In this paper, we present PIXAL, a visual analytics system designed to help an analyst with the task of anomaly reasoning. PIXAL is developed following an iterative design process with professional analysts responsible for anomaly detection. PIXAL is designed to fill gaps in existing tools commonly used by analysts to reason with and make sense of anomalies. PIXAL consists of three components: (1) an algorithm that finds patterns by aggregating multiple anomalous data points using first-order predicates, (2) a visualization tool that allows the analyst to build trust in the algorithmically-generated predicates by performing comparative and counterfactual analyses, and (3) a visualization tool that helps the analyst generate and validate hypotheses by exploring which features in the data most explain the anomalies. Finally, we present the results of a qualitative observational study with professional analysts. These results of the study indicate that PIXAL facilitates the anomaly reasoning process, allowing analysts to make sense of anomalies and generate hypotheses that are meaningful and actionable to business stakeholders.

Index Terms—Predicates, Actionable Hypotheses, Anomaly Detection, Explainable Machine Learning
following an iterative design process with professional data analysts whose jobs involve anomaly detection, reasoning, and reporting. Based on the interviews and the feedback from the analysts, PIXAL is designed with three requirements in mind. First, an anomaly reasoning tool must help an analyst organize and make sense of the collection of anomalous data points. Second, the anomaly reasoning tool must assist the analyst in building trust in the found anomalies. Lastly, the anomaly reasoning tool must enable the analyst in reporting their findings to the business stakeholders and decision makers such that they can take meaningful actions.

To fulfill these design requirements, PIXAL consists of three components. The first is the recursive predicate induction (RPI) algorithm for discovering groupings of anomalous data points. Similar to a regression tree [27], the RPI algorithm takes data points and their assigned anomaly scores and outputs groupings of these points. In particular, the RPI algorithm expresses these groupings as first-order predicates (e.g., \( \text{city} = \text{"Boston"} \) \& (\( \text{precipitation} > 7.6 \)) \& (\( \text{month} \in [\text{Nov, Dec, Jan}] \)), and has two unique properties that can aid anomaly reasoning. First, the RPI algorithm can return multiple groups of anomalies (as predicates) that may overlap the same data points. Having access to different groupings can help analysts reason about how anomalies might be related to multiple different underlying phenomena. Second, the RPI algorithm provides the likelihood that data points in grouping have high anomaly scores. Comparing the data points in a grouping to the rest of the data with a Bayesian t-test [39] produces a Bayes factor corresponding to the degree of evidence that each predicate contains anomalies.

The second component of PIXAL is the PixalExplorer tool that allows analysts to fine-tune and build trust in the predicates generated by the RPI algorithm. At its core, PixalExplorer is an engine that can visualize any first-order predicate as a histogram that shows the distribution of anomaly scores for the data points it contains. Analysts can make modifications to a predicate produced by the RPI algorithm to perform counterfactual analyses, superimpose two or more predicates to make comparisons, or refine the predicate to better reflect their domain knowledge. PixalExplorer provides an interface that supports the analyst in specifying and managing the predicates, and GUI elements (such as sliders) to reduce the burden of repetitive typing during the analysis.

Finally, the third component of PIXAL is Pixalate, a visualization tool to help analysts generate hypotheses about observed anomalies that can be used in a report for business stakeholders and decision makers. Pixalate assists the analyst in making sense of anomaly scores. Rather than reporting predicates directly, which can describe similar data points with high anomaly scores but not why their anomaly scores are high, analysts can use Pixalate to produce reports with higher-level semantic meaning. For example, for the predicate \( \text{city} = \text{"Boston"} \) \& (\( \text{precipitation} > 7.6 \)) \& (\( \text{month} \in [\text{Nov, Dec, Jan}] \)), using Pixalate a business analyst might find that the anomaly highly correlates with a decrease in sales and deduce that the anomalies are likely due to slow sales during winter storms in Boston.

We describe prior research in explainable anomaly detection and visual analytics related to our work.

### 2.1 Anomaly Detection and Explanation

Anomaly detection algorithms typically output anomaly scores that indicate how anomalous each instance is, then classify any instance with an anomaly score above a set threshold as an anomaly. Although the specific methods differ, all of these algorithms aim to measure the degree to which each data point deviates from the rest of the data. For example, the local outlier factor algorithm [8] calculates an isolation score for each instance, and has two unique properties that can aid anomaly reasoning. First, the RPI algorithm can return multiple groups of anomalies (as predicates) that may overlap the same data points. Having access to different groupings can help analysts reason about how anomalies might be related to multiple different underlying phenomena. Second, the RPI algorithm provides the likelihood that data points in grouping have high anomaly scores. Comparing the data points in a grouping to the rest of the data with a Bayesian t-test [39] produces a Bayes factor corresponding to the degree of evidence that each predicate contains anomalies.

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To evaluate the effectiveness of PIXAL in supporting analysts’ anomaly reasoning, we conducted an interview study with three professional data analysts whose jobs involve anomaly detection. The analysts reported that they found PIXAL to be effective in facilitating reasoning and hypothesis-generation, suggesting the potential of PIXAL as a tool for helping them perform anomaly reasoning with real-world problems. In summary, our work on PIXAL makes the following contributions:

- We introduce PIXAL, a visual analytics system that supports anomaly reasoning.
- PIXAL consists of three integrated components that together help analysts aggregate and refine anomalous data points into higher-level, semantically meaningful reports.
- We conducted an interview study with three professional data analysts who validated the effectiveness of PIXAL.

