Explaining Groups of Points in Low-Dimensional Representations

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Abstract

A common workflow in data exploration is to learn a low-dimensional representation of the data, identify groups of points in that representation, and examine the differences between the groups to determine what they represent. We treat this as an interpretable machine learning problem by leveraging the model that learned the low-dimensional representation to help identify the key differences between the groups. To solve this problem, we introduce a new type of explanation, a Global Counterfactual Explanation (GCE), and our algorithm, Transitive Global Translations (TGT), for computing GCEs. TGT identifies the differences between each pair of groups using compressed sensing but constrains those pairwise differences to be consistent among all of the groups. Empirically, we demonstrate that TGT is able to identify explanations that accurately explain the model while being relatively sparse, and that these explanations match real patterns in the data.

1. Introduction

A common workflow in data exploration is to: 1) learn a low-dimensional representation of the data, 2) identify groups of points (i.e., clusters) that are similar to each other in that representation, and 3) examine the differences between the groups to determine what they represent. We focus on the third step of this process: answering the question “What are the key differences between the groups?”

For data exploration, this is an interesting question because the groups often correspond to an unobserved concept of interest and, by identifying which features differentiate the groups, we can learn something about that concept of interest. For example, consider single-cell RNA analysis which uses datasets that measure the gene expression levels of many genes for sampled cells whose cell-types are unknown. Because gene expression and cell-type are closely related, the groups of points that can be seen in a low-dimensional representation of the dataset often correspond to different cell-types (Figure 1). By determining which gene expressions differentiate the groups, we can learn something about the connection between gene expression and cell-type.

One common method for answering this question is manual interpretation and one simple way to do that is to calculate the Difference Between the Mean (DBM) value of each feature between a pair of groups. For example, consider using DBM to explain the differences between the cells in Group 3 and Group 17 from Figure 1. In this case, DBM’s explanation contains many hundreds of non-zero elements, which is far too many to be understood by a person (Figure 2). If we make DBM’s explanation sparse by thresholding it to include only the $k$ largest changes, it is no longer an effective explanation because it no longer reliably maps points from Group 3 to Group 17 (Figure 3). More generally, manual interpretation can be time-consuming and typically ad-hoc, requiring the analyst to make arbitrary decisions that may not be supported by the data.

Another, more principled, method is statistical hypothesis testing for the differences between features across groups. However, the trade-off between the power of these tests and their false positive rate becomes problematic in high-dimensional settings.

Additionally, there is another key shortcoming of both man-
ual interpretation and statistical testing: they do not make use of the model that learned the low-dimensional representation that was used to define the groups in the first place. Intuitively, we would expect that, by inspecting this model directly, we should be able to gain additional insight into the patterns that define the groups. With this perspective, answering our question of interest becomes an interpretable machine learning problem. Although there are a wide variety of methods developed in this area (Ribeiro et al., 2016; Lundberg & Lee, 2017; Wang & Rudin, 2015; Caruana et al., 2015; Ribeiro et al., 2018; Zhang et al., 2018), none of them are designed to answer our question of interest. See Section 2 for further discussion.

We want a counterfactual explanation because our goal is to identify the key differences between Group A and Group B using the low-dimensional representation and the most natural way to do this is to find a transformation that causes the model to assign transformed points from Group A to Group B. Additionally, we want a global explanation because we want to find an explanation that works for all of the points in Group A and because we want the complete set of explanations to be consistent (i.e., symmetrical and transitive) among all the groups. See Section 3.2 for further discussion of our definition of consistency in this context. Hence, our goal is to find a Global Counterfactual Explanation (GCE). Although the space of possible transformations is very large, we limit it to a translation in this work because their interpretability can be measured easily using sparsity.

Contributions: To the best of our knowledge, this is the first work that explores GCEs. Motivated by the desire to generate a simple (i.e., sparse) explanation between each pair of groups, we derive an algorithm to find these explanations that is motivated by compressed sensing (Tsai & Donoho, 2006; Candès et al., 2006). However, the solutions from compressed sensing are only able to explain the difference between one pair of groups. As a result, we generalize that problem setting to find a set of consistent explanations among all groups simultaneously. We call this algorithm Transitive Global Translations (TGT).

We demonstrate the usefulness of TGT with a series of experiments on synthetic, UCI, and single-cell RNA datasets. In our experiments, we measure the effectiveness of explanations using correctness and coverage, with sparsity as a proxy metric for interpretability, and we compare the patterns the explanations find to those we expect to be in the data. We find the TGT clearly outperforms DBM at finding sparse explanations of the model and that its explanations match domain knowledge. 1

1Code for all algorithms and experiments is available at https://github.com/GDPlumb/ELDR

2. Related Work

Although interpretability is often loosely defined and context specific (Lipton, 2016), we categorize existing methods along two axes in order to help demonstrate how a GCE differs from existing types of explanations. Those two axes are the explanation’s level and its form.

The first axis used to categorize explanations is their level: local or global. A local explanation explains a single prediction made by the model (Ribeiro et al., 2016; Lundberg & Lee, 2017; Plumb et al., 2018). (Kauffmann et al., 2019) studies a problem closely related to ours of explaining why a point was assigned to its cluster/group. A global explanation will explain multiple predictions or the entire model at once (Wang & Rudin, 2015; Caruana et al., 2015; Ribeiro et al., 2018).

