Categorical anomaly detection in heterogeneous data using minimum description length clustering

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ABSTRACT

Fast and effective unsupervised anomaly detection algorithms have been proposed for categorical data based on the minimum description length (MDL) principle. However, they can be ineffective when detecting anomalies in heterogeneous datasets representing a mixture of different sources, such as security scenarios in which system and user processes have distinct behavior patterns. We propose a meta-algorithm for enhancing any MDL-based anomaly detection model to deal with heterogeneous data by fitting a mixture model to the data, via a variant of k-means clustering. Our experimental results show that using a discrete mixture model provides competitive performance relative to two previous anomaly detection algorithms, while mixtures of more sophisticated models yield further gains, on both synthetic datasets and realistic datasets from a security scenario.

1 INTRODUCTION

A wide variety of anomaly detection techniques have been studied, considering numerical, categorical, and mixed data [8]. Anomaly detection, or outlier detection, is based on different strategies for estimating the degree to which individual data points differ from the norm exhibited by the dataset as a whole. This challenge is usually compounded by the fact that annotated training data indicating whether data items are normal or abnormal may be unavailable, unbalanced, or unrepresentative of future observations. For example, in a security setting, past attacks may not be representative of future yet-to-be-invented attacks, and attack data is typically sparse, so training an accurate binary classifier is likely to either overfit to the past attacks, or suffer low accuracy against known attacks. We consider unsupervised anomaly detection.

Most work on unsupervised anomaly detection has focused on continuous, numerical data. In this paper, we focus on categorical data, for which several different techniques have been studied [24]. One of the most effective classes of techniques is based on the minimum description length (MDL) principle [10]. According to the MDL principle, we measure how well a model fits the data by how well it compresses the data, plus a cost associated with representing the model itself. The idea is to avoid overfitting by trading off model complexity for accuracy: for example, in the limit, a model that contains a dictionary listing each possible data value would compress the data very well, but be penalized highly for model complexity, since the model contains a copy of all of the different possible values of data records. In the MDL-based approach to anomaly detection [2, 21], we first apply MDL to select a “good” model of the data, and then use the compressed size of each data item as its anomaly score.

Two examples of anomaly detection based on MDL have been studied and shown to perform well: the OC3 algorithm [21] based on an itemset mining technique called Krimp [26], and the CompX algorithm [2]. Broadly speaking, both take a similar approach: first, a model \( H \) of the data that compresses it well is found using a heuristic search, balancing the model complexity \( L(H) \) (number of bits required to compress the model structure/parameters) against the data complexity \( L(X|H) \) (number of bits required to compress the data given the model). Once such a model \( H \) is found, we assign to each object \( x \in X \) a score corresponding to the object’s compressed size \( L(x|H) \) given the selected model. Intuitively, if the model accurately characterizes the data as a whole, records that are representative will compress well, yielding a low anomaly score, while anomalous or abnormal records should compress poorly. If this were not the case, then a more accurate model (compressing the data better) could be obtained by giving the normal records shorter codes and anomalous records longer codes.

While effective, these approaches have some limitations. They work well for homogeneous datasets, for which it is reasonable to assume that there is a single process that generates the observed data. However, the compression models they consider take no account of the possibility that the data represents a mixture of records generated by different data sources. If the data is heterogeneous, there may be further opportunities for compressing it more effectively, by choosing among several different models instead of using a single one.

We illustrate the potential benefits of mixture modeling using geometric intuition. Figure 1 illustrates some data points in a two-dimensional space, with three large clusters \( (a,b,c) \), and a small cluster \( (d) \). If we consider a single model of the data, the “center” of the dataset (illustrated with a star) is closest to the points \( (d) \), while points \( (a,b,c) \) are approximately equidistant. Thus, if we used distance from the center as an anomaly score, it would be difficult to distinguish the anomalous cluster from the three main clusters. If, on the other hand, we recognize that most of the data fall into three main clusters, then we would see that the points \( (d) \) are not close to any of these clusters, even though they are close to the average behavior of the dataset as a whole.

We have emulated this situation in a categorical setting by generating synthetic data with 1000 samples drawn from three discrete distributions corresponding to the large clusters \( (a,b,c) \), and seeding
In this paper, we propose an MDL-based anomaly detection technique that exploits this opportunity to detect and exploit heterogeneities in datasets to improve anomaly detection. Our approach is partly inspired by work using Krimp for clustering [25]. This work proposed both top-down and bottom-up clustering strategies, using Krimp’s compression metric to assess the quality of clusters, and comparing the quality of clusterings obtained for different values of $k$. They found up to 40% improvement in compressed size. The top-down algorithm they presented is similar to the k-means algorithm for clustering numerical data [6], and is similar to other MDL-based clustering algorithms [13]. They observed this approach generalizes to any MDL-based technique but did not explore this insight or consider applications to anomaly detection.

Based on this observation, we consider the value of MDL-based clustering as a basis for anomaly detection. Essentially, the idea is to first identify a clustering for the data (and, in the process, assign each data item to the most appropriate cluster). Next, a score is assigned to each data item based on combining the cost of compressing its cluster number, together with the cost of compressing the data itself using the corresponding model. Both components would be required to decompress the data, since, without the cluster number, the receiver would not know which basic model to use to decompress the data.