# 2 Related Work

We describe prior research in explainable anomaly detection and visual analytics related to our work.
on a particular instance. LIME [38] generates local explanations for individual predictions by approximating a model’s decision function with an explainable model trained on a local subspaces. The advantage of local-explanation approaches is that it can help an analyst detect and diagnose a failure point – for example, identifying an erroneous feature in an ML model or a bad actor in social-network analysis. However, conversely local-explanation approaches are less effective in helping analysts with higher-level reasoning. In cases where the analyst needs to understand a phenomenon or a reason behind the anomalies, global-explanation approaches may be more appropriate. For example, TrafficAV [17] combines network traffic analysis with a decision tree model to detect malware behavior in network traffic generated by mobile applications. This system generates feature weights that explain the characteristics of each family of malware. A similar approach is taken by Carletti et al. [11] which generates weights to explain which features contribute to anomaly scores assigned by the commonly used isolation forest algorithm. Nguyen et al. [34] propose a method for generating global explanations of a variational autoencoder for anomaly detection. Their approach applies a gradient-based fingerprinting technique that explains which features contribute to anomalies for various kinds of attacks.

Our proposed PIXAL system shares the same design goal with global-explanation approaches. However, instead of relying on automated machine learning that is devoid of human judgement and domain knowledge, our visual analytics approach is designed to keep the analyst in control so that they can discover the global explanations that are relevant and meaningful to their domain and analysis context.

### 2.2 Visual Analytics for Anomaly Detection and Analysis

The visual analytics community has a long history in the research and development of systems for anomaly detection, dating back the original visual analytics research agenda proposed by Thomas and Cook [45] and Keim et al. [23]. However, most of these visual analytics systems have been designed to help analysts detect anomalies and outliers (e.g., in fraud detection [14][25][29] and network security monitoring [20][22][35]), or inspect machine learning models to improve detection accuracy, reduce false positives, debug models, etc. [15][21][45]. Few systems exist that directly support the analyst in discovering the potential reasons behind the anomalies and reporting the findings to business stakeholders and decision makers.

Some notable exceptions include the S itu system [19], which provides cyber network analysts with a contextual understanding of suspicious behaviors to aid in decision making. Similar to our design, Situ also utilizes unsupervised anomaly detection algorithms for identifying potential suspicious data and provides analysts with an interactive interface to make sense of the anomalies. Where our approach differs is that our system automatically generates potential explanations, thus reducing the analysts’ need to synthesize the anomalies to gain the contextual understanding.

Other visual analytics systems exist for helping analysts explore and gain insight into the characteristics of data, which inevitably includes detecting and discovering outliers. Examples include systems in the domains of space-time and trajectories analysis (e.g., [34][20][31]), network security (e.g., [52][53][55] and surveys by Shiravi et al. [44] and Zhang et al. [54]), and systems such as Voila [9] – used in urban development scenarios – and TargetVue [10] – used in social media analysis – that can help an analyst discover suspicious behavior in dynamic and heterogeneous data by comparing current event sequences to statistical models of previously observed data.

Similar to S itu, most of these examples are designed for specific domains. Further, they emphasize fluid data exploration but often lack support to assist an analyst in reasoning about anomalies and reporting the findings. PIXAL differs from the prior work in that it is designed to be domain-agnostic and focuses specifically on anomaly reasoning and reporting. In the next section, we describe the challenges and design requirements for a visual analytics system designed for anomaly reasoning.

### 3 Design Requirements and Motivation

The design of PIXAL is inspired and informed by interviews with five professional data analysts at an (automotive) insurance company and one analyst in the health care industry. All analysts have jobs that involve anomaly detection and reporting. Each of the interviews lasted 30 minutes and was conducted over video conferencing due to COVID-19 restrictions. During the interviews, participants were asked to describe their duties, problems that they frequently face, and tools or techniques that they commonly use for their tasks.

#### 3.1 Analysts’ Workflow and Practice

All six analysts describe a similar anomaly detection workflow. First, most (5 out of 6) analysts use off-the-shelf machine learning techniques to detect anomalies in their data (with one analyst using custom queries and scripts). The analysts then manually inspect the resulting anomalous data points, sometimes with the use of visualizations and additional machine learning techniques (e.g., clustering). All analysts reported exploring data in detail within Jupyter notebooks, or similar interactive programming environments. These environments allow a number of useful operations, including generating statistical summaries, filtering, and visualization. Most (4 out of 6) analysts also reported using commercial data exploration tools, like Tableau or Qlik, for investigating data. Ultimately, all analysts report that their goal with anomaly detection is to discover patterns that are generalizable and can be reported to their managers or business stakeholders. In their experience, reporting individual anomalous data points is not useful in practice because the managers and stakeholders cannot take meaningful actions without some higher-level explanation of the anomalies.

#### 3.2 Gaps and Needs in the Workflow

Across all the steps in the analysts’ workflow, the analysts report three tasks that are the least supported and therefore most burdensome. First, the analysts describe the need to organize the anomalous data points (found by the anomaly detection algorithms) into meaningful groupings. Analysts report that grouping similar anomalies together helps them to formulate hypotheses about the root causes of the anomalies. However, this process is time-consuming because there can be nearly infinite ways to group and interpret the data. The analysts need to explore these groupings through a series of trials-and-errors before finding the most meaningful groupings.

