKit-Learn Regression Model can be used here. The user can also provide the strings "gaussian_process" or "linear" for these most commonly used regressors.
`changability_scores`	A python dictionary of the w_i scores described in Section 3.1.2. If this is not specified, a score of 1 will be assigned to each of the variables specified.
`probability_prediction_function` (Compatibility Option)	Function mapping an [n rows x `features_in` columns] DataFrame to (n x 2) probability matrix. Example: `lambda x: model.predict(x).reshape(-1,2)`
`class_prediction_function` (Compatibility Option)	Function mapping an [1 rows x `features_in` columns] DataFrame to integer representing the predicted class. Example: `lambda x: model.predict(x).argmax()`

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Our method is implemented as a "explainer object", into which a end-user passes a model to be explained, the data used to train the model and the target variable of the model. This object, with an "explain" method calls a "searcher" object which generates "single variable explainer" objects. These are scored by "scorer" object. "Sub-classes" can be created for any of these objects to specalise the method for a given situation. The user can also specify additional optional parameters that guide the counterfactual process as outlined in Table 1.

We include an example of the code required to run our method in Listing 1.

```
# Example to run our method on the MNIST Dataset.

import sklearn

from sklearn.datasets import fetch_openml
from sklearn.model_selection import train_test_split
from sklearn.neural_network import MLPClassifier
from sklearn.pipeline import make_pipeline
from sklearn.preprocessing import StandardScaler

from tuneable_counterfactuals_explainer.explainer import Explainer

data = fetch_openml('mnist_784', parser='auto')
train_x, test_x, train_y, test_y = train_test_split(
    data.data[data.target.isin(['0', '1'])],
    data.target[data.target.isin(['0', '1'])],
    test_size=0.2
)

model = MLPClassifier(hidden_layer_sizes=(200,200),alpha=1, max_iter=1000, \\solver='
    adam', verbose=10,  random_state=21,tol=0.000000001)
model = make_pipeline(StandardScaler(), model)
model.fit(train_x, train_y)

explainer = Explainer(
    model,
    train_x,
    'target',
    regressor='linear',
    bounding_method='minmax',
    override_variable_bounds=(0, 255)
)

result = explainer.explain(train_x.iloc[0], additional_threshold=0.25)
```

Listing 1. Minimum required code to run methodology. We begin by loading in the training data and training the underlying model using SciKit-Learn [59]. We then create an Explainer object specifying the use of Linear Surrogate Models. We then use the "explainer.explain" function to explain the decision of the black-box model on a specified example from the training data. By adding the additional threshold of 0.25, we specify that the counterfactual must have a class probability (of the opposite class to the initial classification) of at least 0.75.

3.3. Evaluation Methodology

We evaluate our method by training simple models on simple data-sets and evaluating how the counterfactuals generated by our model compare to those generated by some existing methodologies for generating counterfactuals. While this is not an exhaustive comparison, we have chosen some methodologies with existing publicly available implementations as valuable points of comparison. As our framework is available as an easily installable Python package, this accurately compares what other options domain experts will have at their disposal to explain machine learning models. We will use qualitative and quantitative metrics to evaluate our counterfactuals compared to those generated by other models.

3.3.1. Evaluation Metrics

We examine several quantitative metrics to analyse the performance of our algorithm.

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An ideal algorithm to generate counterfactuals will be able to generate them quickly. However, since the performance of our algorithm is highly dependent on the hardware used, we do not include a speed evaluation of our method.

Additionally, as we want our counterfactual to be close to the original data point, we compare the distance to the original data point in terms of both the L_1 and L_2 norms.

Similarly, we want our counterfactuals to change as few features as possible, so we also compare the number of feature changes. Furthermore, we often want our counterfactual to be plausible — coming from a distribution similar to the original training data set — so we shall also measure the standardized L_2 distance to the nearest training data point.

Some of our qualitative metrics will include those used by [63]. We want our counterfactuals to be both unambiguous and realistic. However, we also want them to reflect the model accurately. We also qualitatively examine what we learn about the model from the counterfactuals, and how useful such a counterfactual may be to a user.

3.3.2. Evaluation Data-Sets

As we discussed in Section 2.3.3, these counterfactual explanations can be useful in financial and medical situations, so we evaluate our methodology on these. Since our methodology can be easily visualized on image datasets, we also evaluate it on this.

Financial Data-Set

Our first evaluation uses a simulated data set [64][1]. We made this decision due to the lack of publicly available data sets for which appropriate documentation of their data collection methods exists. Since this project aims to evaluate the methodology for explaining models rather than the models themselves, it is unlikely that using a simulated data set will significantly affect our results. This dataset will allow us to evaluate the causal explanations that our methodology can generate.

This data set contains 12 features (Age, Annual Income, Home-ownership, Employment length (in years), Loan intent, Loan grade, Loan amount, Interest rate, Loan status, Percent income, Historical default and Credit history length) and 32581 examples. It should be noted that we dropped the "loan_intent" column and reversed the "loan_status" column such that 0 indicates a default. This allowed us to use this as a proxy for whether the individual should receive the loan. Similarly, we converted all remaining categorical columns into numerical columns. An example processed loan applicant is included in Table 2

Table 2. This table shows an example loan applicant within the simulated loans dataset. This applicant should not have been awarded the loan as they defaulted on the loan (indicated by "loan_status" = 0). Our model makes this prediction correctly.

