The Visual Exploration of Aggregate Similarity for Multi-dimensional Clustering

James Twellmeyer[1], Marco Hutter[1], Michael Behrisch[2], Jörn Kohlhammer[1,3] and Tobias Schreck[2]
[1] *Fraunhofer IGD, Darmstadt, Germany*
[2] *University of Konstanz, Konstanz, Germany*
[3] *Technische Universität Darmstadt, Darmstadt, Germany*

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Abstract: We present a visualisation prototype for the support of a novel approach to clustering called TRIAGE. TRIAGE uses aggregation functions which are more adaptable and flexible than the weighted mean for similarity modelling. While TRIAGE has proven itself in practice, the use of complex similarity models makes the interpretation of TRIAGE clusterings challenging. We address this challenge by providing analysts with a linked, matrix-based visualisation of all relevant data attributes. We employ data sampling and matrix seriation to support both effective overviews and fluid, interactive exploration using the same visual metaphor for heterogeneous attributes. The usability of our prototype is demonstrated and assessed with the help of real-world usage scenarios from the cyber-security domain.

1 INTRODUCTION

Let Bob be a security analyst. Bob has set up spam traps to capture spam messages. Bob knows that most messages are sent as campaigns, but he can only collect individual messages. Piecing together the campaigns could give Bob valuable insights into the threat landscape. Bob decides to cluster the spam messages.

Cluster analysis is an exploratory technique aimed at grouping data entities, such that entities in the same group are similar and entities in different groups are dissimilar. The definition implies the existence of a similarity model. Let D be a data table consisting of d attributes (columns) and n entities (rows). In this paper we focus on multi-dimensional (MD) similarity models, i.e. models which include similarity information from all d attributes.

A well known MD similarity model was proposed by Gower and extended by Kaufman and Rousseeuw (Gower, 1971; Kaufman and Rousseeuw, 2009). It can be applied to datasets containing primitive attributes of different types (such as numeric and ordinal attributes), but cannot be applied to structured attributes (such as Bob's email addresses and keyword sets). In these cases, many authors, such as Kaufman and Rousseeuw or Everitt et al., advocate the aggregation of by-attribute similarity functions, $S_1,\dots,S_d$, with a weighted mean. (Kaufman and Rousseeuw, 2009; Everitt et al., 2011) The by-attribute similarities are weighted with respect to perceived attribute importance. For example, let x and y be two entities with 4 attributes in Bob's dataset. Bob obtains a vector σ of four similarity values by applying the four by-attribute similarity functions $S_1,\dots,S_4$ as follows:

$$\begin{aligned}\sigma &= (S_1(x,y),S_2(x,y),S_3(x,y),S_4(x,y))\\ &= (0.1,0.4,0.8,0.4).\end{aligned} \tag{1}$$

Bob then uses the weighted mean with a weight vector w to aggregate the by-attribute similarities in σ to a single MD similarity for x and y as follows:

$$\begin{aligned}S_{WM}(x,y) &=< w,\sigma >\\ &= (0.1,0.4,0.4,0.1)\cdot(0.1,0.8,0.9,0.2)^T\\ &= 0.71\end{aligned} \tag{2}$$

However, Thonnard et al. claim that this approach does not work for datasets like Bob's (Thonnard et al., 2010). Instead, these authors proposed TRIAGE, which replaces the weighted mean with other aggregation functions, such as the ordered weighted average (OWA) or the discrete Choquet integral. OWAs were introduced by Yager and include a sorting step prior to the application of a weight vector (Yager,

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1988). For example, if Bob decided to apply OWA to σ in Equation 1 using the weight vector w in Equation 2, he would do so as follows:

$$\begin{aligned} S_{OWA}(x,y) &= < w, sort(\sigma) > \\ &= (0.1, 0.4, 0.4, 0.1) \cdot (0.9, 0.8, 0.2, 0.1)^T \\ &= 0.5 \end{aligned} \tag{3}$$

The Choquet integral enables the weighting of both individual attributes and data subspaces (Choquet, 1954). These aggregation functions provide users with more flexibility when modelling multi-dimensional similarity. The OWA can be made more robust with respect to outliers by simply giving the largest and smallest similarities a low weight (see Equation 3). The Choquet integral can be configured to adapt to automatically to data subsets with different statistical properties. However, this flexibility and adaptability comes at the cost of an increased complexity. Beliakov et al. provide an practical introduction to aggregation functions for the interested reader (Beliakov et al., 2007).