Second, the analysts discuss the need to manually inspect the outputs of the automated anomaly detection algorithms. The purpose of the inspection is two-fold: (1) the analysts note that anomaly detection algorithms lack domain knowledge. Sometimes flagging a data point as anomalous is accurate from an algorithmic standpoint, but would be inappropriate given the domain context (and vice versa). Resolving such ambiguities requires human knowledge and domain expertise. (2) Through the inspection process, the analyst can build trust and confidence in the found anomalies. No analysts in our interviews felt comfortable reporting the outputs of an anomaly detection algorithm without inspecting the results first. Analysts currently rely on manual programming in tools such as Jupiter notebooks to inspect the data. Integrated support for comparing groups of anomalies that combines visualization with scripting will greatly reduce the analysts’ effort when inspecting and building trust in their data.

Lastly, all analysts note the difficulty in producing reports for stakeholders and decision makers. Since stakeholders and decision makers are often not savvy in data science, they require explanations at a higher semantic level that are not just statistical probabilities, distributions, and p-values. Producing these high-level explanations is difficult because these reports need to be connected to business logic, the explanations need to be human-readable, and there needs to be intuitively understandable evidence to support the findings. Currently there is no tool that can support the analysts in this report-preparation task and each analyst completes this step in their own ad hoc fashion.

#### 3.3 Design Requirements

Our interviews with the analysts highlighted the current technology gaps in supporting their anomaly reasoning and reporting tasks. Based
on the feedback from the analysts, we summarize the currently unsupported tasks into three design requirements. We assert that a visual analytics system for anomaly reasoning must support these requirements:

(R1) Organize: The system must support an analyst in organizing anomaly data points found by a detection algorithm. Ideally the system can suggest multiple and diverse organizations that might suggest possible reasons behind the anomalies.

(R2) Inspect, Refine, and Build Trust: The system must support the analyst in building trust in the found anomalies by allowing the analyst to inspect and refine the anomalies.

(R3) Report: The system must support the analyst in discovering higher-level explanations of the anomalies such that these findings can be reported to stakeholders and decision-makers who might not be savvy in data science.

4 PIXAL System Overview

There are three components to PIXAL. Each component addresses one of the three design requirements, which are: (R1) the RPI algorithm: an algorithm for automatically grouping anomalous data points into meaningful groupings, (R2) PixalExplorer: a visualization tool for supporting an analyst in inspecting and building trust in the found anomalies, and (R3) Pixalate: a visualization tool for helping an analyst generate hypotheses and a report of their findings.

Figure 2 shows a high-level overview of how PIXAL supports an analyst’s workflow. Prior to using PIXAL, an analyst would run an anomaly detection algorithm over the input data, resulting in an anomaly score for each of the data points. PIXAL is agnostic to the specific algorithm used to generate the scores and can accept anomaly scores as either numeric values or binary labels.

The RPI algorithm takes the data points and the accompanying anomaly scores as input and generates groupings of anomalies. The groupings are represented using first-order predicate logic. An important property of the RPI algorithm is that it can generate multiple and possibly overlapping predicates, which can be used by analysts to explore different plausible reasons behind the anomalies.

Second, the PixalExplorer visualization takes the (multiple) predicates generated by the RPI algorithm and allows the analyst to inspect, explore, select, and refine them. PixalExplorer provides visualizations and interaction techniques that support the analyst in performing counter-factual and comparative analyses to assess and build trust in the predicates. Irrelevant or meaningless predicates can be discarded during this process while potentially interesting predicates can be fine-tuned and examined in more detail.

The output of PixalExplorer is a set of “verified” predicates, which the Pixalate visualization tool takes as input. As these predicates only describe what data points are included in the predicate (i.e., the what), the purpose of Pixalate is to help the analyst discover the possible reasons behind these anomalies (i.e., the why). In addition to helping the analyst test hypotheses, Pixalate can be used to create reports that are suitable for a stakeholder or a decision-maker who might not have expertise in data science.

In the following sections we describe each of the components in more detail.

5 Recursive Predicate Induction Algorithm

Conceptually the recursive predicate induction (RPI) algorithm is similar to that of a decision tree (for discrete labels) or a regression tree (for real values) in that it is meant to generate “human readable” groupings of (anomalous) data points. In order to support anomaly reasoning, the RPI algorithm uses two interlocked processes to generate groupings.

5.1 Generating Multiple Anomaly Groupings

Inspired by systems like Scorpion [50], DIFF [1], iDiff [41], Slice Finder [17], and the Cascading Analysts Algorithm [40], RPI algorithm uses first-order predicate logic to represent groupings of anomalous data. The idea is to recursively partition the data using values along the data dimension as “split points.” However, instead of having one split point per decision level as decision trees or regression trees, the use of predicates allows for “partitioning” along the dimensions, resulting in first-order features such as \(10 < \text{var} < 20\) or \(\text{id} \in [1, 3, 10]\). When recursively applied, the features produced by our algorithm form a predicate \(p\): a union of \(k\) first-order features:

\[ p = \bigcup_{i=1}^{k} \{ f_i \} \]  

The RPI algorithm follows a bottom-up recursive process similar to Slice Finder [17]. Specifically, the algorithm starts with initializing \(n = \sum_{i=0}^{d} b_i \) “base predicates”, where \(d\) is the number of data dimensions and \(b_i\) is the cardinality of the data dimension \(i\) if it contains categorical data and number of bins if it contains numeric values (note: bin size is a hyperparameter of the algorithm). At each step of the recursion, a predicate \(p\) is expanded to include another base predicate, resulting in a new predicate \(p'\). The Bayesian hypothesis score (see next Section, 5.2 for detail) is calculated for both \(p\) and \(p'\). If \(p'\) has a better score than \(p\), \(p\) is replaced with \(p'\) and the recursion continues. Otherwise \(p\) joins with another base predicate and is reevaluated. If \(p\) cannot be improved further, \(p\) is returned.

