# "How can we generate counterfactual explanations for ML models that predict the number of contributors to DNA samples?".

## What do experts look at when determining the NOC?

In forensic work, DNA evidence is often analyzed using *Short Tandem Repeats (STR)*. These STR are specific tracks of repeated short DNA sequences of about two to six base pairs long, that have been proven to show high variability between individuals. These parts of the DNA or *loci* have been defined by CODIS, which is the United States national DNA database. One individual can have two different amounts of repeats for a single locus; one inherited from the mother, and one from the father. These thus represent the alleles for this certain region of the DNA. These STR are measured by a process called electrophoresis, which produces an electropherogram. An example can be seen in Figure 1. We will not go into detail about the measuring process, but will provide information about how these results are interpreted. In Figure 1, we only see the locus TH01 with two clear peaks at six and nine repeats. The repeat sequence for TH01 is AATG, so on one chromosome of this individual the AATG sequence is repeated six times on that location, while on the other chromosome it is repeated nine times. The y-axis represents the quantity of information found, measured in Relative Fluorescence Units (RFU). This is also referred to as peak height.

The first step of DNA STR profile interpretation is to determine whether a sample has originated from a single source, or if the sample is a mixture [1, 2]. This is usually easily discerned by looking at the Maximum Allele Count (MAC), which is a measure of the locus with the most alleles present. If this number is bigger than 2, the sample could be considered a mixture since a single human has at most 2 alleles at a given locus; one from the mother and one from the father. Determining the exact number of contributors is difficult, since most DNA profiles are not as clear cut. There are many factors that can obscure the number of contributors.

* Allele sharing: If two donors have the same allele at a locus, we speak of allele sharing. This frequently occurs when donors are relatives, since brothers and sisters share a lot of DNA. It might be difficult to distinguish if an allele is shared between donors, or if a single donor simply is homozygous for this allele; in both cases, the peak height for that allele is higher.
* Allele drop-out: If the DNA was degraded, for example due to sunlight, some parts of the DNA might not be present in the sample to measure. It is also possible that the amount of the DNA available is so small, that the alleles fall below a certain noise filter. Because of this low quality or quantity of DNA, some allele fragments might not show up in the profile at all, which is called drop-out.

These factors can decrease the number of alleles found in a certain profile, which could lead to an underestimation of the number of contributors. There are also factors that could lead to an overestimation of alleles present in a sample:

* Stutter or drop-in: During the process of measuring the STRs, a STR fragment can “slip” from the template. This could cause the electropherogram to measure this strand to have one repeat fewer, since the slipped part of the fragment is not correctly measured. In this way, a small stutter peak is found in the profile just before the valid peak.
* Other noise: The measuring process is not perfect, so some random noise or blobs might show up in the electropherogram, that do not contain any information about the DNA.

Stutter peaks and noise are often filtered out using certain thresholds. As a result, some DNA information might also be lost due to a low-quantity donor.

In general, it is more difficult to discern the NOC, when the number of donors increases.

It is important to make a correct assumption of the number of contributors, since the following steps rely on this number to determine correct evidence in criminal cases. When an incorrect NOC is used for further analysis involving the investigation of the DNA profiles, the results are unreliable [3]. It is possible to rerun the software with a different number of contributors, but

The Maximum Allele Count approach to determine the NOC is quite simple, but it is unreliable due to the factors discussed prior. Performance in general is quite poor, especially with 3 or more contributors [1, 4, 5]. On average, when assessing mixtures between 2-5 contributors, the MAC cannot obtain correct predictions for more than 70% of samples [6]. When looking at 4-person mixtures, more than 70% of the samples are characterized as 2-, or 3-person mixtures using only the MAC approach [5].

Often experts use MAC in combination with the Total Allele Count (TAC), which measures the total number of alleles across all loci. However, this measure suffers from the same obscuring factors as the MAC.

**nC-tool [7]:** Estimates the NOC by simulations performed on the TAC. This achieves better results than using the MAC only, obtaining correct predictions for roughly 76% of 2-5 person mixtures [6].