Feature	Value
`person_age`	22.0
`person_income`	40000.0
`person_emp_length`	4.0
`loan_grade`	1.0
`loan_amnt`	14125.0
`loan_int_rate`	11.49
`loan_percent_income`	35.0
`cb_person_default_on_file`	0.0
`cb_person_cred_hist_length`	3.0
`person_home_renting`	1.0
`person_home_mortgage`	0.0
`person_home_own`	0.0
loan_status	**0.0**
model_1_prediction	**0.0**

[1] https://www.kaggle.com/datasets/laotse/credit-risk-dataset

This data set contains only a small amount of missing data: 3116 loans were missing interest rate data, and 895 were missing employment rate information. For this reason, we chose to remove these 3943 data points.

This dataset represents a realistic, practical example of the use of counterfactuals. Applicants for loans can be given realistic, actionable, advice for how to increase their likelihood of being accepted for a loan.

MIMIC

The MIMIC (Multi-parameter Intelligent Monitoring in Intensive Care) II data set [65] contains physiological signals and vital signs time series captured from patient monitors, along with comprehensive clinical data for tens of thousands of Intensive Care Unit (ICU) patients. We use a smaller pre-processed version of this data set produced by [66], which contains information about the patient, such as age, gender, weight, BMI, information as to if and when the patient entered ICU, information about the patient's clinical and medical history.

MNIST

MNIST [67] is a large data set of labelled handwritten digits. It contains 70000 individually labelled 28 by 28 images with pixel values being integers from 0 to 255. This handwritten digit data set is standard across research in this field [21], presenting a valuable point of comparison.

We include this dataset as, despite it not being practically applicable to our specific use case, it makes it easy to visualize the process of generating these counterfactuals.

3.3.3. Training the Underlying Models

For the medical and financial datasets, we train a simple multi-layer perceptron (MLP) classifier with two hidden layers of size 20 to evaluate our explanation methodology. We select a subset of useful columns in the dataset for this purpose. For the MIMIC data, we kept the "age", "bmi" and "weight" features, information about when the entered ICU and hospital, and numerical clinical features as listed in Table 3. For the loan dataset, we dropped the "loan_percent_income" feature, as it was implied from other features.

For our image dataset, we use convolution neural network. To make comparisons easier with existing research, we use an architecture similar to what is used in the documentation of commonly used machine learning libraries such as Keras [60].

4. Results and Discussion

4.1. Medical Data-Set

By running our methodology using Gaussian process surrogate models, we can show how our proposed method works on medical data. Consider the patient described in Table 3. Figure 5 shows the counterfactuals generated by our methodology. These counterfactuals are plausible, i.e. taking realistic values for the variables present (we discuss possible correlation within the variables making this not realistic in our Future Work section). They are also unambiguous — they clearly show a change in classification, increasing the probability of death from 0.0 to 0.99.

This presentation of our results highlights a key benefit of our methodology, that it creates sequential counterfactuals. This means that it gives a series of steps that a user can take to change the model's output. This is particularly useful in medical situations, as these can often be actionable where a user (such as a clinician) can take these steps to improve the patient's health. We can use changeability scores to tailor our results here, by assigning higher scores to the features we want to change. For example, we can assign a higher score to the weight feature, as this is something that is easier to change than the age feature. As these scores would be different for each patient, our method allows for a domain expert (such as a clinician) to tune this in a *human-in-the-loop* fashion.

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Table 3. Processed MIMIC patient data for a patient who did not die within 28 days of entering ICU. The first three rows specify biographical information about the patient - including age, weight, and BMI. The next four rows specify when the patient entered both the Hospital and Intensive Care. The remaining rows represent the initial values of the clinical features of the patient. The final row is a boolean value representing if the patient died within 28 days of entering ICU.

Feature	**Value**
`age`	71.3
`bmi`	28.05
`weight_first`	43.6
`icu_los_day`	1.91
`hospital_los_day`	22
`day_icu_intime_num`	7
`hour_icu_intime`	5
`map_1st`	87
`hr_1st`	71
`temp_1st`	97.4
`spo2_1st`	100
`abg_count`	2
`wbc_first`	7.2
`hgb_first`	11.7
`platelet_first`	209
`sodium_first`	139
`potassium_first`	2.9
`tco2_first`	26
`chloride_first`	101
`bun_first`	6
`creatinine_first`	1
day_28_flg	**0.000000**

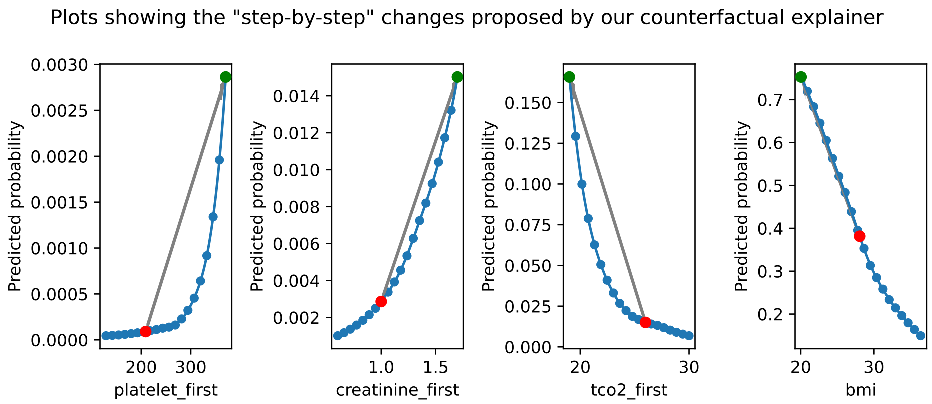

Figure 5. This figure visualises a two stage counterfactual generated by our proposed methodology. In the first step, our framework suggests changing the "hospital_los_day" feature from around $x_i = 23$ to around $x_i = 1$. The second step suggests changing the "bun_first" (blood urea nitrogen at admission time) feature from around 5 to around 41. The blue curve and the blue scatter plot represents the surrogate model and the feature values of the simulated data points used to train it, as in Figure 4.