TRIAGE is well suited to datasets like Bob's. His dataset consists of a mixture of attribute types, some of which are structured. Each cluster may only be visible in a different subset of attributes. This is because spammers attempt to obfuscate their activities by varying the attributes of emails and each spammer uses a different variation strategy.

The TRIAGE approach employs graph-based algorithms to cluster the data, which responds to two further properties of Bob's dataset. Firstly, his clusters vary significantly in size and shape; some campaigns are large-scale (e.g. advertising for fake medication), others are more focused (e.g. phishing attacks on specific organisations). Secondly, the number of clusters cannot be specified a-priori.

1.1 The Problem

The TRIAGE pipeline is summarised in Figure 1. It begins with the data table D. A similarity function S_i is defined for each attribute. Then an aggregation function f is applied to generate a single similarity value for each pair of entities. Finally, a graph-based clustering algorithm is applied to generate MD clusters. To facilitate exploration, the dataset is also clustered for each attribute based on the by-attribute similarities. Each clustering delivers a *null* cluster containing all entities which could not be grouped.

Our goal is not data reduction, but exploration. We group entities automatically to gain insight by examining the groups. But, due to the use of aggregation functions, such as OWA and the Choquet integral, it is not always intuitively clear how the similarities of a given pair of entities were aggregated. Thus, the clusterings which result from TRIAGE are often difficult to interpret.

We present a linked, matrix-based visualisation prototype to support the appraisal and interpretation of a TRIAGE clustering. We developed our visualisation to address two main issues. Firstly, to provide users with a useful overview of the clustering, i.e. the distribution of cluster size and density, and the similarities between clusters. Secondly, to help users understand the internal semantics clusters, i.e. the important substructures, attributes and values.

We cooperated with security analysts during the VIS-SENSE[1] research project. Based on multiple workshops and a field study during this cooperation (Fischer et al., 2014), we derived five essential analytic tasks. We used the taxonomy presented by (Shneiderman, 1996) to formalise them as follows:

(T1) *Overview* of clusters, their size and density distribution.

(T2) *Relate* multi-dimensional clusters to the by-attribute clusters.

(T3) *Zoom* and *Filter* to focus on a few clusters.

(T4) *Relate* entities within clusters to discover substructures.

(T5) *Details-on-demand* to check individual similarities or values.

In the next section we examine related work. In Section 3 we present the usage scenarios which guided our design process and the design itself. Section 4 contains a summary of the execution of usage scenarios with real-world datasets. We also discuss the limitations and potential improvements of our prototype. Finally, we end the paper with our conclusions in Section 6.

2 RELATED WORK

To respond to the tasks **(T1)** to **(T5)**, we need a means to assess and explore both clusterings (**T1**) and individual clusters (**T3**, **T4** and **T5**). An additional requirement is support for the comparison of different clusterings with respect to different attributes (**T2**). We have focussed on techniques supporting cluster analysis in multi-dimensional, heterogeneous datasets. We present an in depth survey of matrix visualisations, since matrices play a central role in our prototype.