In 2019, a Machine Learning (ML) model was created that derived the NOC with an accuracy of roughly 82% [6]. This Random Forest (RF) model was trained based on 590 profiles of 2-5 person mixtures, obtained from **TODO:find how many**  donors. The data used for training was not the original electrophoresis results, but consists of 19 features such as the MAC, locus-specific information, and other statistical features of the data.

Allowing stutter peaks to be counted as alleles [8].

How relatives influence the LR [9]

More contributors, more likely to be estimated to have fewer NOC [10].

**Decision Tree [11]**

Derive NOC from

* Decision tree with

Tested various ML approached (RF / MLP / LDA), showing similar performance to the RF19 model. They obtained very high performance (96%) with a RFC 35 model.

Difference with [2] is “Benschop et al. used 1174 unique donors to construct 590 profiles [20], whereas the PROVEDIt dataset only had 26 unique donors within the 766 profiles used”

This means that the classifiers probably overfit to certain donors.

“In conclusion, the decision tree method for NoC assignment has been shown to be over 77% accurate, with increasing performance with improved stutter and artefact filters”

They used a decision tree to classify peaks as stutter or allele.

**Background STR mixture interpretation [12]**

Information about how statistical analysis is done to determine the LR with the Hd and Hp. Showing that the LR is still the de-facto standard method.

“The peak height information is of benefit for analyzing mixed profiles.”

“The effect of incorrect estimation of the number of donors (caused by allele sharing) to the LR value was examined by Benschop (…) and was illustrated to exert a great effect on the LR” [3]

**Background about NFI-used software for LR calculation DNAStatistX**

Shows the importance of correct NOC estimations: under-assigned number of contributors can cause the model the fail calculating the LR because the observed peaks cannot be well explained.

Also includes the NOC model + the generic RF11 model (with a lower accuracy of ~

Also includes the LoCIM method for inferring the major contributor.

With EuroForMix, we can solve the probability of a peakheight at certain loci and alleles, given the unknown alleles for each contributor (given the NOC), with a Gamma distribution. Thresholds are also upheld. Because we do not know the alleles for each contributor, the probabilities for these alleles are estimated from the allele frequencies from the population.

# Evaluation

Dependence between features must be visualized in explanations

The quality of explanations is sometimes evaluated by performing a quantitative evaluation of a user study. Users are asked to perform a certain task and the explanations help support this task. How well and how fast the humans can accomplish the task is measured as accuracy and efficiency respectively [13, 14]. Subjectively, users were asked for their preference of explanation type in a 1 versus 1 fashion and asked to provide reasons.

Explanations should have few features, as humans pick usually just a few reasons. They should be specific to the problem at hand, and every instance should be explained in the same deterministic way [15]. Deterministic, or consistent feature attributions [16].

Exploration using several visual aids [17].

Research into XAI has shown the need for comparison and evaluation of methods [18-24], and the recent interest in the implementation of counterfactual explanations [18-22]. Although there are a few key components highlighted by these surveys, they also mention that the evaluation must be done specifically to certain applications [22]. One could specify a specific goal to be achieved by the explanations which should be tested [23]. Also the relevance of explanations to a certain audience [24].

What does the NOC machine learning problem look like?

The dataset consists of 590 samples of mixtures between 1 and 5 contributors.

Any machine learning model learns to map the profile to a single output .

Where are the input features of a profile, which are all continuous variables. Currently in the RFC19 model. The target constitutes a multi-class classification problem in the current model, and for any other classifier. The target could be changed to be to correspond to a regression model.

Which model-agnostic counterfactual explanation techniques exist and what problems can they be applied to?

One of the first papers on counterfactual explanations was written to bring up discussion on the “right to explanation” in automated decisions made by black-box algorithms [25].