4.2. Financial Data-Set

4.2.1. Qualitative Evaluation and Complex Narratives

We qualitatively evaluate the performance of our methodology on financial data.

Beginning with equal changeability scores on the applicant described in Table 2, (with an additional threshold of 0.3 and 20 samples used to train each surrogate model) suggests that the applicant should have a higher income (Figure 6). However, this may not be useful to an applicant, as this is not actionable. By setting this variable's changeability score to zero, we can use our methodology to get more practically useful results.

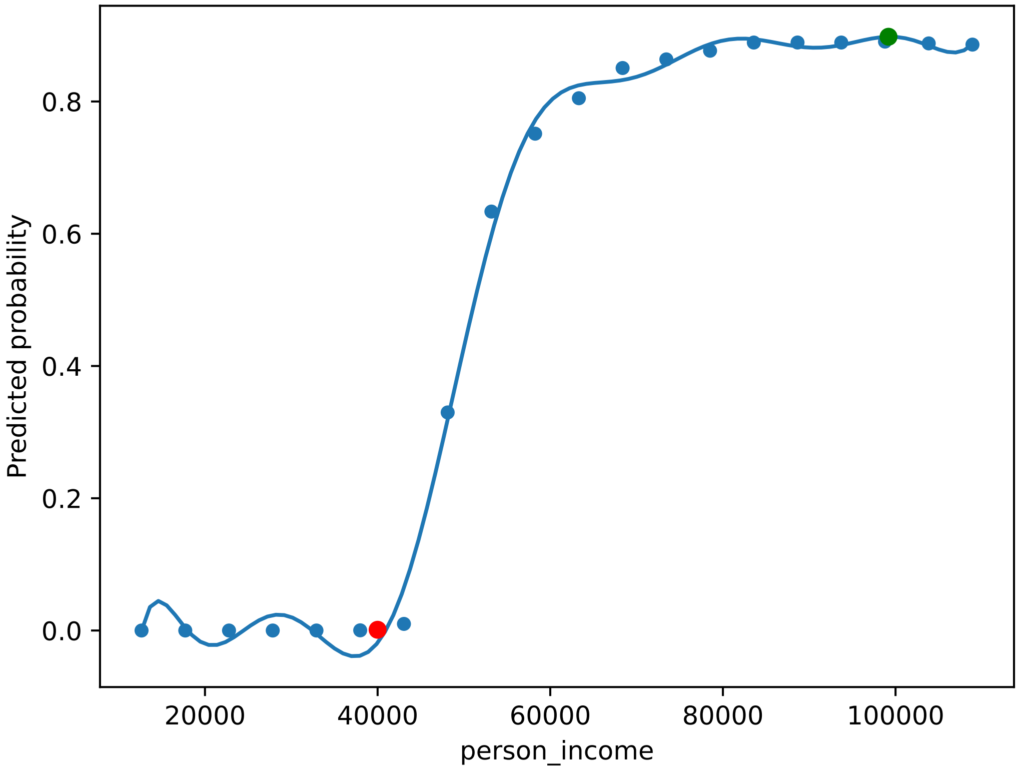

Figure 6. Running our methodology on the example in Table 2, with equal changeability scores and an additional threshold of 0.3, we produce a single stage counterfactual which recommends changing the "person_income" feature from around 40000 to around 95000. In this plot we have shown the initial value of the feature in red and the new value of the feature in green. The blue line represents the surrogate model for the effect of the "person_income" field and the blue dots represent the hypothetical instances used to train the surrogate model.

For sake of example, let us also suppose that the applicant cannot change the size of the loan they are applying for, nor their age, nor their housing situation. In this situation, our model was unable to generate a counterfactual.

This intuitive process for setting these changeability scores, allows for the generation of complex narratives to explain the decisions of machine learning models (in human interpretable ways) [68]. This result suggests that the model (which approximates the automated decision-making system), is highly dependent on opaque and/or fixed features. Thus, our approach offers an understanding of how the model makes decisions, which can help in creating fair models.

Included in Table 4, is an example of an applicant who our model predicted should be awarded the loan. We can ask the question "why should they be awarded the loan?" by finding counterfactuals which would not be awarded the loan. As shown in Figure 7, our method says that the applicant would not be awarded the loan if they had a lower income.

Table 4. This table shows an example loan applicant within the simulated loans dataset. This applicant should have been awarded the loan as they did not default on the loan (indicated by "loan_status" = 1). Our model makes this prediction correctly.