[1] http://www.vis-sense.eu

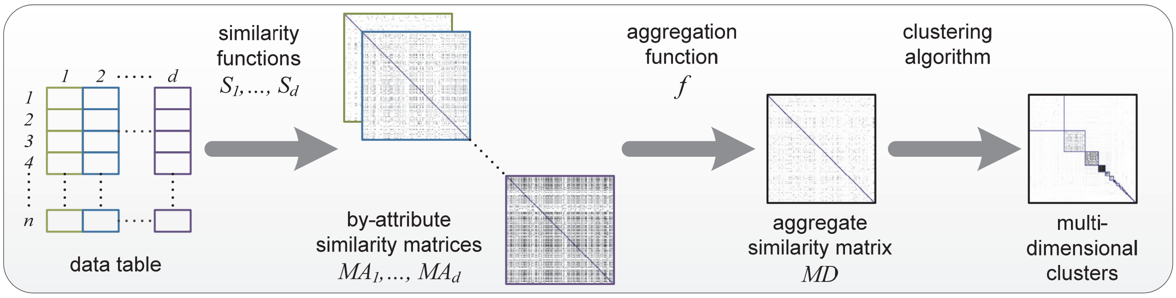


Figure 1: The generic multi-dimensional clustering pipeline. Starting with the input data table, a similarity matrix is calculated for each attribute. An aggregation function is applied to fuse the by-attribute similarities. Finally, the clustering algorithm is executed to obtain multi-dimensional clusters.

Exploring Heterogeneous Data. Classical spreadsheets were extended in the 1990s to support larger datasets and improved interaction. Prominent examples include TableLens (Rao and Card, 1995) and Focus (later InfoZoom) (Spenke et al., 1996). Spreadsheets are simple, compact and intuitive, but sorting is the only meaningful way to compare attributes. To maintain the table metaphor the same sorting must be applied to all attributes. Thus, it is often impossible to find a sorting which exposes dependencies between three or more attributes.

Parallel Coordinate Plots (PCPs) are an established technique for the visualisation of multidimensional data. They suffer from chronic overplotting, but have been subject to many optimisations to improve readability in cluster-identification tasks. However, Holten and van Wijk showed that many of these changes had no measurable effect (Holten and van Wijk, 2010). Li et al. also showed that scatterplots perform better than PCPs in the judgement of correlation between attributes (Li et al., 2008).

Sankey diagrams have also been used for cluster comparison tasks (Lex et al., 2010). They are similar to PCPs, but overplotting is reduced by plotting entity groups rather than individual entities. Lines between groups indicate entity co-occurrence. The width of lines is proportional to the number of entities which co-occur. The technique suffers from two major drawbacks; when the number of clusters is large then edge crossings reduce readability, and two clusterings must be adjacent to one another to enable effective comparison.

Matrix Visualisations. All the above techniques are focused on visualising *entities*. An alternative is to visualise the *similarity* between entities. Similarity-based projections and node-link diagrams with edge-weight-based layouts include this similarity information implicitly. However, visualising the similarity matrices themselves provides analysts with direct access to a similarity-based view of the data.

Matrices are an established method for the visualisation of relational data. They were first proposed as a visual aid for exploratory data analysis by Jacques Bertin in 1967 (Bertin and Berg, 2010). While matrices are used in the statistics and data-mining communities, node-link diagrams have generally been preferred by the visualisation community. Recently, increases in dataset size have led to renewed interest in matrices, because they are more compact than node-link diagrams. Prominent examples are Matrix Zoom (Abello and van Ham, 2004), Matrix-Explorer (Henry and Fekete, 2006), NodeTrix (Henry et al., 2007) and GreenTea (Wong et al., 2013). Matrix Zoom supports the navigation of large, hierarchically clustered graphs, exploiting the hierarchy to enable zooming while optimising the use of screen real estate and RAM. However, the cluster hierarchy is an essential prerequisite for the system. MatrixExplorer provides the user with two coordinated views (a matrix and a node-link diagram) on the same data. NodeTrix takes this approach one step further by combining the views to a hybrid visualisation. GreenTea provides a linked visualisation of one graph as a node-link diagram and a matrix of the shortest-path distances between nodes. MatrixExplorer, NodeTrix and GreenTea do simplify certain tasks, but they sacrifice the compactness of the matrix.

Both Ghoniem et al. and Keller et al. conducted user studies comparing matrices and node-link diagrams (Ghoniem et al., 2005; Keller et al., 2006). They came to the conclusion that matrices were a better choice for large, dense graphs in information retrieval tasks. Except for node and edge count estimations (considered by Ghoniem et al.), these tasks are not applicable to our use case, but encouraging nonetheless.