The second axis we use to categorize explanations is their
form: feature attribution, approximation, or counterfactual. A feature attribution explanation assigns a value measuring how each feature contributed to the model’s prediction(s) (Lundberg & Lee, 2017; Sundararajan et al., 2017). Importantly, it is necessary to define a baseline value for the features in order to compute these explanations. An approximation explanation approximates the model being explained using a function that is simple enough to be considered directly interpretable (e.g., a sparse linear model or a small decision tree) across some neighborhood, which could be centered around a point or could be the entire input space (Ribeiro et al., 2016; Plumb et al., 2018; Wang & Rudin, 2015; Caruana et al., 2015; Ribeiro et al., 2018). A counterfactual explanation finds a transformation of the input(s) such that the transformed version of the input is treated in a specific way by the model (Zhang et al., 2018; Dhurandhar et al., 2018; Goyal et al., 2019; Dhurandhar et al., 2019).

For various reasons, it would be challenging to use other types of explanations to construct a GCE. Local explanations would have to be aggregated in order to produce an explanation that applies to a group of points and it would be highly nontrivial to ensure that the resulting “aggregated group explanations” are consistent. For feature attribution and local approximation explanations, it is difficult to guarantee that the baseline value or neighborhood they consider is defined broadly enough to find the transformation we want. For global approximation explanations, we might not be able to approximate a complex model well enough to find the transformation we want because of the accuracy-interpretability trade-off that stems from the complexity constraint on the explanation model (Lipton, 2016).

### 3. Global Counterfactual Explanations

We will start by introducing our notation, more formally stating the goal of a GCE, and defining the metrics that we will use to measure the quality of GCEs. We do this under the simplifying assumption that we have only two groups of points that we are interested in. Then, in Section 3.1, we will demonstrate the connection between finding a GCE and compressed sensing. We use that connection to derive a loss function we can minimize to find a GCE between a single pair of groups of points. Finally, in Section 3.2, we will remove our simplifying assumption and introduce our algorithm, TGT, for finding a set of consistent GCEs among multiple groups of points.

**Notation:** Let \( r : \mathbb{R}^d \rightarrow \mathbb{R}^m \) denote the function that maps the points in the feature space into a lower-dimensional representation space. The only restriction that we place on \( r \) is that it is differentiable. Suppose that we have two regions of interest in this representation: \( R_{initial}, R_{target} \subseteq \mathbb{R}^m \). Let \( X_{initial} \) and \( X_{target} \) denote their pre-images. Then, our goal is to find the key differences between \( X_{initial} \) and \( X_{target} \) in \( \mathbb{R}^d \) and, unlike manual interpretation or statistical testing, we will treat this as an interpretable machine learning problem by using \( r \) to help find those key differences.

**Defining the Goal of GCEs:** At a high level, the goal of a GCE is to find a transformation that takes the points in \( X_{initial} \) and transforms them so that they are mapped to \( R_{target} \) by \( r \); in other words, \( r \) treats the transformed points from \( X_{initial} \) as if they were points from \( X_{target} \). Formally, the goal is to find a transformation function \( t : \mathbb{R}^d \rightarrow \mathbb{R}^d \) such that:

\[
r(t(x)) \in R_{target} \quad \forall x \in X_{initial}
\]

Because we are using \( t \) as an explanation, it should be as simple as possible. Since they are very simple and their complexity can be readily measured by their sparsity, we limit \( t \) to a translation:

\[
t(x) = x + \delta
\]

**Measuring the Quality of GCEs:** To measure the quality of a GCE we use two metrics: correctness and coverage. Correctness measures the fraction of points mapped from \( X_{initial} \) into \( R_{target} \). Coverage measures the fraction of points in \( R_{target} \) that transformed points from \( X_{initial} \) are similar to. Mathematically, we define correctness as:

\[
cr(t) = \frac{1}{|X_{initial}|} \sum_{x \in X_{initial}} \mathbb{1}[\exists x' \in X_{target} \mid ||r(t(x)) - r(x')||_2^2 \leq \epsilon]
\]

And coverage as:

\[
cv(t) = \frac{1}{|X_{target}|} \sum_{x \in X_{target}} \mathbb{1}[\exists x' \in X_{initial} \mid ||r(x) - r(t(x'))||_2^2 \leq \epsilon]
\]

Clearly, correctness is a necessary property because an explanation with poor correctness has failed to map points from \( X_{initial} \) into \( R_{target} \) (Equation 1). However, coverage is also a desirable property because, intuitively, an explanation with good coverage has captured all of the differences between the groups. Defining these metrics requires that we pick a value of \( \epsilon \).

Observe that, if \( X_{initial} = X_{target} \) and \( t(x) = x \), then \( cr(t) = cv(t) \) and we have a measure of how similar a group of points is to itself. After \( r \) has been learned, we increase \( \epsilon \) until this self-similarity metric for each group of points in the learned representation is between 0.95 and 1.