Two reasons that the authors mention which are also relevant to the current case:

1. Understand why a decision was made
2. Understand how a different decision could be made if certain conditions were changed

In short, a counterfactual explanation is a statement that shows how the instance would have to change to yield a different outcome, or formally:

“Score *p* was returned because variables *V* had values (*v*1, *v*2 , . . .) associated with them. If *V* instead had values (*v*1*'*, *v*2*'*, . . .), and all other variables had remained constant, score *p'* would have been returned.”[25]

For one instance, multiple possible counterfactuals exist, and it is often the question which one is most appropriate. Counterfactuals are purposefully constructed to be minimal, meaning that minimal changes are made to the instance in question. In this way, the changed instance can still be related to the original. It is desirable to present multiple explanations, which correspond to altering different aspects of the original instance. These aspects could also be case-specific.

To generate counterfactuals, we minimize:

Where is the original instance, and is the counterfactual, which we want to find to be as close to as defined by a certain distance function . The outcome of the prediction by the model should be the desired outcome . The desired outcome is balanced to the distance by a weight , where a larger value favors the desired outcome, and a lower value favors less change made to the original instance.

The choice of the distance function is important. The authors found the or Manhattan distance, weighed by the inverse median absolute deviation to be most useful. It is used to normalize each feature, and is robust to outliers. However, the authors recognize that this distance metric should be catered towards specific problems, audiences, and data.

Any suitable optimization algorithm can be used to solve this problem. If access to the gradients of the machine learning model are given, optimization is faster. However, since we aim to look at model-agnostic methods, we disregard this statement.

“Principally, counterfactuals bypass the substantial challenge of explaining the internal workings of complex machine learning systems”

“As the working memory of humans can contain around seven distinct items”

They tested on the LSAT dataset, which is a regression dataset predicting their entrance exam scores (3 input variables).

Pima Diabetes Database: whether Pima women are likely to develop diabetes or not (8 input variables).

One of the authors of this original paper, continued to make contributions with regards to mixed input features (categorical, numerical, other embeddings) which are not quite relevant to our problem; and diverse explanations [26]. The latter entails that once a type of counterfactual is generated, future counterfactuals do not make the same feature changes.

They also use a natural language form with automatically filled-in values to create a more natural explanation rather than a data point and its feature values.

Tested on the LSAT dataset again, showing that the heavily unbalanced dataset was counteracted with this approach: only 6% of students were black, but this strong bias was found.

Also showed how the original method by Wachter et al. uses a brute-force method which is not viable for a large dataset.

Only applicable to linear classifiers.

Evaluate based on domain knowledge if feature importance values are viable and legal. They claim that this approach yields “coherent and informative diverse explanations” based on reasoning about the problem. They claim that a user study would be most appropriate to evaluate whether explanations help people understand why a certain decision has been made.

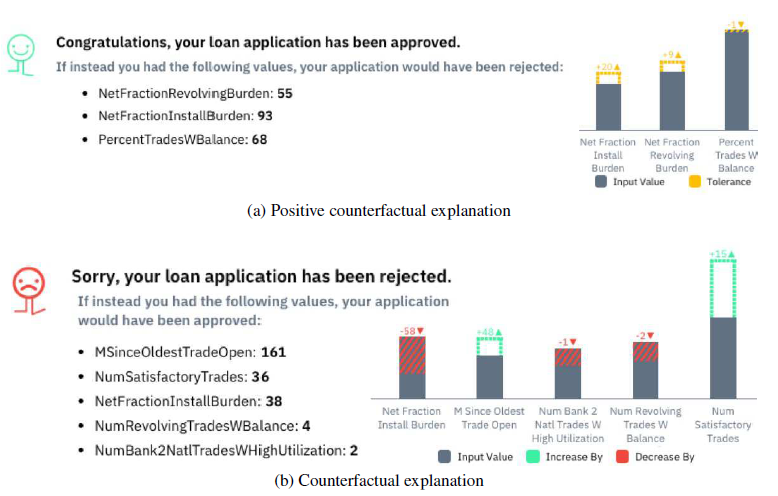
Code: <https://bitbucket.org/ChrisRussell/diverse-coherent-explanations/>

Since then, many varieties of counterfactual methods have been generated.