Feature	Value
Age	22.0
Income	50508.0
Length of Employment	5.0
Grade	0.0
Loan Amount	6000.0
Loan Interest Rate	5.42
Loan Amount as Percent of Income	12.0
Credit History Default on File	0.0
Lenght of Credit History (Year)S	3.0
Renting Indicator	1.0
Home Mortgate Indicator	0.0
Home Ownwership Indicator	0.0
Loan "Status"	1.0
Our Prediction	1.0

We can again use changeability scores to get more tailored explanations. For example, if we restrict what features can be changed to only "length of employment", "interest rate", "credit history length", and "age" (overall, roughly equivalent to applying for the loan later), we are still able to generate a counterfactual. We have included this below:

```
First, change loan_int_rate to 15.2. Then, change person_age to 31.9. Finally, change
    person_emp_length to 7.8
```

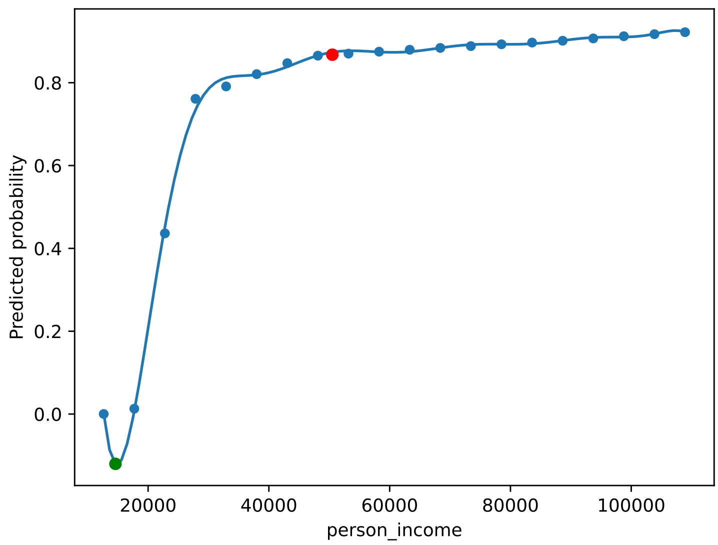

Figure 7. Running our methodology on the example in Table 4, with equal changeability scores and an additional threshold of 0.3, we produce a single stage counterfactual which recommends changing the "person_income" feature from approximately 17000 to approximately 50000. In this plot we have shown the initial value of the feature in red and the new value of the feature in green. The blue line represents the surrogate model for the effect of the "person_income" field and the blue dots represent the hypothetical instances used to train the surrogate model.

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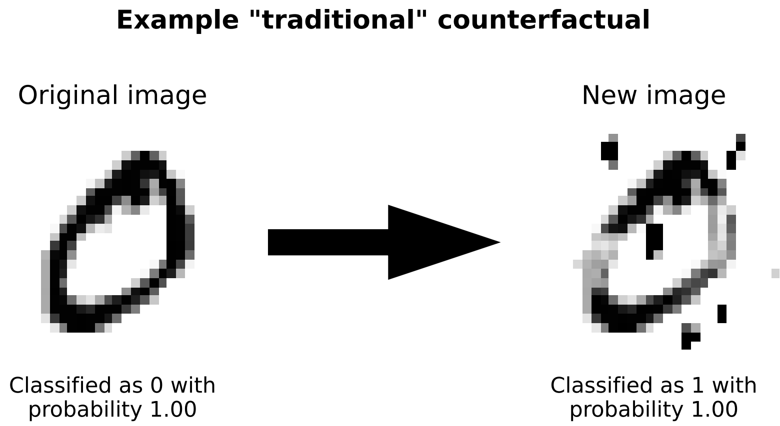
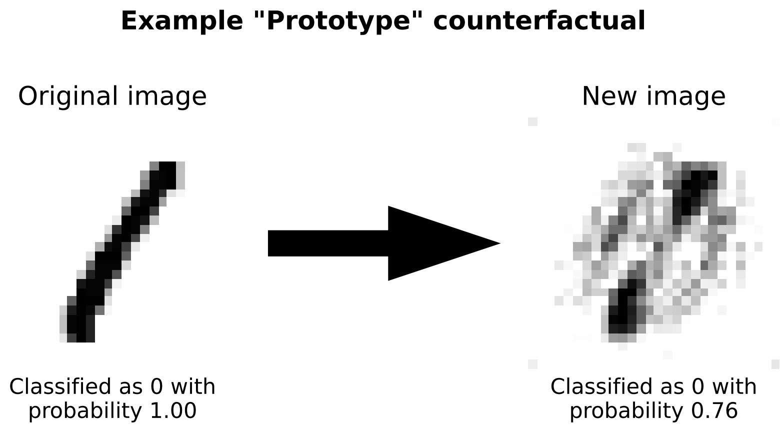
4.3. Image Dataset

We applied our methodology, alongside other points of comparison previously discussed, to the MNIST dataset. We use linear surrogate models and allowing features to take values between the 10% and 90% quantiles of the training data.

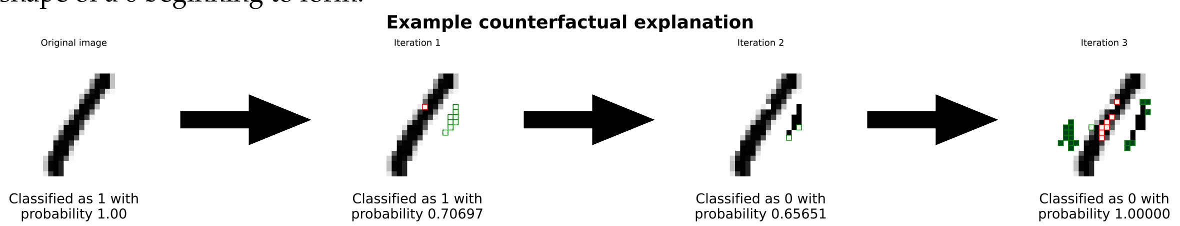
We can see a step-by-step example of this in Figure 8c. Further examples are included in Figure 9



(a) Example counterfactual generated with the methodology of [17]. In this example, the left picture shows the original image, and the right-hand side shows the counterfactual. We see that this example is almost adversarial in nature, producing images that a human would likely classify as a 0 but that trick the model into thinking is a 1.