**A Simple Illustration:** We will now conclude our introduction to GCEs with a simple example to visualize the transformation function and the metrics. In Figures 4, 5, and 6, the data is generated from two Gaussian distributions...
with different means and $r(x) = x$. We use DBM between Group 1 and Group 0 as the translation/explanation. In Figure 4, the two distributions have an equal variance and, as a result, the translation is an effective explanation with good correctness and coverage. In Figures 5 and 6, Group 0 has a smaller variance than Group 1. Because a simple translation cannot capture that information, the translation has poor coverage from Group 0 to Group 1 while its negative has poor correctness from Group 1 to Group 0. This illustrates the connection between correctness and coverage that we will discuss more in Section 3.2.

3.1. Relating GCEs and Compressed Sensing

We will now demonstrate how the problem of finding a GCE between a pair of groups is connected to compressed sensing by starting with an “ideal” loss function that is too difficult to optimize, and making several relaxations to it.

In principle, Equations 1, 3, or 4 define objective functions that we could optimize, but they are discontinuous and hence difficult to optimize. To progress towards a tractable objective, first consider a continuous approximation of correctness (Equation 3):

$$\text{loss}_{\text{mean}}(t) = \frac{1}{|X_{\text{initial}}|} \sum_{x \in X_{\text{initial}}} \min_{x' \in X_{\text{target}}} ||r(t(x)) - r(x')||_2^2$$  (5)

This loss could be optimized by gradient descent using autodifferentiation software, although doing so might be difficult because of the $\min$ operation. Consequently, we consider a simplified version of it:

$$\text{loss}_{\text{mean}}(t) = \frac{1}{|X_{\text{initial}}|} \sum_{x \in X_{\text{initial}}} ||r(t(x)) - \bar{r}_{\text{target}}||_2^2$$  (6)

where $\bar{r}_i = \frac{1}{|X_i|} \sum_{x \in X_i} r(x)$. ³

Next, we are going to make use of our restriction of $t$ to a translation, $\delta$, and assume that $r$ is a linear mapping: $r(x) = Ax$ for $A \in \mathbb{R}^{m \times d}$. Although this assumption about $r$ will not be true in general, it allows us to connect a GCE to the classical compressed sensing formulation. Under these constraints, we have that:

$$\text{loss}_{\text{mean-linear}}(\delta) = \frac{1}{|X_{\text{initial}}|} \sum_{x \in X_{\text{initial}}} ||A(x + \delta) - \bar{r}_{\text{target}}||_2^2$$  (7)

By setting its derivative to zero, we find that solving $A\delta = \bar{r}_{\text{target}} - \bar{r}_{\text{initial}}$ yields an optimal solution to Equation 7. Observe that this is an underdetermined linear system, because $m < d$, and so we can always find such a $\delta$.

Recall that, in general, we want to find a sparse $\delta$. This is partially because because we need the explanation to be simple enough to be understood by a person, but also because the explanation is hopefully modeling real world phenomena and these phenomena often have nice structure (e.g., sparsity). Then, because we are finding a GCE by solving $A\delta = \bar{r}_{\text{target}} - \bar{r}_{\text{initial}}$, we can see that $\bar{r}_{\text{target}} - \bar{r}_{\text{initial}}$ is the model’s low-dimensional measurement that we are trying to reconstruct using the high-dimensional but sparse underlying signal, $\delta$. This is exactly the classical compressed sensing problem formulation. As a result, we will add $l_1$ regularization to $\delta$ as an additional component to the loss function as is done in both linear and non-linear compressed sensing (Blumensath, 2013).

Consequently, we could consider finding a GCE by minimizing the linear compressed sensing loss:

$$\text{loss}_{\text{cs}}(\delta) = ||A(\bar{x}_{\text{initial}} + \delta) - \bar{r}_{\text{target}}||_2^2 + \lambda ||\delta||_1$$  (8)

where $\bar{x}_i = \frac{1}{|X_i|} \sum_{x \in X_i} x$. Or, by removing the assumption that $r(x) = Ax$, minimizing the more general version that

³Note that $\text{loss}_{\text{mean}}$ clearly optimizes for correctness and it does not directly penalize coverage. However, because $\text{loss}_{\text{mean}}$ encourages $r(t(x))$ to be close to $\bar{r}_{\text{target}}$, it is optimizing for correctness at the expense of coverage. In Section 3.2, we will discuss why this is not as harmful as it seems in our setting where $t$ is a symmetrical translation.

⁴Note that DBM solves this but does not consider sparsity.
we use for our experiments:
\[
\text{loss}(\delta) = ||r(\bar{x}_{\text{initial}} + \delta) - \bar{r}_{\text{target}}||_2^2 + \lambda||\delta||_1 \tag{9}
\]

### 3.2. Computing GCEs

We have thus far limited ourselves to explaining the differences between \( l = 2 \) groups of points labeled as \( X_1 \) (“initial”) and \( X_2 \) (“target”), and focused on learning an explanation \( t_{1 \rightarrow 2} \) from \( X_1 \) to \( X_2 \). However, this is not a realistic setting because this labeling was arbitrary and because we usually have \( l > 2 \).