One method proposes to expand on Wachter et al. by adding *positive counterfactuals*, which were catered towards the HELOC loan applications dataset [27]. These explanations are created when the desired outcome is already achieved, but a certain margin of value ranges is presented for which the outcome will also hold. They achieve this by setting the target to represent the decision boundary, which would entail .

In our case, that would still yield the same explanations since we have no explicit positive or negative case.

A second change they propose, is to weigh certain features based on their relevance or importance. This is achieved by adding a weight vector to the original distance metric [27]. They use two strategies to obtain a relevance score for each feature. The first is using global feature importance (ANOVA) scores between feature and target, which should result in a smaller set of feature changes. The second is based on K-Nearest Neighbors to find instances close to the original stance, but with the desired result. The changed features can then be weighted according to this local area, giving more value to features that have historically been known to vary (since neighboring points exist).

**Nice visualization **

This original notion of a counterfactual explanation was translated into a more conversation-like statement [28].

*“Your loan application has been declined. If you were a skilled employee instead of an unskilled –*

*resident, your loan application would be accepted.”*

A different approach to finding factual and counterfactual explanations is based around building a simple classifier around a local neighborhood of the point of interest [29]. This local neighborhood is created with a genetic algorithm, after which this feature space is described using a decision tree. The path down the tree that corresponds to the current label thus explains the actual prediction, while any path that leads to a different outcome could be interpreted as a counterfactual. They measure minimal changes to be the number of split conditions that need to be changed in order to change the prediction.

In comparison to LIME and Anchors, this approach thus supports contrastive explanations. Also the local neighborhood is explored through a genetic algorithm, which produces higher quality training data.

The genetic algorithm is still based around a notion of finding instances that look like x, but are different than x (in feature values). They generate both instances with the same, and different outcomes to x.

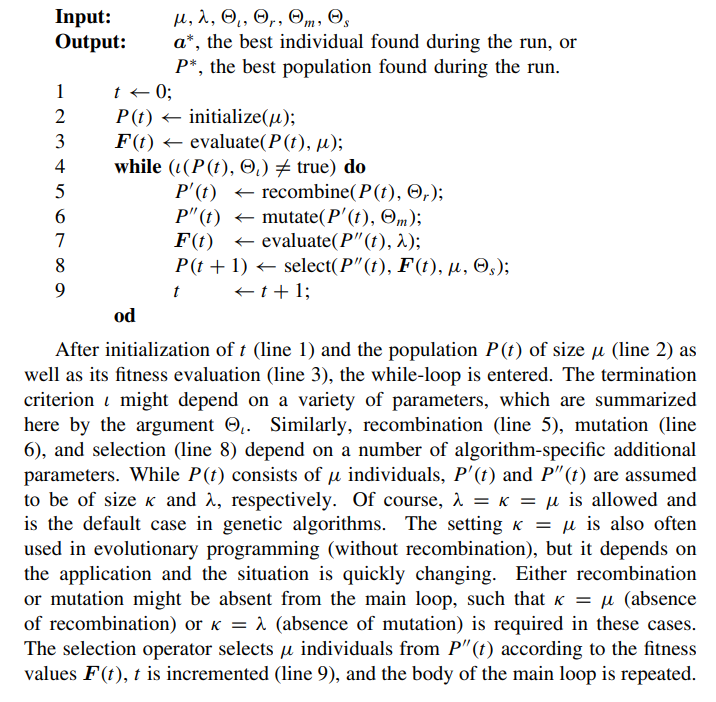


Figure : Basic evolutionary algorithm

* Fitness function: defined based on distance to the original instance
* Crossover/recombination: defined based on 2 features crossing over from parents to children.
* Mutation: defined based on 2 features mutating slightly from parent to child.

Evaluated based on correct classifications of the instances with the decision tree mimic model as compared to the original black-box. Evaluated on various (binary) classification datasets, mostly obtaining outputs with higher fidelity than LIME, even for the local neighborhood.