In this paper, we consider several instances of this idea. Our main contribution is to demonstrate that clustering techniques can improve the anomaly detection performance of a variety of MDL-based models. After introducing notation and a framework for MDL algorithms (Section 2), we consider a naive MDL-based anomaly detection technique called AVC, which is a slight variant of the AVF algorithm [14] in which the data is fit to a product of independent Bernoulli distributions. We consider AVC, Krimp/OC3, and CompreX as instances of the MDL framework, and describe a meta-algorithm that uses a clustering strategy to fit a mixture model to the data (Section 3). We then present experimental evaluation (Section 4) using common datasets as well as data from a realistic security setting which demonstrates that clustering can improve anomaly detection performance (measured using AUC or nDCG score) significantly, while also imposing higher computational cost. Interestingly, the benefits of clustering are much more significant for AVC compared to Krimp/OC3 or CompreX, illustrating that the more sophisticated compression techniques used by the latter are already flexible enough to deal with heterogeneous data. In some cases, clustering using mixtures of AVC models actually outperforms (mixtures of) Krimp or CompreX models, while also being faster.

2 BACKGROUND

We assume familiarity with basics of information theory and the MDL principle [9, 10]. We consider the following framework for selecting and fitting models to data according to the MDL principle. (We employ what Grünwald [10] calls ”two part crude MDL”, which is well-behaved when large amounts of data are available.) We consider an MDL scenario to be specified as follows:

- A space of observations $X$
- A space of hypotheses $H \in \mathcal{H}$
- A global hypothesis codelength function $L : \mathcal{H} \to \mathbb{R}$ satisfying the Kraft inequality $\sum_{H \in \mathcal{H}} 2^{-L(H)} \leq 1$.
- A function $L(-|-) : X \times \mathcal{H} \to \mathbb{R}$, such that for each hypothesis $H$ the associated codelength function $x \mapsto L(x|H)$ takes a data item $x \in X$ to its compressed size, again satisfying the Kraft inequality $\sum_{x \in X} 2^{-L(x|H)} \leq 1$.

Given a MDL scenario $(X, \mathcal{H}, L)$, a learner is an algorithm $F : X^n \to \mathcal{H}$ that attempts to find $H$ minimizing $L(H) + \sum_{x \in X} L(x|H)$. It is not required that a learner finds a global optimum $H_{\min}$; we also allow for $F$ to be nondeterministic or randomized. Familiar probability distributions, with their associated parameter estimation techniques, provide a ready source of MDL-based learning techniques, but our

Figure 1: Geometric intuition

Figure 2: Results of (a) pure and (b) mixture modeling for anomaly detection in synthetic data. Red vertical lines indicate anomalies, while the black vertical line indicates the average codelength.
framework also permits viewing any family of compression algorithms (indexed by hypotheses corresponding to parameterizations, code tables, etc.) as an MDL-based learning technique.

For the purpose of this paper we assume the size of the dataset under consideration is a fixed constant $n$.

**Uniform processes.** As a simple case we consider the trivial MDL scenario $\mathcal{U}_X$ corresponding to a uniform probability distribution over a finite set $X$. In this case, there is only one hypothesis, $\star$, representing the uniform distribution, and the hypothesis codelength function is $L(\star) = 0$, while the observation codelength function is $L(c_1|\star) = -\log(\frac{1}{m}) = \log |X|$.

**Bernoulli processes.** We consider Bernoulli processes, generating 0,1 values, specified by a probability $p$ of generating a 1 and $1-p$ of generating a 0. The hypotheses we might seek to learn about such a process are the probabilities $p$; to avoid degeneracy we require $0 < p < 1$. To avoid having to specify real numbers infinitely precisely, we consider precision to $[\log n]$ bits, where $n$ is the number of data items under consideration. We represent a hypothesis as $m$ interpreted as a rational number $m/n$ where $0 \leq m \leq n$. The codelength of such a hypothesis is $L(m) = [\log n]$, we encode $m$ using $[\log n]$ bits.

Given a sequence of $n$ independent 0/1 values we may estimate $p = \frac{n_1}{n}$ where $n_1$ is the number of 1’s occurring in the sequence. This choice would be optimal, if we wish to compress the sequence minimizing the sum $\sum_{i=1}^n L(x^i|\mathcal{H})$ so that there is no need to deal with data values that were not observed in the input. However, this leads to degeneracy in the case where some value never appears in the input, which means that future observations of unseen values have probability 0, and hence infinite codelength. To avoid this problem, we generally apply a so-called Laplace correction to the counts, by taking $p = (n_1 + 1)/(n + 2)$ to ensure that both outcomes have nonzero probability.

Thus, the codelength of a 0 or 1 value $x$ is $-\log p$ if $x = 1$ and $-\log(1-p)$ otherwise; we may write this concisely as $L(x|\mathcal{H}) = -[x = 1] \log p - [x = 0] \log(1-p)$, where $p = (m+1)/(n+2)$ is derived from $\mathcal{H} = (m,n)$ as above. (We write $[\phi]$ for 0 if $\phi$ is false and 1 if $\phi$ is true.) Finally, we take the learning function $F$: $(0,1)^* \rightarrow \mathcal{H}$ to be

$$F(x^1, \ldots, x^n) = \sum_{i=1}^n x_i$$

**Categorical processes.** We can generalize the above discussion of two-valued Bernoulli processes to $k$-valued categorical processes $\mathcal{C}_k$. A categorical distribution over $k$ outcomes $1, \ldots, k$ is specified by the $k$ probabilities $p_1, \ldots, p_k$ of the different outcomes, up to precision $[\log n]$; since one of them is redundant, the data of a hypothesis is given by $(m_1, \ldots, m_{k-1})$ and the associated codelength $L(H) = (k-1)[\log n]$. From this, we may extract $p_1, \ldots, p_k$ by taking $p_i = (m_i + 1)/(n + k)$ where $i < k$ and $p_k = 1 - \sum_{i<k} p_i$, again applying Laplace correction to avoid degeneracy. Furthermore we may encode a given outcome $x$ according to hypothesis $H$ as $\sum_{i=1}^k \log p_i$.