Unfortunately, the naive solution of using compressed sensing to independently produce explanations for all \( O(l^2) \) pairs of groups will fail to satisfy two desirable properties related to the internal consistency of the explanations. For instance, we would like \( t_{1 \rightarrow 2} \) to agree with \( t_{2 \rightarrow 1} \), a property we call symmetry. Additionally, we would like \( t_{1 \rightarrow 3} \) to agree with the combined explanations \( t_{1 \rightarrow 2} \) and \( t_{2 \rightarrow 3} \); we call this transitivity.

TGT will use compressed sensing to find the explanation between a pair of groups, but set up the structure of the problem to constrain those explanations to be consistent (i.e., symmetrical and transitive). Formally, symmetry requires that \( t_{i \rightarrow j} = t_{j \rightarrow i}^{-1} \) and transitivity requires that \( t_{i \rightarrow k} = t_{j \rightarrow k} \circ t_{i \rightarrow j} \) for any \( j \).

Our approach to finding a consistent set of explanations will be to enforce the consistency constraints by design by computing a set of explanations relative to a reference group. We will assume that \( X_1 \) is the reference group and will find a set of basis explanations \( t_2, \ldots, t_l \), where \( t_i = t_{1 \rightarrow i} \), that we will use to construct any of the possible explanations between any pair of the groups of points.\(^3\) Algorithm 2 describes how \( t_{i \rightarrow j} \) can be constructed from \( t_2, \ldots, t_l \).

**Overview of TGT.** We now have all of the pieces necessary to actually compute a GCE: a differentiable loss function to measure the quality of \( t_{i \rightarrow j} \), \( l_1 \) regularization to help us find the simplest possible explanation between \( X_i \) and \( X_j \), and a problem setup to ensure that our explanations are consistent across \( X_1, \ldots, X_l \). At a high level, our algorithm for computing a set of GCEs, which we call TGT, will proceed to sample random “initial” and “target” groups from the set of all groups, construct that explanation from the set of basis explanations (Algorithm 2), and then use Equation 9 as a loss function to update the explanation using gradient descent (Algorithm 3).

Algorithm 1: TGT: Calculating GCEs with a Reference Group. Note that, because \( \lambda \) is applied to all of the explanations, we cannot tune it to guarantee that each explanation is exactly \( k \)-sparse.

```
Input: Model: \( r \)
Group Means: \( \bar{x}_i \) (feature space) and \( \bar{r}_i \) (representation space)
for \( i = 1, \ldots, l \)
l_1 \text{ Regularization Weight: } \lambda
Learning Rate: \( \alpha \)
Initialize: \( \delta_2, \ldots, \delta_l \) to vectors of 0
while not converged do
    Sample \( i \neq j \) from \( \{1, \ldots, l\} \)
    Construct \( t_{i \rightarrow j} (\delta_{i \rightarrow j}) \) using Algorithm 2
    Calculate objective: \( v = \text{loss}(\delta_{i \rightarrow j}) \) using Equation 9
    Update the components of \( \delta_{i \rightarrow j} \) using Algorithm 3
end while
Return: \( \delta_2, \ldots, \delta_l \)
```

Algorithm 2: How to construct any explanation between an arbitrary pair of groups, \( t_{i \rightarrow j} \), using the set of basis explanations relative to the reference group, \( t_2, \ldots, t_l \).

```
Input: \( i, j \)
if \( i = 1 \) then
    Return: \( t_j \)
else if \( j = 1 \) then
    Return: \( t_i^{-1} \)
else
    Return: \( t_j \circ t_i^{-1} \)
end if
```

Algorithm 3: How to update the basis explanations, \( \delta_2, \ldots, \delta_l \), based on the performance of \( \delta_{i \rightarrow j} \). This essentially splits the signal from the gradient between the basis explanations used to construct \( \delta_{i \rightarrow j} \). Note that it does not maintain any fixed level of sparsity during the update.

```
Input: \( i, j, \alpha, \nabla v \)
if \( i = 1 \) then
    \( \delta_j = \delta_j - \alpha \nabla v \)
else if \( j = 1 \) then
    \( \delta_i = \delta_i + \alpha \nabla v \)
else
    \( \delta_j = \delta_j - 0.5 \alpha \nabla v \)
    \( \delta_i = \delta_i + 0.5 \alpha \nabla v \)
end if
```

\(^3\)Importantly, the transitivity constraint also ensures that our choice of how we label the groups does not influence the optimal solution of our algorithm.

\(^6\)The pseudo-code leaves out some of the details of the optimization process such as how often we sample new “initial” and
3.3. Controlling the Level of Sparsity

Because neither TGT or DBM is guaranteed to produce a \( k \)-sparse explanation, we will threshold each of the explanations to include only the \( k \) most important features (i.e., the \( k \) features with the largest absolute value) for our experiments. This is done after they have been calculated but before their quality has been evaluated. Importantly, TGT has a hyper-parameter, \( \lambda \), which roughly controls the sparsity of its explanations; as a result, we will tune \( \lambda \) to maximize correctness for each value of \( k \).

The fact that \( \lambda \) is tuned for each value of \( k \) raises an interesting question: “Does TGT use a subset of the features from its \( k_2 \)-sparse explanation for its \( k_1 \)-sparse explanation when \( k_1 < k_2 \)?” Naturally, we would like for the answer to be “yes” because, for example, it does not seem like a desirable outcome if a 2-sparse explanation uses Features A and B but a 1-sparse explanation uses Feature C.