Where LIME generates something like: ““if the duration in months had been higher than the value it is for x, the prediction would have been, on average, 0.11 less 0 (or 0.11 more 1)”, which is not very intuitive to understand. In comparison to Anchors: “ANCHOR requires the apriori **discretization** of continuous features, while LORE benefits of the capabilities of decision trees to split continuous features”. “In summary, ANCHOR shows better precision than LORE at the expenses of generality and stability of the produced explanations.”

We can also use the gradient of the loss with respect to the input, which can be followed over the input space with an optimizer (e.g. Adam) until we find an instance x\*, that typically lies on the decision boundary between y^ and y\* [30].

A mask is used to only change certain attributes. We pick which feature to change by first applying the original gradient function, and sorting which features are changed most. Then select the top n features to change, and incorporate those only into the mask. This mask is set to 1 for those features and multiplied by the gradient at each iteration of gradient descent (after obtaining the gradient, before applying it to the weights of the optimizer).

CADEX was compared to finding training samples with a different classification with the nearest L2 distance, and found that CADEX finds “closer” samples to the original.

CADEX also finds attributes to change that SHAP does not consider to be important.

They tested transferability to other classifiers, finding an 86% agreement rate between RF and NN.

Code: <https://github.com/spore1/cadex>

Some have used existing techniques like SHAP to formulate contrastive explanations [31]. They formulate their counterfactual as “‘Why [predicted-class]”, and “Why not [desired-class]?’”. Using the instance of interest, SHAP values are generated for the target class.

First SHAP values are generated for the target- and predicted class.

Then, counterfactual instances (in the training data) are identified using a nearest-neighbor approach (n=50 at a time), only changing features that contribute negatively for the target class.

A concise effort has been made to summarize the most important desiderata of counterfactual explanations [32]. For *completeness*, it is important to make emphasize the conditions of the counterfactual. This means that the explanation must include the phrase “had <variables x, y> changed to be <value a, b>, the classification outcome would have changed*, provided you do not change <variable z>”*. This also entails *contextfulness*. Others are: “soundness – truthfulness of the explanation with respect to the predictive model; interactiveness – interactive explanations are better than static ones; actionability – explanations that give the user suggestions how to change the model’s prediction are preferred; coherence – explanations should agree with the user’s mental model; complexity – the complexity of an explanation should be tuned to the user’s ability and knowledge; and parsimony – shorter explanations are more comprehensive.”

An investigation of the dis- and advantages of counterfactual explanations has shown some insight into the results [33]. It is good to show multiple counterfactuals. It is good to be able to show different levels of parsimony. It is good to show context.

An analysis of the assumptions made by counterfactual arguments has shown that changes deemed to be “actionable”, might not have the desired results; e.g. increasing income, might cause a person to change their job, which would decrease their length of employment [34]. This also highlights the fact that features are often correlated, and changing one value might impact another.

Another point the authors make is that in order to come up with a distance metric, the feature values must be normalized to make them comparable. However, one feature might have a more diverse distribution of values than another, or a certain feature might have a large amount of zeros for instance. These are often based on the training data, but might not align with the worldly reality; e.g. is one year of work experience equal to an increase in salary of 1000eu or 5000eu. It is better to recommend a feature change of something that has little cost to change, though this could conceal real reasons for a certain decision of immutable features such as race.

Here, again it is highlighted that there also must be a notion of what must *not* be changed.

Multi-Objective Counterfactuals (MOC) method [35]. Uses a distance metric based on four objectives, which are optimized simultaneously.

Counterfactual explanation x’ for x:

1. the prediction f(x’) is close to the desired outcome y’
2. x’ is close to x in feature space
3. x’ differs from x in only a few features
4. x’ is a plausible data point based on the training data

Based on L1 distance (2) for numerical features. The final objective (4) is based around finding the L1 distance between x’ and the k (=1) nearest neighboring data points (as an empirical approximation whether it is a plausible data point given the training data).

To minimize this joint problem, NSGA-II was adapted. For the crowding distance sorting, the method not only considers distances in the objective space, but also in the input space. In this way, they are kept if the feature values vary greatly in addition to their objective values. This corresponds better to the users’ desires.

Actionable features are also taken into account, meaning that feature values are capped to represent more realistic values.