(b) Example counterfactual generated with the methodology of [52]. As in the above image, the left picture shows the original image, and the right-hand side shows the counterfactual. We can see the shape of a 0 beginning to form.



(c) Example counterfactual generated with our proposed methodology applied to an example that the underlying model is sure is a 1. The first picture shows the original image, with the final showing the counterfactual. The middle images show some of the steps taken to get from the original image to the counterfactual. Highlighted in red are pixels that have been “turned off” - have a new value lower than the previous value. Similarly, highlighted in green are those which have a new value greater than the previous value. We see our method begins by creating a rounded shape around the 1, before clearing a hole inside of it.

Figure 8. Counterfactuals generated with our methodology, alongside comparable methodologies [17,52].

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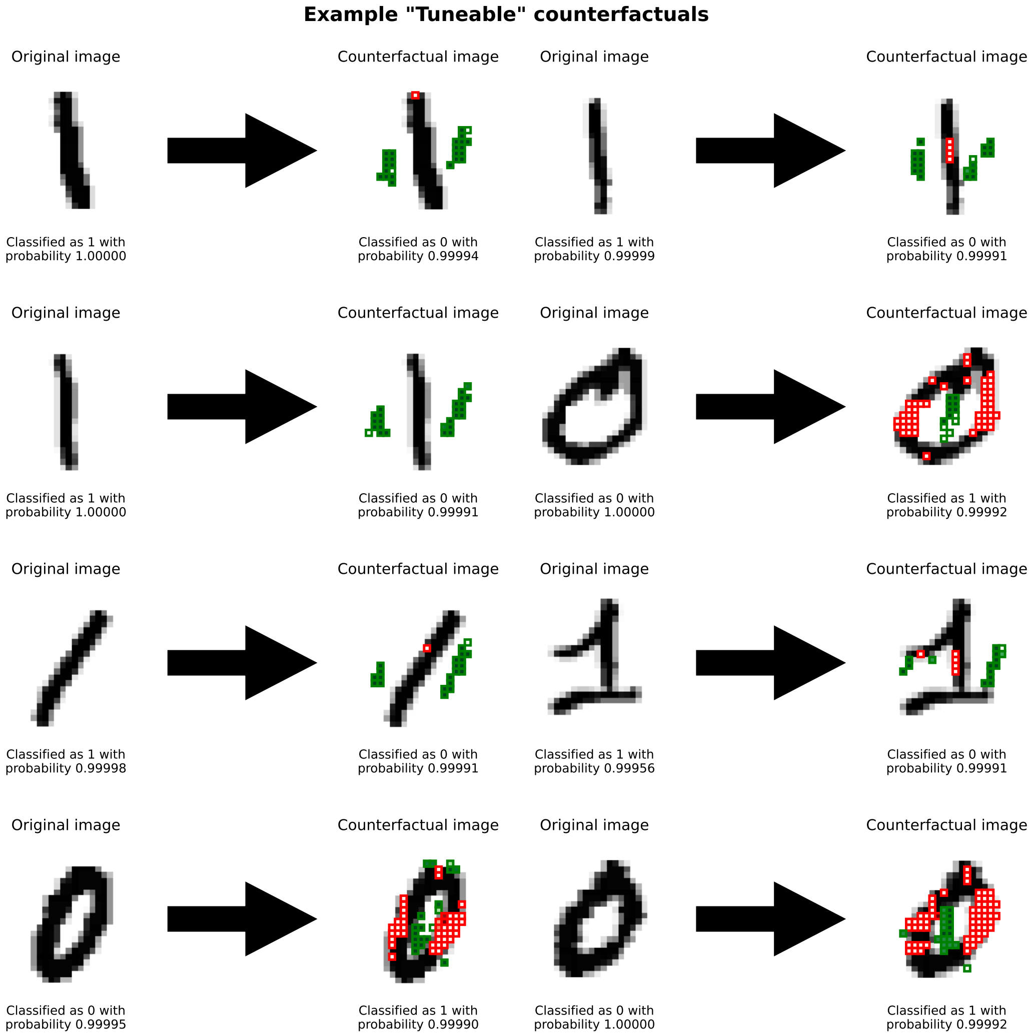

Figure 9. This image shows a range of counterfactuals generated using our methodology. For each pair, the left shows the original image, with the right showing the new counterfactual example. Highlighted in red are pixels that have been "turned off" - have a new value lower than the previous value. Similarly, highlighted in green are those which have a new value greater than the previous value.

These counterfactuals give us insight into how the model makes its classification decisions. In some sense, it begins to "cut-open" the 1 to make it look more like a 0.

Similarly, running the previously described existing methodologies on this example, lead to different, almost adversarial counterfactuals. These are shown in Figures 8a and 8b.

We can see a clear qualitative difference in the types of counterfactual generated between our methodology and the two comparison methods. In a sense, our method works more to transform the image from a 0 into a 1, while the other methods work to perturb the image from a 0 into a 1. Since our method chains together single pixel changes, there is an inbuilt incentive for our method to change fewer pixels (as each change is costed by the scoring function). This is not the case for the other methods, which can change many pixels at once. This can lead to our counterfactuals being more human-interpretable.