Suppose we have two explanations between Group \( i \) and Group \( j \): \( e_1 \) which is \( k_1 \)-sparse and \( e_2 \) which is \( k_2 \)-sparse with \( k_1 < k_2 \). To address this question, we define the similarity of \( e_1 \) and \( e_2 \) as:

\[
similarity(e_1, e_2) = \frac{\sum_{i \in |e_1|} \mathbb{I}_{e_2[i] \neq 0}}{|e_1|}
\]

This metric captures how much of \( e_1 \)’s explanation uses features that were also chosen by \( e_2 \).

Note that this metric also includes the run to run variance of TGT.

4. Experimental Results

Our experimental results are divided into two sections. In the first section, we demonstrate that TGT is better at explaining the model than DBM is when we restrict the explanations to varying degrees of sparsity. In the second section, we move beyond assessing whether or not TGT explains the model and demonstrate that it also appears to capture real signals in the data.

4.1. TGT’s Efficacy at Explaining the Model

From an interpretable machine learning perspective, our goal is help practitioners understand the dimensionality-reduction models they use in the data exploration process. We measure the quality of GCEs using correctness (Equation 3) and coverage (Equation 4) at varying degrees of sparsity.

We trained the model from (Ding et al., 2018) on the UCI Iris, Boston Housing, and Heart Disease datasets (Dua & Graff, 2017) and a single-cell RNA dataset (Shekhar et al., 2016). This model learns a non-linear embedding using a neural network architecture which is trained to be a parametric version of t-SNE (Maaten & Hinton, 2008) that also preserves the global structure in the data (Kobak & Berens, 2018). We then used that visualization to define the groups of points. This representation and grouping is shown for the single-cell RNA dataset in Figure 1; all of them can be found in the Appendix A.1.

Next, because the acceptable level of complexity depends on both the application and the person using the explanation, we measured the effectiveness of the explanations produced by TGT and DBM at explaining the model for a range of sparsity levels.

**Explanation effectiveness at different levels of sparsity.** The results of this comparison are in Figure 7. As we can see, TGT performed at least as well as DBM and usually did better and that TGT’s explanations are quite similar to each other as we ask it to find sparser explanations. Note that all of these metrics are defined for a single pair of groups and so these plots report the average across all pairs of groups.

**Exploring a Specific Level of Sparsity.** Looking at Figure 7, we see that TGT’s performance: is almost as good when \( k = 1 \) as when \( k = 4 \) on Iris, drops off sharply for \( k < 5 \) on Boston Housing, and drops off sharply for \( k < 3 \) on Heart Disease.

On the single-cell RNA dataset, we see that TGT significantly outperforms DBM when \( k = 250 \) (Appendix A.2 Figure 16); note that this comparison becomes significantly more favorable for TGT for smaller \( k \). We show the pairwise correctness and coverage metrics for these levels of sparsity in Figure 8.

**Figure 3, but with TGT.** In Figure 3, we showed that DBM
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Figure 7: A comparison of the effectiveness of TGT to DBM at explaining the model (measured by correctness and coverage) at a range of sparsity levels. Note that TGT performs as least as well as DBM and usually does better. Looking at the similarity metric, we see that TGT is fairly consistent at picking a subset of the current features when asked to find an even sparser solution.

does not produce a good 250-sparse explanation for the difference between Group 3 and Group 17 from Figure 1. For the sake of an easy comparison, a similar plot that uses TGT’s 250-sparse explanation is in Figure 9; it is a much better explanation of the model.

4.2. TGT’s Efficacy at Capturing Real Signals in the Data

In the previous section, we demonstrated that TGT provides accurate explanations of the model that learned the low-dimensional representation. However, in practice, there could be a mismatch between what the model itself learns and the true underlying structure in the data. In this section, we evaluate empirically whether or not TGT provides explanations that match underlying patterns in the data.

We begin with an experiment on a synthetic dataset with a known causal structure and demonstrate that TGT correctly identifies this structure. This also serves as an intuitive example of why a sparser explanation may be as effective as a less-sparse explanation. Next, we leverage the labels that come with the UCI datasets to compare TGT’s explanations to some basic domain knowledge. Finally, we then modify the UCI datasets and demonstrate that TGT is able to identify those modifications. Together, these results indicate that TGT is identifying real patterns in the data.

Synthetic Data with a Known Causal Structure. By specifying the causal structure of the data, we can know which differences are necessary in the explanation, since they are the causal differences, and which differences are unnecessary, since they are explained by the causal differences. We found that TGT correctly identified the causal structure of this dataset and that DBM did not.

We used the following procedure to generate each point in our synthetic dataset: $x_1, x_2 \sim \text{Bern}(0.5) + \mathcal{N}(0, 0.2)$, $x_3 \sim \mathcal{N}(0, 0.5)$, and $x_4 \sim x_1 + \mathcal{N}(0, 0.05)$. The causal structure of this dataset is simple. $x_1$ and $x_2$ jointly cause 4 different groups of points. The explanation for the differences between these groups must include these variables. $x_3$ is a noise variable that is unrelated to these groups and, as a result, should not be included in any explanation. $x_4$ is a variable that is correlated with those groups, since it is caused by $x_1$, but does not cause those groups. As a result, it is not necessary to include it in any explanation.