For optimization, all \(n\) base predicates are expanded in parallel. After each step of the recursion, all predicates are considered for merging if two predicates are the same (e.g., \(p_1 = \{f_a, f_b\}\) is the same as \(p_2 = \{f_a, f_b\}\) since the features in a conjunctive first-order predicate are order invariant).

5.2 Bayesian Hypothesis Testing

Given a predicate \(p\), the purpose of Bayesian hypothesis testing is to determine if \(p\) describes a subset of data that is statistically significantly more anomalous than the rest of the data. Conceptually, this can be described as a function \(g\):

\[ K = g(D, p(D)) \]  

where \(p(D)\) represents the subset of data instances that satisfy the predicate \(p\) as it is applied over the dataset \(D\). The metric – if it is greater than some threshold, \(p(D)\) will be considered to be significantly more anomalous than \(D\). With Bayesian hypothesis testing, \(K\) is formally defined as:

\[ K = \Pr(D|H_1) \Pr(D|H_0) \]  

where \(D\) is a set consisting of both the full dataset \(D\) and the subset of data \(p(D)\) such that \(D = \{D, p(D)\}\). \(H_1\) is the null hypothesis that the subset \(p(D)\) is not different from the rest of the data \(D\), and \(H_1\) is the alternative hypothesis (that \(p(D)\) is different from \(D\)).

\(K\), as expressed in Equation 3, is commonly referred to as the Bayes factor [23]. Since \(K\) represents the odds, or the likelihood ratio of the (marginal) likelihood of the two competing hypotheses, the values of Bayes factors are consistent in that they are invariant to differences in the definition of anomaly score. As such, there is a universal interpretation of the values of \(K\). \(K\) less than 0.3 suggests no or bare evidence for the alternative hypothesis (\(H_1\)). Values between 3.2 and 10 suggest substantial evidence; 10 to 100 is strong evidence; and \(K > 100\) is decisive evidence [22]. Compared to traditional hypothesis testing (such as \(p\)-values used in Slice Finder [17]), Bayes factors can express evidence to different degrees beyond just an accept/reject threshold.

In the RPI algorithm, we compute Equation 3 using the JZS Bayes factor introduced by Rouder et al. [39], which has been implemented as a library available in R. For the full definition of the JZS Bayes factor as a Bayesian hypothesis test, we refer to Equation 1 in the work by Rouder et al. [39] (p. 231).

In the context of anomaly reasoning, we note a number of benefits using the Bayes factor for determining the similarities between subsets of data. First, higher values of \(K\) represent more confidence in the explanation (that \(D\) and \(p(D)\) are different in their degrees of anomalousness). Second, the range of values of \(K\) is consistent and

**Note:** For the full citation, please refer to the original paper or the provided bibliographic entry. See the snippet for more details.
invariant to the size or complexity of the data \( D \). Lastly, \( K \) increases not just as the average anomaly score in \( p(D) \) increases but also as the number of data points in \( p(D) \) increases. This follows from the intuition that the more anomalous data points a grouping contains the more confidence we should have that the grouping is meaningful.

### 5.3 Practicabilities

In addition to the benefits of Bayes factors, the other advantages of the RPI algorithm over other grouping algorithms is that the RPI algorithm provides the analyst with multiple overlapping groupings for the same data points. However, being able to generate multiple overlapping groupings requires taking a recursive approach to searching the space of possible predicates rather than greedily maximizing Bayes factor. While the RPI algorithm only takes approximately 10 seconds to run on small datasets (10k rows and 10 dimensions), larger datasets (100k rows, 30 dimensions) can take 20+ minutes, while large datasets (1 million rows, 100 dimensions) can take hours to complete. The potentially long running time means that in practice the RPI algorithm is best suited for online computation. We discuss the use of the RPI algorithm in an interactive visual analytics environment further in the Discussion Section (Section 10.2).

### 6 PixalExplorer

The output of the RPI algorithm is a set of predicates and their associated evidence scores (\( K \)). With PixalExplorer, an analyst can examine these predicates in more detail. The analyst can inspect each predicate, discard a predicate, (manually) generate new predicates, or refine (edit) an existing predicate. These operations allow the analyst to perform counter-factual (i.e., “what-if”) analyses and comparisons between predicates to produce the final predicates for the reporting phase.

As shown in Figure 3, PixalExplorer is a visualization tool that can render any first-order predicate (based on the input data) as a distribution in a histogram. The y-axis of the histogram represents count and the x-axis the range of the anomaly scores. Multiple predicates can be visualized at the same time using different colors, allowing for superpositional comparisons of the predicates’ distributions.