Finally, the learning function that identifies the best hypothesis for the data is:

$$F(x^1, \ldots, x^n) = \sum_{i=1}^n [x^i = 1], \ldots, \sum_{i=1}^n [x^i = k-1]$$

**Independent products.** Given two MDL scenarios $X = (X, \mathcal{H}_1, L_1)$ and $Y = (Y, \mathcal{H}_2, L_2)$, we can combine them independently to form a scenario over pairs $(x,y) \in X \times Y$ by taking a product $X \times Y$. The hypotheses $\mathcal{H} = \mathcal{H}_1 \times \mathcal{H}_2$ for the product are pairs of hypotheses for $X$ and $Y$. The hypothesis codelength function is defined by taking sums of codelengths: $L(\mathcal{H}_1, \mathcal{H}_2) = L_1(\mathcal{H}_1) + L_2(\mathcal{H}_2)$. The data codelength function is also defined by taking sums, using the respective hypotheses: $L((x,y)|(\mathcal{H}_1, \mathcal{H}_2)) = L_1(x|\mathcal{H}_1) + L_2(y|\mathcal{H}_2)$.

Finally, given learning functions $F_1, F_2$ for $X$ and $Y$ respectively, the learner function $F$ is defined as:

$$F((x^1, y^1), \ldots, (x^n, y^n)) = (F_1(x^1, \ldots, x^n), F_2(y^1, \ldots, y^n))$$

Likewise, we can also consider $n$-ary products $\prod_{i=1}^n X_i = X_1 \times \cdots \times X_m$ whose behavior is determined by iterating binary products.

## 3 MDL-BASED ANOMALY DETECTION

We now consider several instances of the above framework and their use for anomaly detection. In each case, we follow the same recipe as proposed in previous work [2, 21]: first induce a good model of the data according to the MDL principle, that compresses the dataset as a whole; then assign each element an anomaly score corresponding to its compressed size using the model. We can then inspect the highest-scoring data items as being the most anomalous.

The first instance of this framework, called Attribute Value Compression (AVC), is a slight variation of a known anomaly detection algorithm called Attribute Value Frequency (AVF) [14], but is based on optimal compression of each attribute independently. Thus, it is limited in that it cannot exploit interdependencies among attributes. Next, we recast the Krimp/OC3 and CompreX algorithms as instances of the above framework, though we abstract over the details. Finally, we describe a generic strategy (i.e. a meta-algorithm) for learning mixtures of MDL hypotheses, given a basic learner such as AVC, Krimp or CompreX. Given a learner $F$ for component models, the meta-algorithm produces a learner for $k$-mixture models $F^*$, using the MDL principle to find a suitable value for $k$.

### 3.1 Basic models

**Attribute Value Coding.** Given a binary or categorical dataset with $m$ attributes $X_1, \ldots, X_m$ each corresponding to a Bernoulli or categorical process, we define the Attribute Value Coding algorithm as the learner induced by taking the product of the optimal learners for the components $X_1, \ldots, X_m$. Concretely, $F_{AVC}$ calculates the frequencies of the values of each attribute independently and $L_{AVC}(X_1, \ldots, X_m)$ then encodes each attribute $x_i$ with codelength $-\log p_i$ where $p_i$ is the probability of attribute $i$ having value $x_i$. For example, when the attributes are all binary, the probabilities first calculated as $p_i = \frac{1}{m} \sum_{j=1}^m x_{ij}$ and the score of each element $x$ is $L(x|\mathcal{H}) = \sum_{i=1}^m -([x_j = 1] \log p_j + [x_j = 0] \log(1-p_j))$.

**Example 3.1.** Here, we introduce a small (extremely simplistic) running example to illustrate AVC. Suppose we have the following dataset:

| id  | abc.com | xyz.com | evil.com |
|-----|---------|---------|----------|
| $P_{17}$ | 1       | 1       | 0        |
| $P_{42}$ | 1       | 1       | 0        |
| $P_{1337}$ | 0       | 0       | 1        |
| $P_{607}$ | 1       | 1       | 0        |
where $P_{17}, P_{42}, P_{1337}, P_{007}$ are four distinct processes and $abc.com$, $xyz.com$ and $evil.com$, three attributes corresponding to network addresses accessed by the processes.

$P_{17}$ and $P_{42}$ access both $abc.com$ and $xyz.com$ and are both processes with innocuous activity while $P_{1337}$ and $P_{007}$ are malicious processes ($P_{1337}$ a naive attacker that only accesses $evil.com$, and $P_{007}$ a more sophisticated attacker that accesses all three addresses in order to attempt to camouflage its behavior).