GAP (Wu et al., 2010), MIMatrixViz (Bremm et al., 2010) and CLUSION (Strehl and Ghosh, 2003) are pure matrix visualisations, and thus most similar to our approach. GAP combines an entity similarity matrix, an attribute similarity matrix and a data-table heatmap in a single display. The approach enables the simultaneous exploration of both clusters and attribute subspaces. MIMatrixViz enables the simultaneous display of two matrix representations of the same data. It supports zooming, panning and details on demand and provides a customised matrix seriation (also known as matrix sorting or reordering) algorithm. CLUSION uses a coarse seriation algorithm to provide users with a quick, compact overview of a dataset partitioned into a predefined number of clusters of similar size. The authors compared their approach with PCP and projection techniques to illustrate the usefulness of matrices in cluster assessment. Behrisch et al. present a different take on matrices (Behrisch et al., 2014). The authors support navigation in large sets of matrices with the help of a novel distance function. While this work is related to ours, the focus is more on matrix search and retrieval tasks than on the simultaneous display of multiple views on the same data.

We go beyond the state of the art by using multiple, linked matrices (one per attribute) to provide multiple views of the data. We use the matrices as a generic visual metaphor, which remains consistent across heterogeneous attribute types. Our prototype includes established interactive mechanisms, such as zooming, panning and seriation. Finally, we have included an interactive sampling mechanism to enable the fluid exploration of large datasets at multiple levels of detail. Our prototype enables the easy comparison of by-attribute and multi-dimensional clusterings, to help users to validate clusterings and discover interesting data subspaces. Through zooming and resampling users can examine single clusters in detail to understand why they were formed.

3 DESIGN AND IMPLEMENTATION

To guide our design process we defined a series of typical usage scenarios. We use these scenarios to present and assess the usability of our approach in Section 4. The scenarios are as follows:

(S1) Assess the overall clustering; i.e. the number, density and distribution of clusters **(T1)**. Identify interesting attributes **(T2)**.

(S2) Assess the null cluster (i.e. the entities which could not be grouped). Identify structures in the null cluster which may indicate the presence of groups which were missed, and thus a poor clustering **(T2)**. Remove the null cluster and resample the data **(T3)**.

(S3) Assess an MD cluster in its context. Assess its quality (i.e. density and semantics) and similarity to other clusters **(T2)**. Identify those attributes which contributed most to the formation of the cluster and those attributes which did not contribute to the formation of the cluster **(T2)**.

(S4) Focus on one MD cluster **(T3)**. Apply local sorting to reveal substructures **(T4)**. Relate the substructures to clusters in attributes **(T2)**. Formulate a domain-dependant interpretation of the cluster, using the values involved (i.e. find the story behind the cluster) **(T5)**.

Our prototype (shown in Figure 2) is a coordinated display of similarity matrices. One matrix for each attribute and a multidimensional (MD) similarity matrix are displayed simultaneously. All the matrices are symmetric, meaning that the rows and columns are interchangeable. We apply the same sorting to the rows and columns of each matrix to ensure that the symmetry is clearly visible. However, we sort each matrix individually, such that the structures relevant for that matrix stand out. Each row (or column) corresponds to a single entity in the dataset. Each matrix cell contains the similarity score between the corresponding column entity and row entity. The cells are all in the range $[0,1]$, which is mapped to a colour map generated in accordance with Ware's guidelines (Ware, 2013); light cells indicate low similarity and saturated cells indicate high similarity. Each matrix can be zoomed and panned. Hovering over any cell in the matrix causes a tooltip to be shown containing the pair attribute values corresponding to the cell together with their similarity score.

The matrix entries are initially sorted by cluster label using the coarse seriation method described below. Thus, entities in the same cluster are placed adjacent to one another, which normally results in a block-diagonal form (see Figure 3). Each block on the diagonal of the matrix corresponds with a cluster in the dataset. We will use the terms *diagonal block* and *cluster* interchangeably when referring to the matrix visualizations.