We then generated a dataset consisting of 400 points created using this process and trained an autoencoder (Kramer, 1991) to learn a two dimensional representation of the
When we inspect the explanations, shown in Table 1, we artificially add a known signal to the dataset by choosing whether or not they are on the Charles River. Finally on the well as equally priced groups of houses that differ mainly in (which is the variable that is not causally related to the groups.

### Table 1: A comparison of the explanations from TGT and from DBM. Note that they are similar except that TGT does not use \( x_1 \), which is the variable that is not causaly related to the groups.

| Explanation | Method | \( x_1 \) | \( x_2 \) | \( x_3 \) | \( x_4 \) |
|-------------|--------|------------|------------|------------|------------|
| 0 \( \rightarrow \) 1 | TGT    | -1.087     | 0.012      | 0.003      | -0.001     |
|             | DBM    | -1.019     | 0.038      | 0.011      | -1.031     |
| 0 \( \rightarrow \) 2 | TGT    | 0.003      | 0.878      | -0.002     | 0.000      |
|             | DBM    | -0.013     | 0.966      | 0.056      | -0.027     |
| 0 \( \rightarrow \) 3 | TGT    | -0.985     | 0.705      | -0.003     | 0.002      |
|             | DBM    | -1.019     | 1.033      | -0.006     | -1.028     |

A visualization of this learned representation is in the Appendix A.1 Figure 14; as expected, there are four distinct groups. Then, we used TGT and DBM to calculate the GCEs between these groups. The pairwise and average correctness and coverage metrics for these solutions are in the Appendix A.2 Figures 17 and 18; observe that the two methods are equally effective at explaining the model.

When we inspect the explanations, shown in Table 1, we see that both TGT and DBM use \( x_1 \) and \( x_2 \), neither use \( x_3 \), and that DBM uses \( x_4 \) while TGT does not. As a result, we have demonstrated that, even in a very simple setting, there is good reason to believe that an explanation that is simpler (i.e., sparser) than the DBM explanation exists and that TGT might be able to find it.

### Qualitative Analysis of the UCI Datasets using the Labels.

Qualitatively, we found that TGT’s explanations agreed with domain knowledge about these datasets. Specifically: On the Iris dataset, its explanations agreed with a simple decision tree because they both relied mostly on the Petal Width to separate the groups. On the Boston Housing dataset, it identified the differences between a set of inexpensive urban houses vs expensive suburban houses as well as equally priced groups of houses that differ mainly in whether or not they are on the Charles River. Finally on the Heart Disease dataset, it found that the difference between a moderate and a low risk group of subjects was that the low-risk group’s symptoms were explained by something other than heart disease and the difference between the moderate and high risk group of subjects is that the former is made up of men and the later of women. For full details, see the Appendix A.3.

### Quantitative Analysis of Modified Versions of the UCI Datasets.

In order to perform a more quantitative analysis, we artificially add a known signal to the dataset by choosing one of the groups of points, creating a modified copy of it, and adding those new points back into the dataset. We can then ask two important questions about TGT’s behavior. First, does TGT correctly identify the modifications we made to the original dataset? Second, do TGT’s explanations between the original groups change when the modified group is added to the dataset? Details of how we setup these experiments and their results are in the Appendix A.4.

We found that TGT does identify the modifications we made and that, in doing so, it does not significantly change the explanations between the original groups. Importantly, this result remains true even if we retrain the learned representation on the modified dataset.

These results are a strong indicator that TGT is finding real patterns in the data because it recovers both the original signal and the artificial signal even when the algorithm is rerun or the representation is retrained.

### 5. Conclusion

In this work, we introduced a new type of explanation, a GCE, which is a counterfactual explanation that applies to an entire group of points rather than a single point. Next, we defined reasonable metrics to measure the quality of GCEs (i.e., correctness and coverage) and introduced the concept of consistency (i.e., symmetry and transitivity), which is an important additional criteria that GCEs must satisfy. Given that, we defined an algorithm for finding consistent GCEs, TGT, that treats each pairwise explanation as a compressed sensing problem. Our first experiments empirically demonstrated that TGT is better able to explain the model than DBM across a range of levels of sparsity. Our next experiments showed that TGT captures real patterns in the data. This was done using a synthetic dataset with a known causal structure and by comparing TGT’s explanations to background knowledge about the UCI datasets. As an additional test, we then added a synthetic signal to the UCI datasets and demonstrated that TGT can recover that signal without changing it’s explanations between the real groups. Importantly, this results remains true even when the representation is retrained.

Although we focused on data exploration in this work, similar groups arise naturally whenever the model being trained uses an encoder-decoder structure. This technique is ubiquitous in most areas where deep learning is common (e.g., semi-supervised learning, image classification, natural language process, reinforcement learning). In these settings, identifying the key differences between the groups is an interesting question because we can observe that “The model treats points in Group A the same/differently as points in Group B”, determine that “The key differences between Group A and Group B are X”, and then conclude that “The model does not/does use pattern X to make its decisions”. We believe that exploring these applications is an important direction of future work that will require more sophisticated transformation functions and optimization procedures.
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A. Appendix

A.1. Learned Representations

The learned representations and the corresponding groups of points for the datasets we studied are in Figures 10, 11, 12, 13, and 14.