To calculate the AVC score of each of the processes and determine which exhibit abnormal behavior, we first compute the frequencies of occurrence ($c_i$, with $i \in \{abc.com, xyz.com, evil.com\}$) of each of the three dataset attributes followed by the probability $p_i$ of each of the attributes having value $x_i$ (where $x_i$ is either 0 or 1):

$$c_{abc.com} = c_{xyz.com} = 3 \quad \text{and} \quad c_{evil.com} = 2$$

$$p_{abc.com=1} = p_{xyz.com=1} = \frac{3}{4} \quad \text{and} \quad p_{evil.com=1} = \frac{1}{2}$$

(the probabilities can be estimated simply by taking $p_i = \frac{c_i}{n}$ where $n$ is the number of data points i.e. processes here)

The AVC scores are then simply calculated as follows:

$$AVC(P_{17}) = -\frac{1}{2}(\log p_{1} + \log \frac{1}{2} + \log \frac{1}{2}) \approx 0.61$$

$$AVC(P_{42}) = -\frac{1}{2}(\log \frac{1}{2} + \log p_{1} + \log \frac{1}{2}) \approx 0.61$$

$$AVC(P_{1337}) = -\frac{1}{2}(\log \frac{1}{2} + \log p_{1} + \log \frac{1}{2}) \approx 1.66$$

$$AVC(P_{007}) = -\frac{1}{2}(\log \frac{1}{2} + \log \frac{1}{2} + \log \frac{1}{2}) \approx 0.61$$

We term this approach "Attribute Value Coding" because it is very similar to a previously-defined anomaly detection technique called "Attribute Value Frequency" (AVF) [14]. The main difference is that, in AVF, we sum the probabilities of each attribute retaining its observed value, not the log-probabilities (i.e. codelengths); hence, AVF does not have a direct reading as an MDL technique, while AVC does. Because AVC scores do not correspond to compressed sizes, it would be meaningless to attempt to use them as a component in a larger MDL-based compression strategy such as the one we propose based on clustering.

**Krimp.** We will also consider the Krimp algorithm as an MDL scenario and learner. In Krimp, a (binary) dataset is compressed by identifying certain subsets of frequently co-occurring attributes. Concretely, in Krimp, the dataset is to be represented by a code table $CT$ which lists the possible subsets and their codelengths, and then each data item is represented by a set of codewords called its cover, so that the length $L(x | CT) = \sum_{y \in \text{Cover}(CT)}|x_i|$, the length of the cover.

In Krimp, a candidate collection of itemsets is mined from the data using standard techniques. The mined itemsets are considered as candidate entries to a code table; those that are useful in improving compression are selected. Krimp performs a heuristic search to try to find a code table that minimizes the compressed size of the data. Different pruning strategies are used to remove candidates which are less effective. The exact details of the search and pruning algorithms do not play an important role here as we will use them as a black box.

However, what is important is that we can assign a cost $L(CT)$ to the code table itself (that is, the number of bits necessary to record or communicate it) and we can assign a cost $L(x | CT)$ to each data item given a code table (that is, the number of bits necessary to communicate a given data item, using a certain code table). These codelengths satisfy the Kraft inequality.

In the MDL scenario corresponding to Krimp, the hypotheses are Krimp’s code tables $CT$, and the codelength functions $L(CT), L(\overline{CT})$ are as defined in previous papers [21, 26]. We write $F_{\text{Krimp}}$ for the Krimp algorithm itself, which selects among the (huge number of) potential code tables one which performs well in balancing the hypothesis codelength against the encoded size of the data.

**CompreX.** We will also describe how to model the CompreX scenario and its MDL scenario. In CompreX, as in Krimp, code tables are used. However, in CompreX, instead of using a single global code table, the input attributes are partitioned and one code table is assigned to encode the attributes in each component of the partition. Thus, the hypotheses $H = \{P, CT_1, \ldots, CT_p\}$ consist of a partition $P = \{P_1, \ldots, P_p\}$ of the attributes, along with one code table for each partition. A hypothesis codelength function $L(H)$ is described in the paper [2] using Krimp’s $L(CT)$ together with an encoding of partitions, and the codelength function for data elements given a hypothesis is derived by adding together the codelengths of the attributes in each part:

$$L(x | H) = \sum_{i=1}^{p} L(p_{Pi}(x) | CT_i)$$

where $p_{Pi}(x)$ is the projection of the attributes of $x$ to the subset $P_i$. Note that once the partition is given, this is essentially a product of Krimp MDL scenarios.

Unlike Krimp, CompreX follows a bottom-up strategy for synthesizing code tables: initially the partition consists of singleton attributes only and the associated code tables are trivial. Using information gain as a heuristic, CompreX greedily merges partition elements and combines their code tables. Itemset mining is not directly performed; nevertheless, CompreX was found to obtain good compression compared to Krimp, indicating that many datasets may contain subsets of highly-correlated attributes for which CompreX’s partitioning strategy works well. We write $F_{\text{CompreX}}$ for CompreX considered as an MDL learner algorithm, relative to an appropriate MDL scenario.

### 3.2 Mixture models

We assume given a basic MDL scenario $X = (X, \mathcal{H}, L)$ and learner $F$ for fitting hypotheses to the data. As mentioned by [25], any such technique can be used as a component in a $k$-means-style clustering technique, which can again be justified by the MDL principle. In this section, we spell out the details in a way that is independent of the choice of $X$ and $F$.