Similarly, our use of changeability scores can be used as an alternative method to guide counterfactuals to be more interpretable. For example, when generating our MNIST counterfactuals, we want to change pixels close to the digit. We can do this by giving these pixels a higher changeability score. We do this by blurring the image, and applying a threshold of 0.05 to these scores. This is shown in Figure 11. This continues to generate counterfactuals that are close to the original image, but also interpretable, demonstrating the flexibility of our methodology. Similarly, our counterfactuals

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are unambiguous — they demonstrate a clear change in classification. Another example is shown in Figure 12.

4.3.1. Comparison with SHAP

As our idea of fitting linear surrogate models is somewhat similar to SHAP values, we include a comparison with SHAP values in Figure 10.

We see that, in this example, the SHAP explainer assigns high importance values to similar areas of the image as our counterfactual explainer chooses to change. In some sense, this is unsurprising considering the similarities between our methodologies.

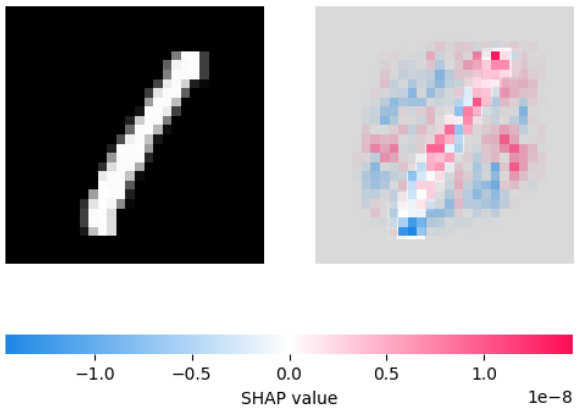

Figure 10. This figure shows the SHAP Values associated with various pixels on this example of an image classified as a 1. We see that the important features to this image correspond to a oval, the shape of a 0, around the 1. This gives us a similar insight to our method which attempts to "fill in" in 0 and draw a circle around the 1.

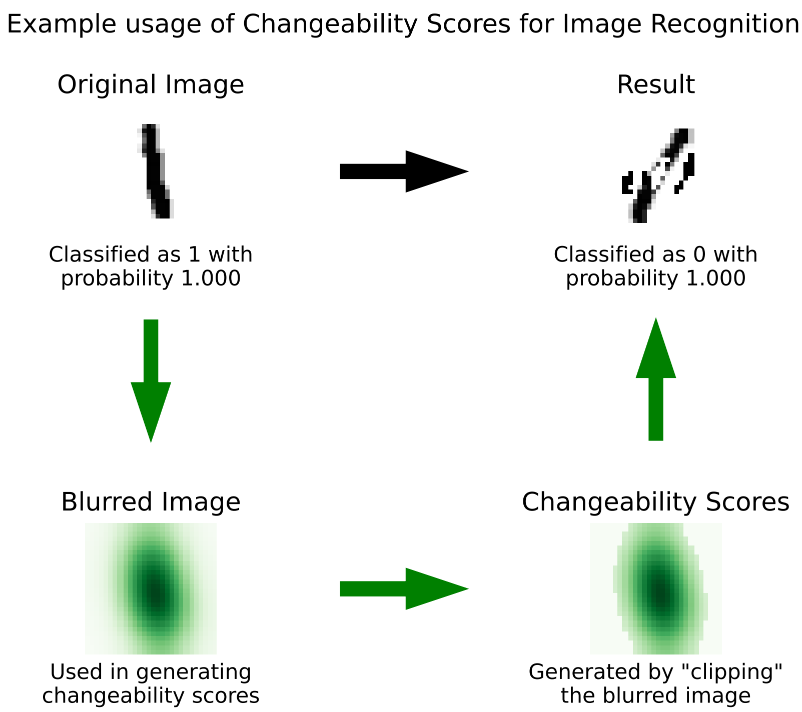

Figure 11. Example counterfactual generated with our methodology using changeability scores derived from a Gaussian blur. We have applied our method to a image originally classified as a 1. We see that, to generate our changeability scores, we first blue the image with a Gaussian, then apply a threshold to the these scores. Using these we are able to produce a simple counterfactual which the model believes is a 0 with probability 0.64. We see that it has created a hole in the centre of the 1, suggesting that the model using this is as a classification criteria.