Frames are overlaid over the cluster boundaries in the matrices to assist the user in cluster perception. We use the grid induced by these cluster boundaries to divide the matrix into brushable regions. When a user clicks on a cluster the entities contained in that cluster are highlighted; all rows and columns corresponding to the entities in the cluster are marked red. Since the matrices are linked, the brushed entities are highlighted in all the matrices simultaneously, not only in the matrix which was clicked. This allows a user to immediately see whether a cluster in one attribute is clustered or scattered in the other attributes.

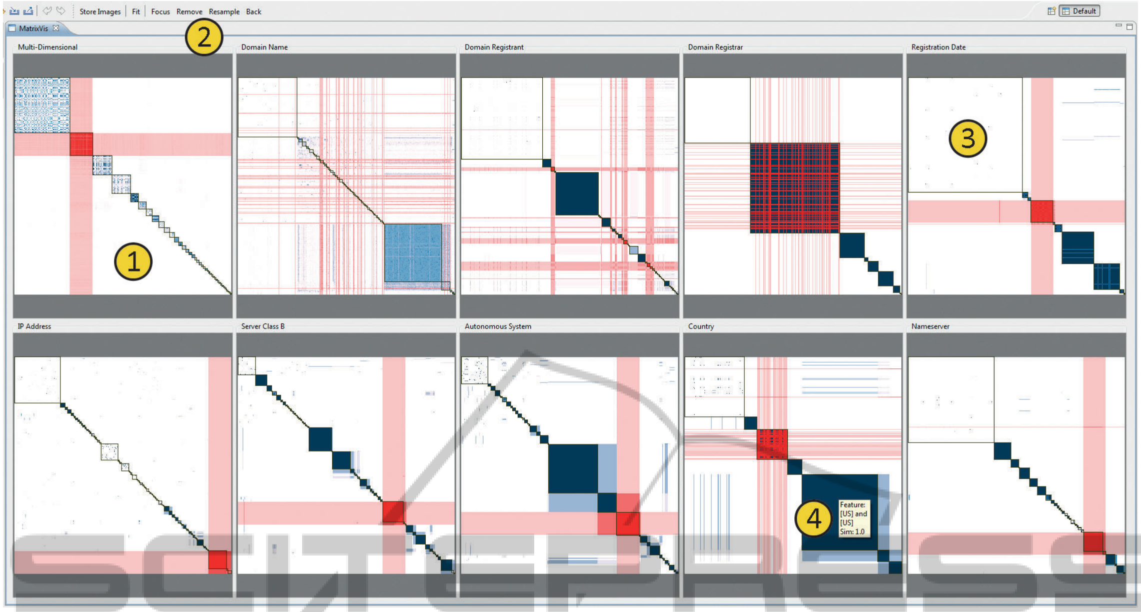


Figure 2: Overview of our prototype, which consists of a coordinated display of matrices. The top left matrix (1) is the multidimensional similarity matrix, the others are by-attribute similarity matrices. Global actions are available in the toolbar (2). Null clusters are always displayed as the top left cluster of each matrix (3). Tooltips reveal data values and similarity scores (4). In this view a cluster in the *Multi-Dimensional* matrix was selected. It is quite salient and, thus, compact. It is easy to see that the attributes *Domain Name*, and *Domain Registrant* did not contribute to the formation of this cluster, since the highlighted entities are scattered in these matrices. The other attributes made clear contributions to the formation of the cluster, since the highlighted entities here are tightly grouped and fall in a single cluster in almost all cases.