Given the MDL scenario $X = (X, \mathcal{H}, L)$, we can construct a new scenario $X^*$ called the $X$-mixture model as follows:

- The observations $X$ are those of $X$.
- The hypotheses correspond to $K$-mixture models of hypotheses $\mathcal{H}$, for all positive $K$. These are tuples $(K, H, \tilde{H}_i)$, where $H$ is a hypothesis for the $K$ possible components specified by $C_k = \{1, \ldots, K\}, \mathcal{H}_k, L_K$, the $K$-valued categorical process model and the $K$ hypotheses $H_1, \ldots, H_K \in \mathcal{H}$ characterize each component.
- Define the encoding for a hypothesis $(K, H, \tilde{H}_i)$ as $L^*(K, H, \tilde{H}_i) = [\log n] + L_K(H) + \sum_{k=1}^{K} L(H_k)$. That is, we encode $K$ (which takes at most $[\log n]$ bits), then the hypothesis for the class
We write $X^*$ for the MDL scenario specified above, and call it the mixture of $X$ models.

Intuitively, this scenario corresponds to the following (nondeterministic) compression algorithm: we guess $K$, a distribution over $K$ class labels, and $K$ hypotheses corresponding to the $K$ components existing in the data. We encode this information and transmit it to the receiver. Subsequently, each data value $x$ can then be transmitted by first encoding the class label $i$ for $x$ (using the hypothesis $H_i$ describing the distribution of class labels), then transmitting $x$ itself using the hypothesis $H_i$.

This nondeterministic algorithm suggests an optimal (but infeasible) compression algorithm: given data $x \in X^*$, find a mixture model hypothesis that yields the optimal codelength $L(H^*) + L(X|H^*)$ given the above scenario. Of course, this naive approach is infeasible since, even if we know an efficient optimal learner for the components $X$, finding the optimal mixture model parameters (equivalently, the optimal clustering minimizing the codelength) might require considering all of the possible partitions. The number of partitions of $n$ is the Bell number $B_n$ which grows very rapidly (e.g. $B_{20} > 50$ trillion).

However, just as for conventional clustering, an iterative greedy approach can be effective, following a similar strategy to the classic $k$-means clustering algorithm. We outline such a strategy below, which is largely the same as in [25]; the main difference is that we use an optimal code for the class labels, instead of ignoring the codelength of the class labels as they do.

The mixture model fitting process is a variant of the $k$-means clustering algorithm, but using MDL hypotheses to represent the clusters, and with codelength assigned to a point by a given cluster playing a role analogous to the distance metric in $k$-means. To find the right $k$, we start with $k = 1$ and increase it until we have found a local minimum. (In practice, we typically detect when increasing $k$ yields diminishing returns, and stop early, since trying all $k$ up to $n$ would be prohibitively expensive.) Similarly to $k$-means, in each iteration, we alternate between estimating the component models based on the current candidate clustering (line 5 in Algorithm 1), and reassigning points to clusters (line 6 in Algorithm 1). However, instead of taking the “mean” of a set of points, which is meaningless for categorical data, we represent a set of points using a hypothesis and we calculate the “distance” of each point as its (idealized) compressed size, were it to be compressed using that hypothesis. The hypotheses may be simple AVC models, Krimp code tables, CompeX hypotheses, or those of any other MDL scenario.