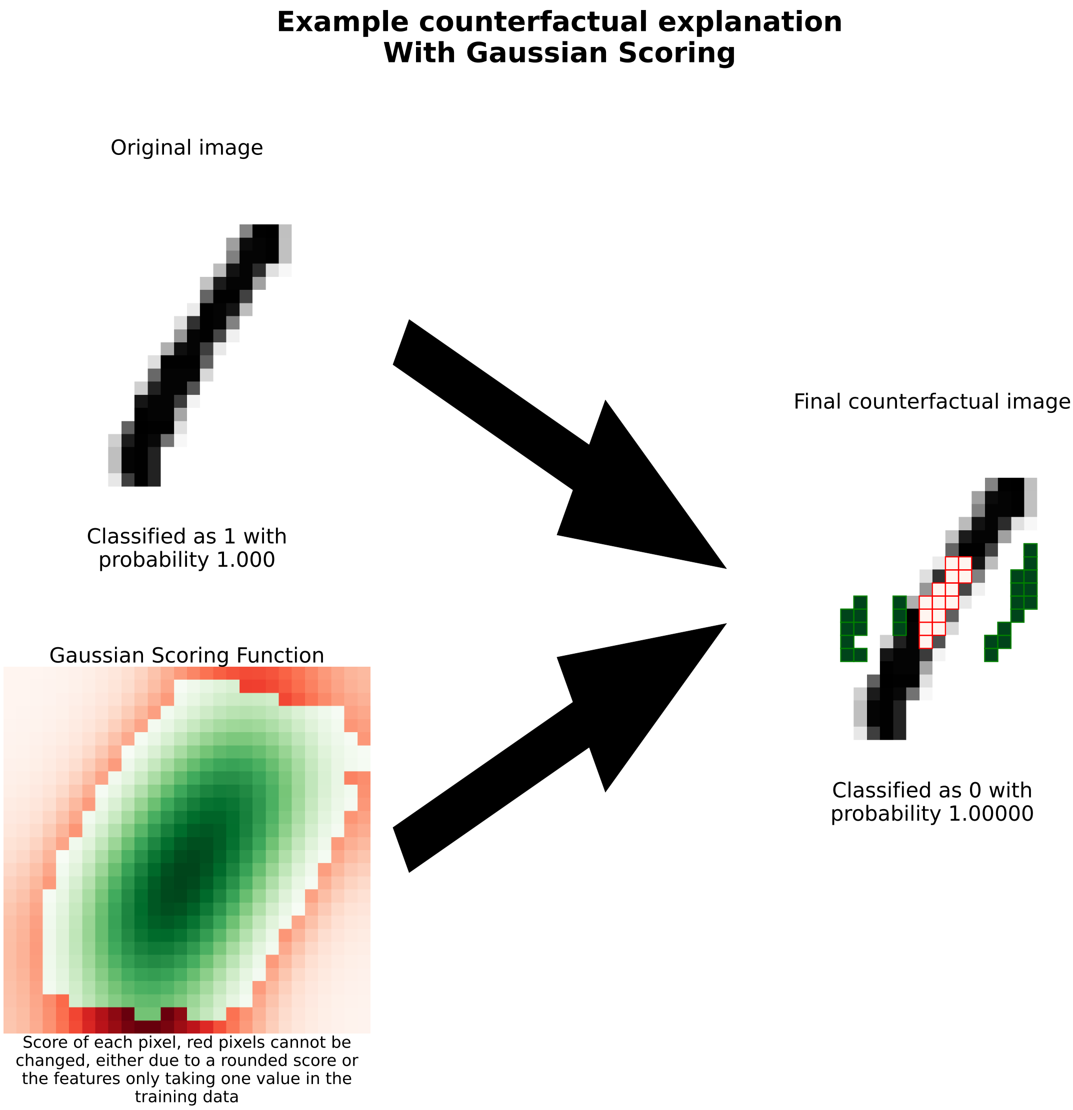

Figure 12. Example counterfactual generated with our methodology. Here, we use the Gaussian scoring function on an image that the underlying model is convinced is a 0 and use our method to transform it into an image that the underlying model is sure is a 1. The top-left picture shows the original image, with the right image showing the counterfactual. In the final image, highlighted in red are pixels which have been turned off - have a new value lower than the previous value. Similarly, highlighted in green are those which have a new value greater than the previous value. We see again that our method begins by attempting to fill in the 0, suggesting the underlying model uses the hole as a classification criteria. The bottom-left image shows our Gaussian scoring function, with the darker pixels showing a higher changeability score. While most of the pixels are in green, the red pixels represent pixels that our method will not change - either because their changeability score has been rounded to zero, or because they do not take a range of values in the training dataset.

4.4. Quantitative Evaluations

Figure 13 shows violin plots of the various quantitative metrics defined in Section 3.3.1. To generate these quantitative results, we randomly sampled 50 images from the original MNIST training dataset. We applied our methodology, and comparable methodologies, to these examples, with a `linear` regressor and a `quantile` bounding method. We then quantitatively compared the counterfactuals generated.

As shown in these plots, compared to comparable methods, our proposed methodology changes fewer features, but changes them by a larger amount (both in terms of L_1 and L_2 distance). In a sense, our counterfactuals are more interpretable, since they change fewer features.