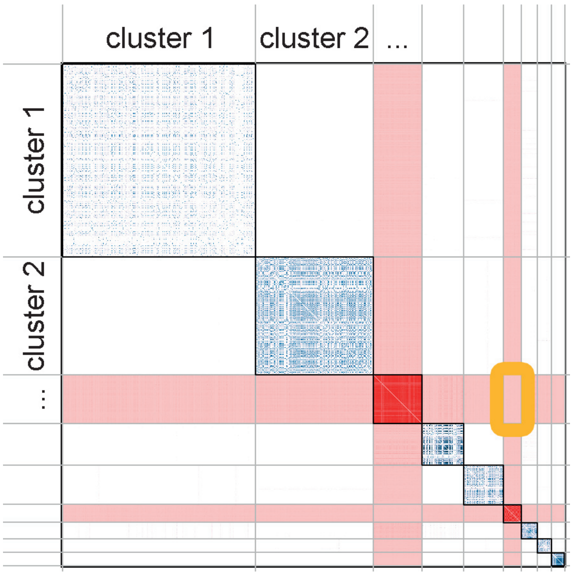


Figure 3: The initial sorting by cluster label produces a block diagonal form. Saturated matrix cells indicate a high similarity. The clusters are overlaid with boundary lines (black). A grid of brushable regions is induced by the blocks (grey lines — not visible in the actual visualisation). Rows and columns corresponding to the selected entities are highlighted (in red). The grid cell framed in orange was clicked to make the current selection. A matrix with empty off-diagonal blocks was chosen to simplify this figure. In general, the off-diagonal blocks are not empty.

When a user clicks on an off-diagonal region the adjacent clusters are highlighted. Arbitrary regions can be brushed by clicking and dragging.

3.1 Interactive Sampling

The datasets we have considered range in size from 5 000 to 10 000 entities. It is generally not useful to display the full-sized matrices, since their allocated screen space is too small and the quadratic increase in memory requirements can lead to RAM exhaustion. Ellis and Dix published a taxonomy and comparison of data reduction strategies for information visualisation (Ellis and Dix, 2007). Sampling was the strategy which fulfilled most of the authors' criteria and was the strategy which the authors had used successfully in the past (Ellis and Dix, 2002). Thus, we employ a sampling mechanism for data reduction.

Our sampling strategy is focused on the MD matrix, since this is the most important matrix in the analysis. When a dataset is loaded, an initial sampling is generated using the following guidelines:

- The sample must contain at least one element from each cluster,
- The sample must be as close as possible to uniformly distributed, and

- The sample must contain approximately N elements, where N is a predefined target sample size.

The first guideline ensures that no clusters are overlooked. At present we use a target size of $N = 1\,000$, which enables an initial period of interactive zooming and panning, and is a reasonable compromise between detail and RAM load.

After the application of filters, the displayed data resolution may become low. A user can then initiate a re-sampling of the data. In this case, the following guidelines are followed:

- The new sample must have the same distribution with respect to the *MD* matrix clusters as the current sample, and
- The sample must contain a maximum of N elements.

Since we know the size of the datasets and clusters a priori the target distributions are achieved by pseudorandomly sampling a targeted number of integer indices from each cluster. When zooming into clusters, the number of entities available may be less than the target size N. In this case, the available entities are simply displayed (i.e. the sample is equal to the dataset).

3.2 Matrix Seriation

Mueller et al. provide a guide to the interpretation of similarity matrices (Mueller et al., 2007b). Important visual features in cluster analysis are on-diagonal and off-diagonal blocks. On-diagonal blocks can be interpreted as strongly connected subgraphs. The darker and denser the blocks are, the higher the edge weights and the degree of connectedness. White space indicates the presence of dissimilar entity pairs. When a lot of white space is present, the block should be reordered to reveal substructures (Mueller et al., 2007b).

Off-diagonal blocks indicate the presence of bipartite subgraphs, i.e. connections between clusters (Mueller et al., 2007b). Again, the darker and denser the blocks, the stronger the inter-cluster connections.

For the initial display of the matrices we follow the same coarse seriation approach as CLUSION (Strehl and Ghosh, 2003). This provides the user with a good initial impression of the number of clusters, their size distribution and density distribution, as well as inter-cluster connections. Due to the different nature of our clustering algorithms, we had to adapt the Strehl and Gosh seriation. In particular, their algorithm delivers cluster labels in an order, which places similar clusters adjacent to one another (Strehl and Ghosh, 2003). In our system this is not the case. Our coarse seriation algorithm is summarised below.