Figure 10: The learned representation and grouping for the UCI Iris dataset

Figure 11: The learned representation and grouping for the UCI Boston Housing dataset

Figure 12: The learned representation and grouping for the UCI Heart Disease dataset

Figure 13: The learned representation and grouping for the single-cell RNA dataset

Figure 14: The learned representation and grouping for the synthetic dataset.

A.2. Pairwise Correctness and Coverage Plots

TGT is much better than DBM for finding 250-sparse explanations on the single-cell RNA dataset (Figures 15 and 16). On the synthetic dataset, TGT and DBM are equally effective explanations of the model (Figures 17 and 18). However, TGT only relied on the two causal variables while DBM included the correlated variable as well.

Figure 15: The pairwise metrics for TGT on the single-cell RNA dataset for 250-sparse explanations.

Figure 16: The pairwise metrics for DBM on the single-cell RNA dataset for 250-sparse explanations.

Figure 17: The pairwise metrics for TGT on the synthetic dataset with no sparsity constraint.

Figure 18: The pairwise metrics for DBM on the synthetic dataset with no sparsity constraint.

A.3. Qualitative Analysis of the UCI Datasets using the Labels

Although the representations we learned for these datasets were trained in an unsupervised manner, the groups that they find often have strong connections to the labels for the datasets; see Table 3, Figure 21, and Table 4. By using the connection between the groups and labels, we will be able to qualitatively assess whether or not TGT is finding real patterns in the data. Because all of the explanations are in terms of feature indices, we have included the mapping from feature index to feature name for each of our datasets in Table 2.

Table 2: The names of each of the figures in the datasets.

| Dataset Feature Name | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
|----------------------|---|---|---|---|---|---|---|---|---|---|----|----|----|
| Iris                 |   |   |   |   |   |   |   |   |   |   |    |    |    |
| Iris Dataset         |   |   |   |   |   |   |   |   |   |   |    |    |    |

Iris Dataset. Looking at Table 3, we can see that the groups in this representation match very closely with the class labels. As a result, we would like to know whether or not the explanations TGT finds are consistent with a model trained
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directly to predict the labels. For this comparison, we used a simple decision tree, which is shown in Figure 19. Looking at TGT’s explanations (Figure 20), we can see that they largely agree with the decision tree since both primarily use Petal Width to separate the classes/groups.

Table 3: The distribution of the labels per group for the UCI Iris dataset (classification).

| Group | Iris Setosa | Iris Versicolour | Iris Virginica |
|-------|-------------|-----------------|---------------|
| 0     | 6           | 44              | 48            |
| 1     | 5           | 122             | 0             |
| 2     | 381         | 0               | 0             |

Figure 19: A small decision tree trained on this dataset. Notice that it relies on the Petal Width feature.

Figure 20: TGT’s 1-sparse explanation of the difference between Group 0 and Group 1 (left) and Group 0 and Group 2 (right). Similar to the decision tree, they rely on the Petal Width feature.

Boston Housing Dataset. Looking at Figure 21, we can see that two comparisons between the groups stand out: Group 0 to Group 2, which shows a significant increase in the price, and Group 3 to Group 5, which has relatively little effect on the price. As a result, we would like to determine what the differences between these groups of houses are that influence their price.

Figure 21: The distribution of the labels per group for the UCI Boston Housing dataset (regression).

Looking at Figure 22, we see that TGT found that the key differences between Group 0 and Group 2 appears to be the difference between a house being in an urban area vs being in a suburb: the proportion of land zoned for large residential lots and B both increase while access to radial highways and tax rates both decrease. It also found that the key differences between Group 3 and Group 5 are, first, moving the house onto the Charles river and, second, decreasing B.

Figure 22: TGT’s 5-sparse explanation for Group 0 to Group 2 (Left) and Group 3 to Group 5 (right).

Heart Disease Dataset. Looking at Figure 4, we see that there are three large groups that stand out: Group 1, which has a balanced risk of heart disease, Group 3, which has a relatively low risk, and Group 6, which has a relatively high risk. As a result, we would like to determine what the differences between these groups of subjects are that influence their risk of heart disease.

Table 4: The distribution of the labels per group for the UCI Heart Disease dataset (classification).

| Group | No Heart Disease | Heart Disease |
|-------|------------------|---------------|
| 0     | 6                | 15            |
| 1     | 46               | 62            |
| 2     | 10               | 1             |
| 3     | 15               | 14            |
| 4     | 4                | 1             |
| 5     | 10               | 7             |
| 6     | 10               | 6             |
| 7     | 2                | 5             |

Looking at Figure 23, TGT found that the key differences between Group 1 and Group 3 are a moderate decrease in chest pain along with having exercised induced angina; these are subjects whose symptoms are explained by exercise induced angina rather than heart disease. It also found that the key difference between Group 1 and Group 6 is that Group 1 is made up of men while Group 6 is made up of women; this is consistent with the fact that heart disease is the leading cause of mortality in women (Bello & Mosca, 2004).