Algorithm 1: Mixture model fitting algorithm

```
Input: a dataset $\tilde{X}$
Output: An $X^*$ hypothesis $(\tilde{K}, \tilde{H}, \tilde{c})$
1 $k = 1$
2 while $k \leq n$ do
3 Randomly assign each $x^i$ to one of $k$ classes. Let $y^j$ be the initial class of each $x^i$.
4 repeat
5 Run $H_j := F_X(x^i | y^j = j)$ to calculate the hypothesis for each class;
6 Re-assign each $x^i$ to the class $j$ minimizing $L(x^i | H_j)$, setting $y^j$ to $j$;
7 Evaluate $c := L^*(K, \tilde{H}, \tilde{c}) + \sum_{i=1}^{n} L^*(x^i | H_j, \tilde{H}_i)$, the cost of the current hypothesis;
8 until a local minimum $c_k$ is reached.
9 Set $k := k + 1$;
end
11 Return the hypothesis $(k, \tilde{H}, \tilde{c})$ achieving minimal $c_k$. convergence are possible; we fix some small $\epsilon > 0$ and iterate until the total compressed size fails to improve by more than $\epsilon$ times the previous size. We may also conduct several trials with different random initializations and take the result that minimizes the compressed size.

Now, to find the best $k$, we consider a range of $k$ values and fit a model with $k$ components for each $k$. Suppose we have constructed models $M_1, \ldots, M_n$ for all possible $k$ values between 1 and $n$. We choose $k$ to be the one for which $L(M_k) + L(X|M)$ is minimized. Of course, it would likely be wasteful to fit models again and again so, by fixing some $\epsilon$, we may terminate the process early if increasing $k$ fails to result in a better fit. In practice, we usually consider $k$ values up to some relatively small number, since $n$ is usually very large.

3.3 Anomaly detection

Let $H$ be the best hypothesis found by the above procedure for some MDL scenario $X$. To perform anomaly scoring we simply assign each $x$ its codelength $L(x|H)$. Because we have required codelength functions to be nondegenerate (i.e. satisfying the Kraft inequality for each hypothesis), $L(x|H)$ is well-defined and finite, even if we consider records $x$ that were not present in the original dataset. Since codelength functions satisfying the Kraft inequality correspond to (sub)probability distributions, the records for which the codelength $L(x|H)$ are largest are precisely those whose conditional probability given $H$ are smallest.

4 EVALUATION

4.1 Datasets

We consider several public datasets collected for evaluation of categorical anomaly detection by Pang [17]. Their characteristics are summarized in the first few columns of Table 1. The datasets range in size up to 2k records and between 22–114 attributes, with between 27 and 60 anomalies. We transformed all datasets to use binary encodings of multivalued attributes to ensure compatibility.
with Krimp. Most of these datasets are derived from standard classification datasets by choosing one class to be the normal class and selecting a few examples of another class to be the anomalies.

We also consider several datasets derived from the DARPA Transparent Computing program, consisting of data about operating system processes in a system under attack by an advanced persistent threat (APT) (see Table 1 lower left for dataset statistics). These categorical datasets are derived from much larger raw provenance trace datasets as described by Berrada et al. [4]; we consider only their ProcessEvent datasets in which each record describes the behavior of an operating system process, and the attributes indicate whether the process ever performed a particular kind of action (read, write, forking another process, etc.) These datasets contain a mix of system and user-level processes describing all of the activity in an operating system. These datasets are drawn from a realistic security application of anomaly detection, and are mostly larger and with a smaller percentage of anomalies, and because of the heterogeneity of the underlying OS processes being recorded we believe they form a more compelling test for our approach than the generic datasets. The datasets include two security evaluation scenarios in which computers running different operating systems were attacked by simulated APT intruders, usually leading to a very small percentage of attack processes which we would like to detect as anomalous.

4.2 Experimental Results

Experimental setup. We implemented AVC and AVC∗ in Python, using libraries for linear algebra to perform the iterative clustering steps efficiently. We also implemented Python scripts that run adapted versions of Krimp/OC3 and CompreX to perform their clustering variants OC3∗ and CompreX∗. We made minor changes to publicly available code for Krimp1 and CompreX2 to enable this. We used the default settings for Krimp, and considered all closed itemsets. For CompreX, we used the default behavior in the publicly available Matlab implementation.

All experiments were run on an HP Elitedesk 800 with Intel i5-6500 CPU and 32GB RAM running Scientific Linux 7.

Evaluation metrics. Following most work on anomaly detection, we report the AUC score resulting from the ranking induced by the anomaly scores, i.e. the area under the receiver operator characteristic curve, which summarizes the effectiveness of anomaly detection at all possible thresholds. For large datasets with very sparse anomalies, the AUC score is not very informative because even a very high score such as 0.999 can correspond to all of the anomalies being found in the top 0.1% of records, but this could still be useless for actually finding anomalies if the dataset has millions of records. As a complement to AUC score, we follow [3, 4] in also reporting the normalized discounted cumulative gain of the rankings, which is widely used in information retrieval to assess the results of search algorithms and assigns proportionately greater weight to rankings that return relevant results (in this case, anomalies) close to the top. Both nDCG and AUC scores are between 0 and 1, with 1 representing the best possible result. Their calculations are otherwise standard and we refer to [4] or other sources for definitions and baseline results using a variety of categorical anomaly detection algorithms.

Research questions and experiments. We ran experiments intended to assess the following research questions:

1. Q1: Can clustering using simple AVC models yield anomaly detection performance competitive with Krimp or CompreX?
2. Q2: Can clustering increase the anomaly detection performance of Krimp or CompreX?
3. Q3: Is the performance overhead of clustering acceptable?

To assess Q1, we evaluated the anomaly detection performance of AVC, Krimp, CompreX, and AVC∗ on the different datasets. The results are summarized in Table 1. In the case of AVC, Krimp and CompreX, the reported result is the result of one run since the result is deterministic. For AVC∗, we ran 10 runs for each dataset with different random initializations, since k-means algorithms are sensitive to initial conditions, and we report the median result from the 10 runs for the k value yielding the smallest compressed sizes.