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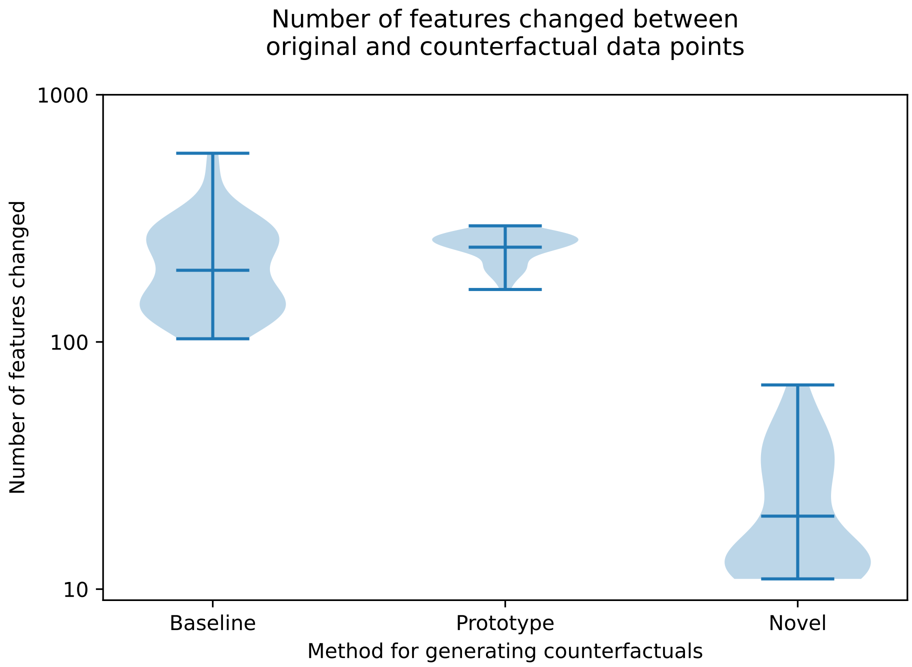
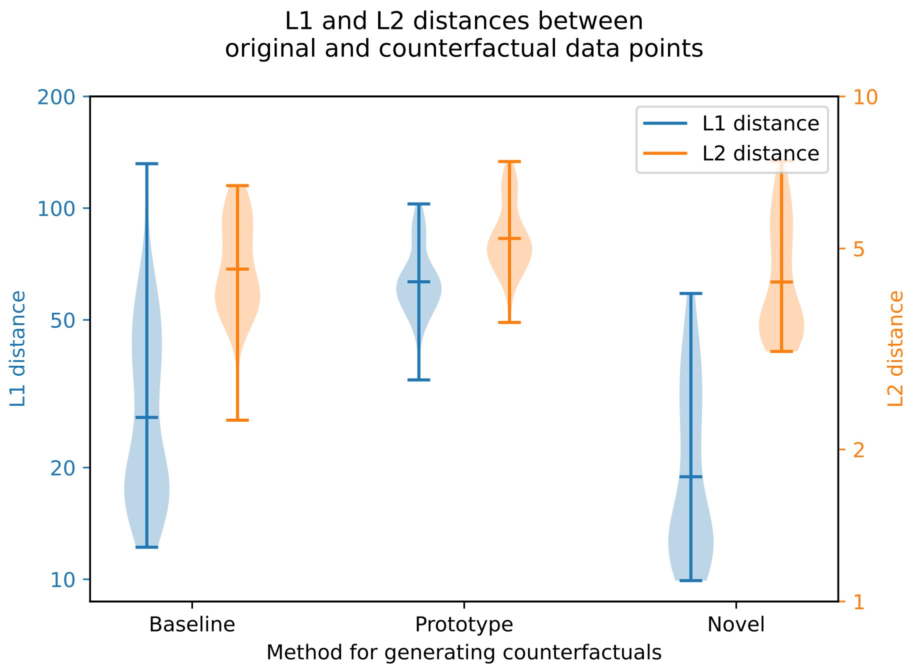


(a) Violin plots of the number of feature changed by each method.



(b) Violin plots of the L_1 and L_2 distances to the original data point for each method.

Figure 13. Plots of quantitative metrics comparing our method (denoted as novel) to two existing methods (denoted as baseline [17] and prototype [52]). To generate these, we applied our method to 25 randomly sampled examples from the MNIST dataset. We used an additional threshold of 0.25 - meaning that the class probability of the resulting counterfactual instances would be at least 0.75. All other optional parameters for our method were set to their default values. We did not specify any particular feature ranges for either our method nor for the comparison methods. We see that our method changes fewer features, while changing them by comparable amounts. This, in some cases, can produce more intuitive counterfactuals.

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5. Conclusions

5.1. Key Contributions

In this work, we develop a methodology to generate counterfactuals to explain black-box models. This method borrows ideas from human-computer interaction research to develop a tuneable, human-in-the-loop explanation method for machine learning models.

From a technical lens, our method can perform on any black box model. Similarly, our method can easily be parallelised at each stage of the search process (Figure 3). Similarly, our system produces sequential counterfactuals (which end-users strongly prefer and regard as more trustworthy [47]).

Furthermore, our code structure is very flexible – not only can any regressor be used for the single-variable explainers, but we also build in various "scoring functions" that provide different counterfactuals for different use cases. For example, our `searcher` system could be modified to not attempt to try and change conflicting features - such as the various housing indicator columns in Table 2. Through the use of changeability scores, our method provides an inherent tuneability that makes it useful in a range of settings. Similarly, by following a step-by-step process, with each step being an inherently explainable model, our explanations are easily interpretable to a non-technical user.

We also see that our method is able to work on a range of input formats, and applications. Here, we show that our approach can work on both tabular and image formats. We show specific applications in the fields of finance, medicine and image recognition.

We evaluated the performance of our approach on a range of data sets. We found that our approach is able to produce, on average, counterfactuals that change fewer features, and change these by larger amounts. Overall, we have shown some benefits of our method compared to some existing methods for generating counterfactuals.

We hope our method can find broad applicability in critical domains such as finance and healthcare, where explainability is important.

5.2. Limitations and Future Work

Our methodology relies on fitting models to the variation of individual features. However, this cannot account for the correlation between different features. One possible methodology for addressing this is to allow a domain expert to form groups of features likely to be correlated and fit simple models to these. By using the training data itself to guide what values are allowed – possibly through an auto-encoder – we can account for these correlations. Similarly, we could implement different strategies into our search method (Figure 3).

There is also scope to conduct extensive user studies into how both how domain experts understand the tunability of our method and how well users respond to the counterfactuals generated. This will be the subject of future work.

We note that our model only aims to change the decisions made by a model, not the "ground truth". A particular example of this is that, in the case of handwritten digits, we have not changed a 1 to a 0, as any human looking at the images would still believe this is a 1. We have only changed the decision made by the model. This is a limitation of any explainable AI method, including ours.

Ethics: No ethics approval was necessary for this work.
Code availability: All code used in this work is available from the following repository:

`https://github.com/JoshanParmar/TuneableCounterfactuals`

Our python package can be installed using pip through

`pip install tuneable-counterfactuals-explainer`

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Data Availability Statement: This study does not generate any data.

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