Only evaluated on the 4 objectives posed, in comparison to other state-of-the-art methods (dice, recourse, whatif, tweaking).

Counterfactual Local Explanations viA Regression (CLEAR) [36]. They highlight the fact that when only generating counterfactuals, there is no notion of why the current prediction was made or how much each current feature contributed to the prediction. They indicate that instead perhaps a neighborhood could be defined around x.

The method is based around

1. creating counterfactuals by searching through the feature space
2. generating a synthetic dataset by sampling features, creating neighborhood around x (using Euclidean distance).
3. Perform regression on the neighborhood dataset.

They only change one feature at a time

They evaluate in comparison to LIME and based on a fidelity measure, which I don’t really understand.

Created an interactive user-based system, that supports a range of *why* questions asked by a user through chat, called Glass-Box [37]. It provides class-contrastive counterfactual explanations, presented in natural language. They used the German credit dataset, which has a binary classification. The class contract in a multi-class classification could be specified.

Three types of questions are allowed: *Why* gives a plain counterfactual. *Why given* gives another counterfactual where some variables are fixed.

Desiderata based on [32]:

* F3: Explanation Target, F4: Explanation Breadth/Scope, F7: Relation to the Predictive System
* O7: Function of the Explanation, O8: Causality vs. Actionability
* U3: Contextfullness, U6: Chronology, U7: Coherence, U8: Novelty, U9: Complexity, U10: Personalisation, U11: Parsimony

They allow the explanation to go further than a single data point, to a subspace of the data.

Tested on AI people (6) and lay persons (11). They were satisfied with the explanations regarding understanding and content.

They used a decision tree to be the ML model and was used to generate the counterfactuals.

Counterfactual Explanations for Robustness, Transparency, Interpretability, and Fairness of Artificial Intelligence models (CERTIFAI) [38].

They use a genetic algorithm based on minimum distance (L1 distance) between counterfactual and instance to be explained.

They use their counterfactuals to evaluate the fairness and robustness of different classifiers.

When sampling counterfactual instances it is important to bring in domain knowledge, especially if the problem is not that simple [39]. This domain knowledge includes taking advantage of the empirical distribution of the data to sample instances that are likely, by capturing the distribution of feature values and feature correlations.

Feature importance techniques fall into two main categories; perturbation- and gradient-based methods [40]. The most prevalent method using perturbations is SHAP. “The highlight of Shapley values is that they enjoy axiomatic uniqueness guarantees. Unfortunately, calculating the exact Shapley value is exponential in d, input dimensionality; however, the literature has proposed approximate methods using weighted linear regression [34], Monte Carlo approximation [61], centroid aggregation [11], and graph-structured factorization [14].”. “review the Shapley value explanations to ensure that the model exhibits expected behavior (i.e., the model uses the same features that a human would for the same task)”. “Organization A found that in practice LIME explanations [50] give unexpected explanations that do not align with human intuition. Recent work [71] shows that the fragility of LIME explanations can be traced to the sampling variance when explaining a singular data point and to the explanation sensitivity to sample size and sampling proximity”. In summary, Shapley values are easy to deploy and have solid motivations from game theory.

As for counterfactuals; they can be applied to any model and data type. Some counterfactuals might not be feasible. It is therefore important to use training data and constraints to guide the process.

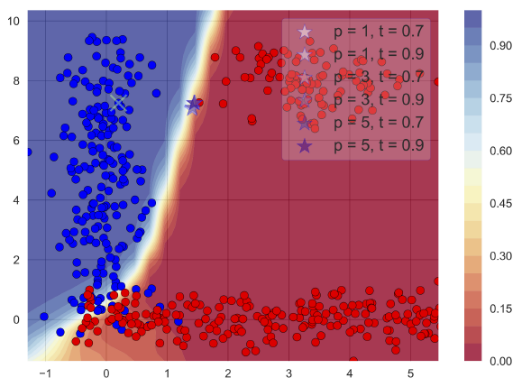
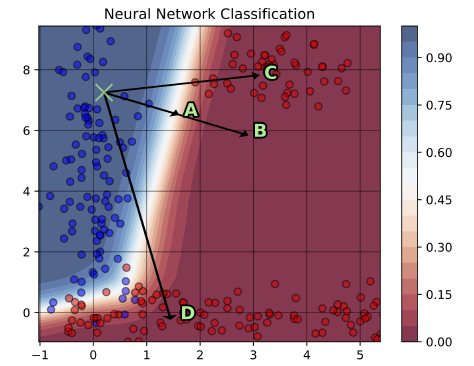
They recommend to determine clear desiderata:

* Identify the target for which the explanation is intended.
* Understand what they are looking for.
* Understand how they will engage with the explanation.

In a paper where counterfactual sets are presented, some desirable properties are listed [41]. One of these is the notion of set coverage, meaning that the counterfactual set should include as many training samples as possible (similarly defined in LORE). They also mention the bounds of the counterfactuals so that they produce **feasible instances**, as well as **provide ranges** instead of unbounded changes. For example; 25C < temp < 35C, instead of >25C.

Also evaluated on distance to factual sample (0-1 using L1-norm)

Feasible and Actionable Counterfactual Explanations (FACE) was developed to overcome the problem of generating counterfactuals that do not align with the **underlying data distributions** [42]. They also focus on actionability of the found counterfactual and argue that there should be an obtainable path to the desired new data point. They argue that D is therefore the best option, though I think C would be more appropriate for our purpose. A is generated by minimizing the L2 norm, and B represents a larger classification margin.



The danger of A and B is that these instances might still be classified wrong due to the low-density areas, which ML models are known to perform unreliably in.

The focus of this paper is to *transform* one data point to another, thereby focusing on actionability.

Their only focus for evaluation is to visualize the path taken by their algorithm. They do show that the counterfactuals by Wachter et al. (left picture) do not fall close to the data distribution.

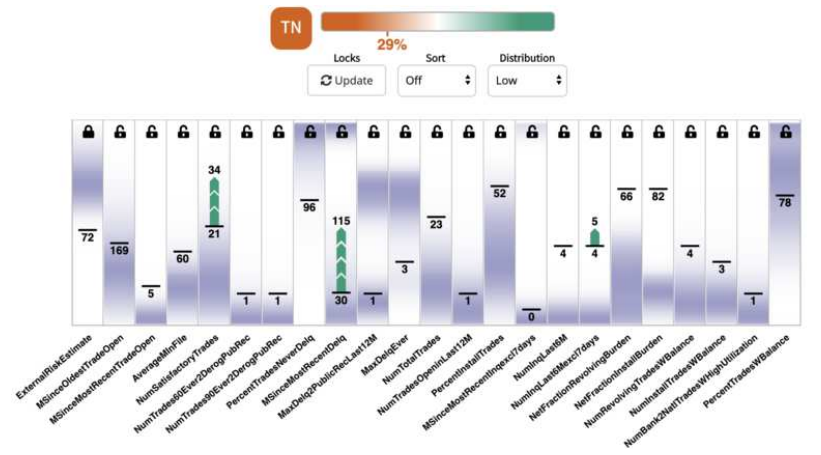
ViCE: visual counterfactual explanations [43]. Their desiderata:

* How does the instance in question lie in comparison to the data?
* Which features are most relevant to the model?
* Which are changes in feature values that would alter the model’s prediction?
* How can we select actionable changes?

Find counterfactuals by finding a minimal set of features, and minimal amounts of changes.

They **discretize the dataset** by fitting a gaussian on each feature, splitting the values into *n* bins such that the middle *n-2* capture 4 standard deviations from the mean, extreme bins capture data points beyond that.

Their algorithm works **by greedily moving feature values across bins** until the predicted class is changed, or until a constraint is reached on the number of features changed / number of bins changed. They start with the instance of interest, and move along the available features to the bins below and above, choosing the one that elicits the most change in the model’s output.



They evaluated on the Home Equity Line of Credit (HELOC) dataset, using the desiderate mentioned previously.

Cannot be used for multi-class in this moment.

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