**Predicate Editing and Refinement:** An analyst can manipulate a predicate in multiple ways. First, a text box (shown in Figure 4) allows the analyst to type in a predicate manually or select an existing predicate and edit its string representation. Alternatively, the analyst can use the GUI elements supported by PixalExplorer to simplify the process. For example, a slider is provided for modifying the ranges of a numeric feature in a predicate, and a dropdown menu for adding or removing values of a categorical feature. Not only do these GUI elements reduce the editing effort, they allow an analyst to quickly perform counter-factual analysis – trying out different value ranges and observing the changes in the visualization interactively.

**Predicate Management:** To aid the analyst in exploring and analyzing multiple predicates, PixalExplorer provides tools to help manage the (potentially many) predicates. Figure 5 shows the panel where the analyst can hide a predicate, remove a predicate from the visualization, change the color of the predicate in the visualization, clone a predicate (to allow for experimentation), delete a predicate, and take the complement of a predicate (i.e., to select the data subset \( D \setminus p(D) \)) from Equation 2. After the analyst has completed their inspection and is satisfied with the final set of predicates, they can export the predicates for use in the next tool, Pixilate.

### 7 Pixilate

The final step of the anomaly reasoning process is for an analyst to come up with hypotheses about the cause of anomalies and prepare a report for a stakeholder or decision maker. Since stakeholders and decision makers are not always well versed in data science, the report needs to provide high-level explanations of the anomalies that the decision makers can relate to.

In order to support an analyst in generating such reports, Pixilate must support the analyst in two tasks. First, the analyst must be able to identify the “why” behind the anomalies that is meaningful to the stakeholder or decision maker. Second, for each of the possible explanations, the analyst must be able to provide the evidence to support the finding. Together, the “why” and its accompanying evidence form a hypothesis about the potential reasoning behind the anomalies that a decision maker can act on. During the reporting process, an analyst often include multiple plausible hypotheses in their reports.

Figure 6 illustrates the visualization interface of Pixilate to support these two tasks. It consists of five panels, which we describe below.

**Predicates View (Panel A):** This view lists all the predicates produced by PixalExplorer. The predicates are sorted by their evidence scores. To begin the investigation and start forming hypotheses, the analyst selects a predicate in this panel, which will update all the subsequent views.

**Distribution View (Panel B):** This view provides a visual confirmation of the distribution of the selected predicate. The Distribution View is the same as the histogram view in PixalExplorer except that it only shows two distributions. The blue distribution represents the selected predicate (i.e., \( p(D) \) in Equation 2) and the grey distribution its complement (i.e., \( (D \setminus p(D)) \)).

**Pivot View (Panel C).** The purpose of the Pivot View is to support the analyst in investigating each of the features in a predicate in more detail (see Equation 1). For example, given a predicate \( \langle \text{locationId} = \text{’location5’} \rangle \land \langle \text{sensorId} \in \{\text{’sensor4’, ’sensor5’, ’sensor7’}\} \land \langle \text{voltage} > 80 \rangle \rangle \), the analyst can pivot on the locationId, the sensorId, or the voltage feature. Pivoting on the locationId feature results in a barchart visualization where each bar represents a location id in the data (with the bar for ‘location5’ shown in blue, see Figure 4b). The y-axis of the barchart represents the average anomaly score.

Importantly, the height of each bar is only based on the subset of the data selected by the predicate. For example, the bar representing the locationId ‘location5’ is based on the data selected with the predicate \( \langle \text{sensorId} \in \{\text{’sensor4’, ’sensor5’, ’sensor7’}\} \land \langle \text{voltage} > 80 \rangle \rangle \). In this sense, the features not selected as the pivot come up with hypotheses about the cause of anomalies and prepare a report for a stakeholder or decision maker. Since stakeholders and decision makers are not always well versed in data science, the report needs to provide high-level explanations of the anomalies that the decision makers can relate to.

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**Exploration View (Panel D):** Once the analyst selects a pivot, the exploration view shows the detail of this selection and allows the analyst to explore further. Inspired by visualization systems such as Tableau [44] and Polestar [49], with the Exploration View the analyst can select different visualization encoding (e.g., change the x or y-axes, the mark type, the colors, or the filters). Initially the Exploration View defaults to using anomaly score as the y-axis – the same as the visualization shown in the Pivot View. As the analyst explores different attributes for the y-axis, they can identify possible reasons that make the predicate anomalous. For example, in Figure 6 the selected pivot in the Pivot View (Panel C) shows that the bars representing ‘sensor4’, ‘sensor5’, and ‘sensor7’ (shown in blue)
have significantly higher anomaly scores than the other sensors. In the Exploration View (Panel D), the analyst has changed the y-axis to temperature. From this visualization, the analyst observes that all three sensors have higher values in temperature, suggesting that the reason for the high anomaly scores for this predicate may be due to increased ambient temperature.

Lastly, the analyst can bookmark a visualization. The visualization can be exported later as the supporting evidence of the analyst’s finding.

**Recommendation View (Panel E):** While the Exploration View supports the analyst in manual exploration, the Recommendation View automatically generates possible reasons for the anomalies in a predicate. These recommendations are generated by computing the correlation between the anomaly scores of a predicate (given a pivot) and the attributes in the input data. Attributes that correlate with anomaly scores (where the correlation coefficient is above .3) are added to the list of recommendations.