9This is a unusually defined feature that is related to the racial demographics of a town. Determining what it means to change this feature depends on a measurement that is not in the dataset.
A.4. Quantitative Analysis of Modified Versions of the UCI Datasets.

Because the UCI datasets are not synthetic datasets, we do not know the underlying process that generated the data and, as a result, it is difficult to quantitatively determine whether or not an explanation is “correct” in the way that we could with the synthetic dataset. Consequently, we performed a series of experiments on modified versions of the original datasets in order to answer two important questions:

- Does TGT correctly identify the modifications we made to the original dataset?
- Do TGT’s explanations between the original groups change when the modified group is added to the dataset?

We found that TGT does identify the modifications we made and that, in doing so, it does not significantly change the explanations between the original groups. Importantly, this result remains true even if we retrain the learned representation on the modified dataset. These results are a strong indicator that TGT is finding real patterns in the data.

How do we modify the datasets? We create a modified version of the original dataset by: picking one of the groups of points in the original dataset, modifying that group of points in some way, and adding that new modified group of points to the original dataset. We will call the original dataset $D$ and the modified dataset $D’$, where $D’ = D \cup G’$ and $G’$ is the modified version of some group of points $G$. The critical choice to make during this process is to determine what modification to apply to $G$ to get $G’$. We chose to add random noise to some of the features of the points in $G$ and used the following two criteria when defining this modification for a particular dataset:

- $G’$ should be approximately within the range/distribution of $D$.
- $r(G’)$ should form its own (approximately) distinct group. Intuitively, if $r(G’)$ does not form its own group, then $r$ thinks $G’$ is similar to some other group in the dataset and, as a result, we would not expect TGT to be able to explain the differences between $G’$ and that group of points.

The modifications we used are in Table 5.

| Dataset | Group Modified | Feature Index | Perturbation Applied |
|---------|----------------|---------------|----------------------|
| Iris    | 0              | 1             | -0.4 + Uniform(-0.1, 0.1) |
| Housing | 1              | 1             | 0.9 + Uniform(-0.1, 0.1) |
|         | 9              |               | -0.5 + Uniform(-0.1, 0.1) |
| Heart   | 1              | 6             | -0.9 + Uniform(-0.1, 0.1) |
|         | 8              |               | 0.6 + Uniform(-0.1, 0.1) |

Experimental Setup: We now have two versions of each dataset: $D$ and $D’$. We also have the original learned representation $r$, which was trained on $D$, and a new learned representation $r’$, which is trained on $D’$. As a result, we have three sets of explanations:

- **Original:** These explain $r$ when applied to $D$
- **Modified:** These explain $r$ when applied to $D’$
- **Retrained:** These explain $r’$ when applied to $D’$

The visualization of the representation for the first setting is in the Appendix A.1 and the later two these settings is in Figures 24, 25, and 26. Note that applying $r$ to $D’$ looks the same as applying $r$ to $D$ except for the fact that there is an additional group from adding $G’$ to $D$ and that applying $r’$ to $D’$ often shows that $r’$ has learned to separate $G’$ from the other groups better than $r$ did.

Figure 24: The learned representation for: $r$ applied to $D’$ (Left) and $r’$ applied to $D’$ (Right) for the Iris dataset

Figure 25: The learned representation for: $r$ applied to $D’$ (Left) and $r’$ applied to $D’$ (Right) for the Boston Housing dataset
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Figure 26: The learned representation for: $r$ applied to $D'$ (Left) and $r'$ applied to $D'$ (Right) for the Heart Disease dataset.

Does TGT correctly identify the modifications we made to the original dataset? In Figure Figures 27, 28, and 29, we can see the explanations TGT found for the difference between $G$ and $G'$ for each of the datasets. If we compare the explanations to the modifications from Table 5, we can see that they identified which features we changed and, approximately, by how much. The error in the estimation of “by how much” is due to the $l_1$ regularization used to find a simple explanation.

Figure 27: The Modified (Left) and Retrained (Right) explanation’s explanation for the difference between $G$ and $G'$ on the Iris dataset.

Figure 28: The Modified (Left) and Retrained (Right) explanation’s explanation for the difference between $G$ and $G'$ on the Boston Housing dataset.

Figure 29: The Modified (Left) and Retrained (Right) explanation’s explanation for the difference between $G$ and $G'$ on the Heart Disease dataset.

Do TGT’s explanations between the original groups change when the modified group is added to the dataset? In Figures 30, 31, and 32, we can see a comparison of the explanations for the differences between the original groups for the Original vs the Modified and the Original vs the Retrained explanations. Adding $G'$ to $D$ did not cause TGT to find significantly different explanations between the groups in $D$. Explaining $r'$ resulted in explanations that were generally similar, but adding another layer of variability (i.e., training $r'$) did add some noise.

Figure 30: The absolute difference between the Modified (Left)/Retrained (Right) explanations and the Original explanations scaled relative to the Original explanations on the Iris dataset.

Figure 31: The absolute difference between the Modified (Left)/Retrained (Right) explanations and the Original explanations scaled relative to the Original explanations on the Boston Housing dataset.

Figure 32: The absolute difference between the Modified (Left)/Retrained (Right) explanations and the Original explanations scaled relative to the Original explanations on the Heart Disease dataset.