To assess Q2, we ran AVC∗, OC3∗ and CompreX∗ on all of the datasets, for different values of k (1, 2, 4, 8, 16, 20 for AVC∗ and OC3∗, but only 1, 2, 4 for CompreX∗ because the running time was prohibitive for higher values of k). Figures 3-4 show selected results from these experiments, plotting relative compressed sizes (bars) and maximum and median AUC or nDCG scores (green and red lines) against k values. In this experiment we ran 10 trials of each algorithm for a fixed value of k and again report medians of AUC or nDCG scores for the 10 runs. For illustration, we also show the maximum AUC or nDCG score achieved in each batch of 10 runs as well as the median; however, in an unsupervised setting we have no way of knowing in advance which of several runs will produce this optimal result.

Finally to assess Q3, we report the average running times (again across 10 runs) of each algorithm on each dataset. These are shown in Figure 5. The reported running times for AVC, OC3, CompreX, AVC∗ and OC3∗ are for 10 runs of the full algorithm, considering all k-values up to 20, with early stopping if a local minimum is identified early. For CompreX∗ we report only a few examples for k-values up to 2 or 4 because each run takes over a minute even for small datasets. In interpreting these results it is important to keep in mind that each base algorithm was implemented in a different programming language: AVC in Python (using libraries such as numpy for efficient matrix manipulations), Krimp in C++, and CompreX in Matlab. Moreover, the wrapper Python code for AVC∗, OC3∗, and CompreX∗ may contribute to higher overhead for these algorithms (for example due to repeated process startup costs) compared to a single-language implementation. Nevertheless, these results allow at least a coarse qualitative comparison among the different techniques.

4.3 Discussion

Effectiveness of AVC∗ compared to OC3 and CompreX. The results in Table 1 show that generally, AVC is not competitive with Krimp/OC3 or CompreX, with the interesting exception of the Probe dataset. However, when we consider mixtures of AVC models in AVC∗, anomaly detection performance increases significantly, leading to the best overall results in 10 cases, compared to 13 for
Categorical anomaly detection in heterogeneous data using minimum description length clustering

Table 1: (Left) Dataset characteristics (N=number of records, M=number of attributes, %Anomaly = percentage of anomalies). (Right) AUC and nDCG scores for Krimp, CompreX, AVC and AVC*. The best score of each kind is highlighted in bold.

| Dataset       | N     | M     | %Anomaly | Krimp AUC | Krimp nDCG | CompreX AUC | CompreX nDCG | AVC AUC | AVC nDCG | AVC* AUC | AVC* nDCG |
|--------------|-------|-------|----------|-----------|------------|-------------|-------------|---------|----------|---------|----------|
| AID362       | 4,279 | 114   | 1.4%     | 0.582     | 0.409      | 0.675       | 0.423       | 0.644   | 0.420    | 0.674   | 0.433    |
| Bank         | 41,188| 52    | 11%      | 0.625     | 0.814      | 0.639       | 0.823       | 0.593   | 0.808    | 0.608   | 0.810    |
| Chess (KRK)  | 28,056| 40    | 0.01%    | 0.321     | 0.220      | 0.622       | 0.263       | 0.645   | 0.244    | 0.673   | 0.254    |
| CMC          | 1,473 | 22    | 2.7%     | 0.559     | 0.402      | 0.580       | 0.458       | 0.589   | 0.474    | 0.600   | 0.414    |
| Probe        | 64,759| 82    | 6.4%     | 0.938     | 0.925      | 0.937       | 0.915       | 0.951   | 0.961    | 0.937   | 0.912    |
| SolarFlare   | 1,066 | 41    | 4%       | 0.792     |            |             |             |         |          | 0.783   | 0.545    |
| Windows S1   | 17,569| 22    | 0.04%    | 0.992     | 0.302      | 0.996       | 0.602       | 0.984   | 0.618    | 0.996   | 0.675    |
| BSD S1       | 76,903| 29    | 0.02%    | 0.976     | 0.436      | 0.976       | 0.542       | 0.882   | 0.525    | 0.975   | 0.516    |
| Linux S1     | 247,160| 24| 0.01%    | 0.887     | 0.340      | 0.887       | 0.299       | 0.821   | 0.264    | 0.887   | 0.407    |
| Android S1   | 102   | 21    | 8.8%     | 0.754     | 0.740      | 0.731       | 0.821       | 0.826   | 0.848    | 0.860   | 0.861    |
| Windows S2   | 11,151| 30    | 0.07%    | 0.857     | 0.242      | 0.856       | 0.223       | 0.808   | 0.230    | 0.881   | 0.240    |
| BSD S2       | 224,624| 31| 0.004%   | 0.936     | 0.249      | 0.904       | 0.211       | 0.873   | 0.191    | 0.917   | 0.186    |
| Linux S2     | 282,087| 25| 0.01%    | 0.873     | 0.387      | 0.873       | 0.469       | 0.824   | 0.306    | 0.856   | 0.358    |
| Android S2   | 12,106| 27    | 0.1%     | 0.884     | 0.328      | 0.930       | 0.780       | 0.906   | 0.305    | 0.907   | 0.629    |

Figure 3: Compressed size and AUC or nDCG score vs. K for Bank and Probe datasets

CompreX and six for Krimp/OC3. (When there is a tie, we give credit to both techniques.) Thus, despite its simplicity, the AVC* algorithm illustrates that a simple MDL-based compression model together with MDL-based clustering yields a competitive anomaly detection technique.

Effect of clustering on anomaly detection. For AVC*, increasing the number of clusters typically improves compression performance. On the other hand, for OC3*, the best compression often results from K = 1 and typically fewer clusters are found. For the generic datasets, increasing K does not always translate to improved anomaly detection performance, even if it improves compressed size. As representative examples, consider the Bank and Probe datasets in Figure 3. Both are compressed more effectively by AVC* for k = 16 or 20 while the best k value for OC3* is 1. Increasing K results in improved median anomaly detection scores by AVC* while for the other situations (Bank using OC3* and Probe using either algorithm) increasing K leads to no improvement. The counterintuitive results for Probe could result, for example, if there are several clusters and all of the anomalies are close to one large cluster but far from representative of the dataset as a whole.

We also consider the results obtained for the APT security datasets. We show the results for Scenario 1 in Figure 4, since the Scenario 1 results for Probe could result, for example, if there are several clusters and all of the anomalies are close to one large cluster but far from representative of the dataset as a whole.
for CompreX*, while OC3* does obtain lower compressed size with 4–8 clusters but the increase in anomaly detection performance is not as significant, with median AUC score nearly unchanged and nDCG score increasing from 0.34 to 0.41. On the other hand, for the Android dataset (the smallest of the APT datasets), AVC* obtains only small improvements in compressed size at $K = 1$, with some associated improvement in AUC and nDCG scores, while both OC3* and CompreX* obtain minimal compressed size at $K = 1$. Again, the general trend is that OC3* and CompreX* find fewer clusters.
5 RELATED WORK

Mixture models and clustering have been used for anomaly detection in numerical and mixed data; for example, the SmartSifter algorithm [27] considers mixed categorical and numerical data, and induces a different mixture model of numerical data for each combination of categorical attributes. SmartSifter also uses an MDL-like logarithmic anomaly score. However, SmartSifter’s running time grows exponentially in the number of categorical attributes, and in practice, scales with the number of combinations of attributes actually present in the data, which makes it unsuitable to datasets with large numbers of categorical attributes. Another approach due to Bouguessa aggregates the results of several anomaly detectors and fits a mixture model to identify anomalous clusters [7].