The recommendations are presented as both a natural language sentence and a visualization. The natural language sentence is generated using a simple grammar that converts a first-order predicate into a sentence. For example, the recommendation “Average humidity is high when locationID is location5 compared to other locationID’s when sensorID is sensor4, sensor5, and sensor7 and voltage is greater than 80” corresponds to the predicate: \( (\text{locationID} = \text{location5}) \land (\text{sensorID} \in \{\text{sensor4}, \text{sensor5}, \text{sensor7}\}) \land (\text{voltage} > 80) \) with the pivot on the LocationID feature and the attribute Temperature as the possible reason recommended by Pixalate for the anomalies in the predicate.

When an analyst clicks on a recommendation, the visualization will be displayed in the Exploration View for further examination and can be bookmarked for later exportation into a report.

**8 Usage Scenario**

We describe our tool with a usage scenario, where an analyst uses Pixal to reason about anomalies in a sales dataset. The dataset used in this scenario is modified from the “Superstore Sales” dataset included with Tableau Desktop (version 2020.4). Each row in the dataset includes the Sub-Category of product sold (e.g., Furniture, Office Supplies), the State it was sold in, the customer Segment (e.g., Consumer, Home Office), Order Date, the Quantity of the product being sold, and the Unit-Price and Unit-Cost of the product being sold. Additionally, the data includes the average temperature and Precipitation on the sales date. In this scenario, an analyst has been tasked by Superstore executives with identifying and reporting anomalous phenomenon in the sales dataset.

The analysts begin by generating anomaly scores for the dataset. The popular open source Python library Scikit-learn includes a number of anomaly detection algorithms, including the isolation forest (iForest) algorithm. Understanding that the Superstore executives will be primarily interested in sales related anomalies (i.e., Quantity, Unit-Price, and Unit-Cost), the analyst runs the iForest algorithm on these features, which then assigns each row in the data an anomaly score.

Next, the analyst imports the Superstore data and the assigned anomaly scores into the RPI algorithm, which produces 7 predicates (ranked by their evidence scores from high to low):

1. Sub-Category in ['Tables']
2. Sub-Category in ['Machines']
3. Sub-Category in ['Copiers']
4. State in ['New York', 'Massachusetts', 'New Hampshire'] & Segment in ['Consumer', 'Home Office'] & 2016-11-8 < Order Date < 2017-1-21
5. 2.74 < precipitation < 4.59 & -0.09 < Temperature < 36.36 & Segment in ['Consumer', 'Home Office']
6. 2016-11-8 < Order Date < 2017-1-21 & State = 'Vermont'
7. State = 'Vermont' & Segment = 'Corporate'

**8.1 Discovering Business Logic**

The analyst notices that the top three ranked predicates are all related to product Sub-Category. This is consistent with the analyst's understanding that the Sub-Category of the product being sold will have a significant effect on the Quantity, Unit-Price, and Unit-Cost. The analyst visualizes the similarities between them, the analyst decides to visualize the three predicates together. Using the text editor in PixalExplorer, the analyst manually types in a new predicate by combining the three, resulting in:

8. Sub-Category in ['Tables', 'Machines', 'Copiers']

The analyst can now see the complete distribution of anomaly scores for the three Sub-Categories together. To verify that this predicate is indeed anomalous, the analyst compares this predicate against the rest of the data. The analyst completes this goal by first cloning predicate 8, and clicking on the “NOT” button in the panel, resulting in a new predicate:

9. NOT(Sub-Category in ['Tables', 'Machines', 'Copiers'])

Figure 5 shows the analyst’s superposition of predicates 8 and 9 to compare their differences. From this visualization, the analyst can see that Machines, Copiers, and Tables (shown in orange) tend to have higher anomaly scores when compared to all other Sub-Categories (shown in blue).

To understand the potential reason behind this anomaly, the analyst copies predicate 8 and opens it in Pixalate. First, the analyst confirms with the Distribution View that anomaly scores are high for Tables, Machines, and Copiers compared to other Sub-Categories. Turning to the Recommendation View, the analyst sees from the visualization and the text description that Unit-Cost and Unit-Price are both higher for Copiers, Machines, and Tables compared to other Sub-Categories.
4, resulting in: Temperature these visualizations in Pixalate and includes them in their report. Segments is also found to be anomalous. This observation gives the mation that high Precipitation are likely due to winter storms with high and low and New Hampshire during the dates between November and January eresis that the decreased sales together with the previous finding, the analyst begins to form the hypoth- mendations that suggest that other states (between the State and Order-Date) will need to be examined closely.

Turning to Pixalate, the analyst first examines the State and then the Order-Date features of predicate 4 in the Pivot View. When piv- oting on State, the analyst observes a recommendation in the Recom- mendation View (see Figure 5) that suggests that the sales Quantity in New York, Massachusetts, and New Hampshire are lower compared to other states (between the Order-Dates 2016-11-8 and 2017-1-21, and in the Consumer and Home Office Segments).

When pivoting on Order-Date, the analyst observes two recom- mendations that suggest that Precipitation values are higher and the Temperature values are lower during the period of interest. To- gether with the previous finding, the analyst begins to form the hypothe- sis that the decreased sales Quantity in New York, Massachusetts, and New Hampshire during the dates between November and January are likely due to winter storms with high Precipitation and low Temperature.