Clustering techniques have been widely considered for numerical (non-categorical) data, while clustering for categorical data (which usually lacks natural metrics) has received much less study; the main approaches considered so far include EM-style algorithms for latent class inference or fitting discrete mixture models [6]; \(k\)-modes which performs clustering with respect to a dissimilarity metric [12]; and MDL-based clustering [13, 25].

The MDL-based clustering approach we adopted is inspired by and similar to those of Kontkanen et al. [13] and van Leeuwen et al. [25], but differs from both in that we consider clustering based on any MDL-based technique, whereas Kontkanen et al. consider a minimax optimal encoding of mixtures of discrete distributions, and van Leeuwen et al. consider Krimp as the base compressor but their approach does not take into account the cost of encoding the inferred classes. The latter do observe that their \(k\)-means-style algorithm could be used with other compressors. Moreover, neither approach has previously been considered as a basis for anomaly detection, whereas previous work on MDL-based anomaly detection has not considered clustering or mixture model fitting. Our work shows that this approach can improve anomaly detection for a variety of MDL techniques, resulting in a new competitive algorithm AVC*, in some cases improving on the performance of Krimp/OC3 and CompreX reported in previous work.

Besides Krimp/OC3 and CompreX, another MDL-based approach to anomaly detection is the UPC algorithm of Bertens et al. [5], which uses a Krimp-style compression algorithm and then looks for objects with unusual combinations of features. The anomaly scores are not directly based on compressed sizes. To the best of our knowledge the only previous work applying clustering to categorical anomaly detection is the ROAD algorithm [22], and a variant based on rough sets called Rough-ROAD [23]. Both algorithms perform clustering based on an ad-hoc metric on categorical data, and neither is based on MDL. ROAD was shown to have better performance than AVF [14] but was not compared with other anomaly detection algorithms such as Krimp/OC3 or CompreX, while Rough-ROAD was compared only with ROAD.

This work has been motivated by the observation that according to the minimum description length principle, the best-fitting model for some data is the one that minimizes the communication cost of the data, including the cost of describing the chosen model. However, to apply MDL requires deciding on a class of models and encoding scheme for them. Moreover, allowing more complex models increases the cost and algorithmic difficulty of searching and fitting the best one. In the limit, we could consider arbitrary compression algorithms as predictive models but then finding the
optimal one would be undecidable. Allowing mixture models and fitting them using clustering is one strategy for enriching the model space, which allows for the possibility of improved compression (that is, better prediction), while remaining relatively algorithmically straightforward. The idea of CompreX, that is, partitioning the columns of a dataset to enhance compression, is another approach. It would be interesting to explore other points on the tradeoff curve between model (and search space) complexity and compression effectiveness.

The public datasets for anomaly detection are drawn from those collected by Pang et al. [18, 19] in their work on feature selection and anomaly detection. Their work demonstrates how unsupervised feature selection could be used to improve categorical anomaly detection, including for CompreX; this is an orthogonal direction for improving anomaly detection effectiveness and performance, and it may be interesting to study whether it can be combined with clustering/mixture modeling.

Our main motivating application has been data gathered from security exercises in a recent DARPA program. These datasets are extracted from a much richer graph dataset in which operating system processes, files, and other resources are represented as nodes, and relationships between them as edges. Anomaly detection and intrusion detection techniques have been developed and applied to these datasets and studied by a number of papers [3, 4, 11, 15, 16, 20], but there is as yet no commonly accepted public dataset of ground truth annotations for evaluating different techniques; we used those developed by the authors of [3, 4] for their binary feature datasets. Comparing or combining our work with the above results obtained by others would be a valuable exercise.

6 CONCLUSIONS
Anomaly detection over categorical data is challenging but has received comparatively less attention than for continuous or numerical data. The previous state of the art is to search for patterns in the data that aid compression, for example using itemset mining or partitioning the columns into mutually informative subsets, and then use the codelength of each record as its anomaly score; according to the MDL principle, the best model is the one that compresses the data best, so once such a model is found, the anomalies are the records compressed poorly by the model.

We observe that in heterogeneous datasets containing mixtures of distinct kinds of records, existing techniques may miss opportunities to improve compression, and hence allowing mixtures of models may improve compression and lead to better-fitting models according to the MDL principle. The idea of fitting mixtures of models to data is not new, and has been used as a basis for MDL-based clustering techniques, we propose the use of mixture models and clustering algorithms to improve the performance of MDL-based anomaly detection. We illustrated this general strategy using three MDL-based anomaly detection techniques as the components of mixture models: simple discrete AVC models, the Krimp algorithm underlying OC3, and the CompreX algorithm.

Our results show that, in many cases, using a k-means-style algorithm finds opportunities for improving compression compared to using a single model. Moreover, we also show that mixture modeling can improve the anomaly detection performance of existing algorithms such as Krimp/OC3 and CompreX, and even that mixtures of simple models provide competitive anomaly detection performance compared to unmixied Krimp or OC3 models. On the other hand, performing iterative clustering to fit a mixture model is more expensive computationally, and our choice of randomized initialization of the clusters may leave room for further improvement since it is well known that randomly initializing clusters is not always the best strategy. Finally, we considered only the case of batch, nonadapative processing and it would also be interesting to consider streaming, adaptive anomaly detection techniques based on incremental clustering.

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