Interestingly, looking ahead at predicate 5, the analyst sees the confirma- tion that high Precipitation and low Temperature of the same Segments is also found to be anomalous. This observation gives the analyst increased confidence in their finding. The analyst bookmarks these visualizations in Pixalate and includes them in their report.

9 Interview Study
We performed an interview study to evaluate the effectiveness of PIXAL in helping data analysts solve anomaly reasoning tasks.

Participants: We recruited three professional data analysts to partici- pate in this interview study. All three participants had experience with anomaly detection as part of their job duties. Two of the analysts work for health care companies, with one of the two having also participated in the initial set of interviews (see Section 8.1). The third analyst works as a data scientist for an academic institution.

Procedure: We walked each participant through a scenario where an analyst uses PIXAL to reason about anomalies in a sales dataset and reports their findings to decision makers. After introducing the dataset, we demonstrated the use of PIXAL on the scenario described in Section 8. The participants were encouraged to ask questions and direct the exploration process in the style of pair-analytics.

Following the tasks each participant was interviewed to provide feed- back on the usability of the tool, comparison to traditional anomaly detection workflows, and how well the explanations generated using PIXAL could be used to communicate to decision makers. Each of these studies lasted 60 minutes and was conducted over video confer- ence due to COVID-19 considerations. With the consent of participants, videos of the interviews were recorded.

9.1 Study Result
We reviewed the qualitative feedback from the interviews and distilled them into six main findings. These findings are grouped by how well PIXAL supports the three design requirements (Section 3.3).

R1 (Organize): Generating Anomaly Groupings: Two out of the three participants agreed that analyzing groups of anomalies is usually preferred over analyzing single anomalies: “Individual anomalies happen frequently and do not necessarily correspond to a persistent issue in the system.” “Someone who is really interested in the data might still investigate individual data points, but predicates will be sufficient for understanding the high-level context in most cases.”

R1 (Organize): Benefits of Multiple Predicates: In addition to bringing focus to persistent groups of anomalies, two out of three partici- pants noted that predicates also have the advantage of being easy to understand: “Understanding the data as predicates instead of the raw data makes it a lot easier to consume, even for someone who knows what they’re looking for.” “The predicates seem flexible and easy to understand. You’re really just talking about grouping with different features.”

All three participants agreed that generating multiple predicates helped with anomaly reasoning: “When we’re trying to explain a group of anomalies we test a collection of hypotheses, having multiple pred- icates lets you compare multiple different classes of anomaly types.” “Anomalies often occur as part of a convoluted chain of events. Multiple

Fig. 5: An analyst compares predicate 8 (orange) and its complement predicate 9 (blue). Observing that anomaly scores are generally higher in predicate 8, they are able to confirm that this predicate contains anomalies and is worth further investigation.

Fig. 6: This figure shows an analysis of a predicate with multiple features using Pixalate. Examining the feature relating to State as the pivot, an analyst identifies the increased Quantity in sales as a potential cause of anomalies in the Recommendation View.
by a human image, but determining what exactly makes it abnormal must be done lyists to reason about hypotheses: “To determine what the anomaly is from an anomaly detection algorithm: “More than individual anomaly points. In particular, one participant in the Two of the three participants R3 (Report): Hypothesis Generation: All the three participants found that the tools provided by PIXAL helped them generate hypotheses in our case study: “PIXAL highlighted three states as anomalous, New York, Massachusetts, and New Jersey. Knowing that anomalies also frequently occur when there is high precipitation and low temperatures, it’s likely that weather in those states in that time period caused a decrease in sales. If we can anticipate this type of weather in the future we could propose a 10% off sale either for specific products or for online orders.” This tool made it easy to reason about how a snowstorm on the upper east coast could be causing anomalies by interfering with sales.”

R3 (Report): Recommendations: All three participants found the recommendations to be useful: “The recommended text and plots work well together. You can quickly compare anomalies to normal data by reading the text and get a better sense of magnitude and overall pattern by looking at the plot.” In particular, participants found the text generated by PIXAL useful for explaining anomalies: “An analyst might not be satisfied by a statistically fragile summary like average quantity, but usually this would be sufficient for reporting purposes.” They also found the visualizations generated by PIXAL useful for explaining anomalies: “The plots help you quickly identify patterns and understand which features might be contributing to anomalies.”

Summary Feedback: All three participants stated that PIXAL would help them reason about anomalies in their job function: “This seems like it would free up a lot of time usually spent digging into individual data points. Even if you are not looking for any particular anomalies this seems like a wonderful tool for exploratory data analysis.” “Pathologists need to be able to report what exactly is occurring that caused a section of an image to be flagged as abnormal. This system could help quickly identify patterns and understand which features might be contributing to anomalies.”

Suggestions for Improvement: Overall, the participants were enthusiastic about the design of PIXAL. When asked about whether there are opportunities for improvement, one suggested a minor feature in the ability to export multiple bookmarks in the same report. Another participant suggested that additional features in PIXAL could help an analyst better identify useful patterns in the anomalies: “The plots generated by PIXAL could include additional features to highlight patterns in anomalies. For example, the reordering the x-axis so that anomalies are grouped together could help highlight differences between them and the normal data.”

10 Discussions and Design Implications

The overall evaluation of PIXAL was very positive. The participants’ feedback suggests that this design of PIXAL can effectively support analysts in performing anomaly reasoning. As PIXAL is developed following an iterative design process, there were prototypes that were not met with similar enthusiasm by during evaluation. In this section we describe two of the lessons learned and the design principles that we distilled from the experience.

10.1 Anomaly Reasoning as a Sensemaking Process

From our interviews with the analysts and our observations of the participants interactions with PIXAL, we posit that the analysts’ process of anomaly reasoning resembles the Sensemaking model proposed by Pirolli and Card [56]. Similar to Sensemaking, anomaly reasoning starts with a large amount of disorganized data. Through the Foraging Loop involving inspection, exploration, refinement, the analyst develops groupings of the anomalies. The analyst then undergoes the Sensemaking Loop in which they develop mental models and hypotheses about the observed anomalies. The process completes when the analyst produces a report (i.e. presentation) that tells a story about the anomalies to stakeholders and decision makers.

The outputs from each component of PIXAL (see Figure 2) also correlate to the amount of Structure in the Sensemaking model. The initial inputs to PIXAL (i.e., the set of data points and their anomaly
When constructing the predicates, the analyst was also able to terminate work. In the context of anomaly reasoning, we explore the potential pitfalls of progressive visualization and steerally exhibit biases when generating the predicates. If an analyst had sometimes led them into making rushed and incorrect choices. Forcing the participants to make such decisions in real-time, the participants were often unable to or were uncertain about how to steer the search spaces early.

In the mixed-initiative approach for an analyst to generate predicates, the left panel provides an analyst with a variety of ways to "steer" the computation, which analysts found difficult to use. The similarity between the anomaly reasoning and the Sensemaking processes suggests a potential commonality in the design process. We leave the confirmation and validation of this observation for future work.

10.2 Mixed-Initiative Anomaly Reasoning Considered Harmful

During our iterative design process we designed a prototype mixed-initiative visual analytics system for anomaly reasoning. However, our evaluation with professional data analysts suggested that this approach could be potentially harmful. In this prototypes, analysts were able to steer the predicate generation process in the RPI algorithm. The analyst was able to suggest potentially interesting features to be included in the predicate (in real time), and the RPI algorithm would react by favoring those features when constructing the predicates. The analyst was also able to terminate a predicate during the search process if the predicate is no longer of interest. Figure 8 shows the interface of this mixed-initiative prototype system.

On the positive side, during an evaluation the participants noted that this prototype met the three design requirements as outlined in Section 3.3. It addition, this approach had the benefit of much faster computation times from the RPI algorithm: rather than searching an exponential space of predicates including potentially irrelevant features, the mixed-initiative approach allowed the analyst to prune irrelevant search spaces early.

However, during the evaluation we also observed significant limitations to the mixed-initiative approach. First, we found that the participants were often unable to or were uncertain about how to steer the predicates. For example, the participants were not able to decide with certainty whether a feature such as precipitation should be included in a predicate that is meant to detect anomalies about business cost. Forcing the participants to make such decisions in real-time sometimes led them into making rushed and incorrect choices.

Additionally, analysts steering the computation would occasionally exhibit biases when generating the predicates. If an analyst had a perceived assumption about what was likely causing the anomalies, their steering would often reflect the bias and direct the computation towards confirming that assumption. Recent research has begun to explore the potential pitfalls of progressive visualization and steering (e.g., 7, 15, 37, 43, 46). In the context of anomaly reasoning, we observe that such bias can be detrimental to the analysts’ abilities to appropriately reason about the anomalies.

11 Limitations and Future Work

Although the PIXAL benefited from the lessons learned from the iterative design and was found to be effective by professional data analysts, we note that there is still room for improvement. In this section we outline some of the limitations of PIXAL.

Integrated Anomaly Detection: One of the analyst expressed the desire to have integrated anomaly detection capabilities in PIXAL. PIXAL currently assumes that the input data and their corresponding anomaly scores have been previously verified. However, while the verification process can be performed as a preprocessing step, the analyst suggested that an integrated solution will allow for opportunities to iterate between anomaly detection and anomaly reasoning in cases where the anomaly detection algorithm performs poorly on the input data.

Improved Recommendations: During the evaluation the participants applauded PIXAL's ability to provide automated recommendations that explained the possible reasons behind the anomalies. We recognize that there are still opportunities to develop more sophisticated algorithms for improved recommendations. To start, the recommendations in PIXAL are currently based on the correlation coefficients between the anomaly scores and each of the data attributes independently. This limits PIXAL to only be able to identify single data attributes as potential reasons and excludes the interactions between multiple attributes as possible explanations. We will investigate other approaches, such as multi-linear regression and KL divergence in the future to improve the recommendations.

12 Conclusions

In this paper, we present PIXAL, a visual analytics system for helping analysts reason about anomalies. PIXAL fills gaps in existing tools for anomaly reasoning: The RPI algorithm helps analysts find logical groupings of anomalous data points by generating and testing predicates using a Bayesian hypothesis testing framework. PixalExplorer allows analysts to visualize and build trust in predicates generated by the RPI algorithm. Pixalate helps the analyst generate and validate hypotheses that might explain the cause of a group of anomalies, and provides support for generating reports that can be presented to stakeholders. We evaluated the utility of Pixal with three professional data analysts who observed PIXAL being used to solve an anomaly reasoning problem. All three analysts found that PIXAL facilitated anomaly reasoning by filling gaps in their current workflow.

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