- The order of the entities in a cluster is randomised to ensure that cluster substructures do not appear in the initial overview (aggregate cluster properties are important in the overview, salient substructures may distract the user).
- A meta-graph is constructed based on the clustering; a node represents each cluster and the aggregate similarity between each cluster pair results in an edge weight.
- Seriation is carried out on the data of the meta-graph and a sorted list of cluster labels is returned.
- The original matrix is sorted by cluster label based on the returned list.

The null cluster is not considered in the sorting process. It is always placed as the top left block on the diagonal.

After applying filters and re-sampling, the coarse seriation loses its usefulness. Due to the random sorting, cluster substructures cannot be seen. To resolve this issue, the user can apply a fine seriation to a matrix by right-clicking. Like Wong et al. we provide a selection of seriation algorithms to the user (Wong et al., 2013).

Most of the seriation algorithms attempt to transform the matrix, such that its non-zero elements are close to the diagonal. It is important to note that the results of many of the algorithms are dependent on the initial sorting of the matrix (Mueller et al., 2007a). Thus, the application of multiple seriations sequentially can lead to an improved overall visual result.

In addition to the interactions described above we provide a set of functions which can be applied to all matrices simultaneously:

Refit all the displayed matrices to maximise their use of display space. This function is useful when the available display space changes.

Remove the selected entities from the current display.

Focus on the selected entities by removing all unselected entities from the current display.

Re-sample the dataset (described in detail above).

Back go one step back in the interaction history.

4 USAGE SCENARIOS

To present and assess the usability of our approach we carried out the scenarios defined in Section 1 with three datasets from the cyber-security domain.

Table 1: A summary of the three datasets used for the usage scenarios.

Dataset	Entities (n)	Attributes (d)	MD Clusters	Null Cluster Size
SGNET	10 162	22	21	931 (9% of entities)
HARMUR	5 852	10	42	1 866 (32% of entities)
419SCAM	4 688	6	103	(Null cluster removed)

The first dataset is a subset taken from the SGNET project (Leita and Dacier, 2008), the second is a subset from the HARMUR project (Leita and Cova, 2011) and the third is a subset from the 419SCAM email archive (Isacenkova et al., 2013). The SGNET dataset is a collection of malware samples collected from a globally deployed network of honeypots. It contains attributes regarding the source host, destination host, exploit used to spread the malware and various descriptive attributes of the malware itself. The HARMUR dataset is a collection of blacklisted websites. It contains the domain names, information on the host servers and details on the registration of the domains. The 419SCAM email archive contains a set of real scam emails which employ a variety of strategies to extract money from innocent citizens (e.g. bogus sales or prizes). The attributes extracted include telephone numbers and email addresses found in the body of the email, the subject line and header information.

Each dataset consisted of a heterogeneous mixture of attributes. Each dataset had already been clustered and we had access to the raw data, the similarity matrices and cluster labels for each attribute, as well as the aggregated (MD) similarity matrix and cluster labels. A summary of the properties of the datasets is shown in Table 1.

We used a single screen with a resolution of 1920 x 1080 to carry out the usage scenarios. The prototype was optimised to make maximal use of a screen of this size. In the following paragraphs we discuss our observations when carrying out each of the usage scenarios.

Scenario (S1): The number of clusters, their size and density could be perceived for all attributes. This was also the case when the display was crowded (e.g. when viewing the SGNET dataset.) Redundant attributes could easily be identified, since they showed similar block-diagonal patterns. Less useful attributes could be also be identified; these either had large null clusters or consisted of a very large number of small clusters.

The different types of similarity functions used led to visually distinct matrices (see Figure 4). Simple matching led to a clean block-diagonal structure with dark blocks and white off-diagonal regions. Similarity matrices resulting from string comparison were more noisy. The MD matrices were generally noisier than the others; the SGNET matrix had numerous salient off-diagonal blocks, the other two matrices had fewer.

Uneven textures within on-diagonal blocks alluded to the presence of sub-clusters. These textures were strongest in the MD matrices.

The smallest clusters were difficult to assess without zooming, due to the small amount of screen space they occupied. This was particularly problematic in the 419SCAM dataset.

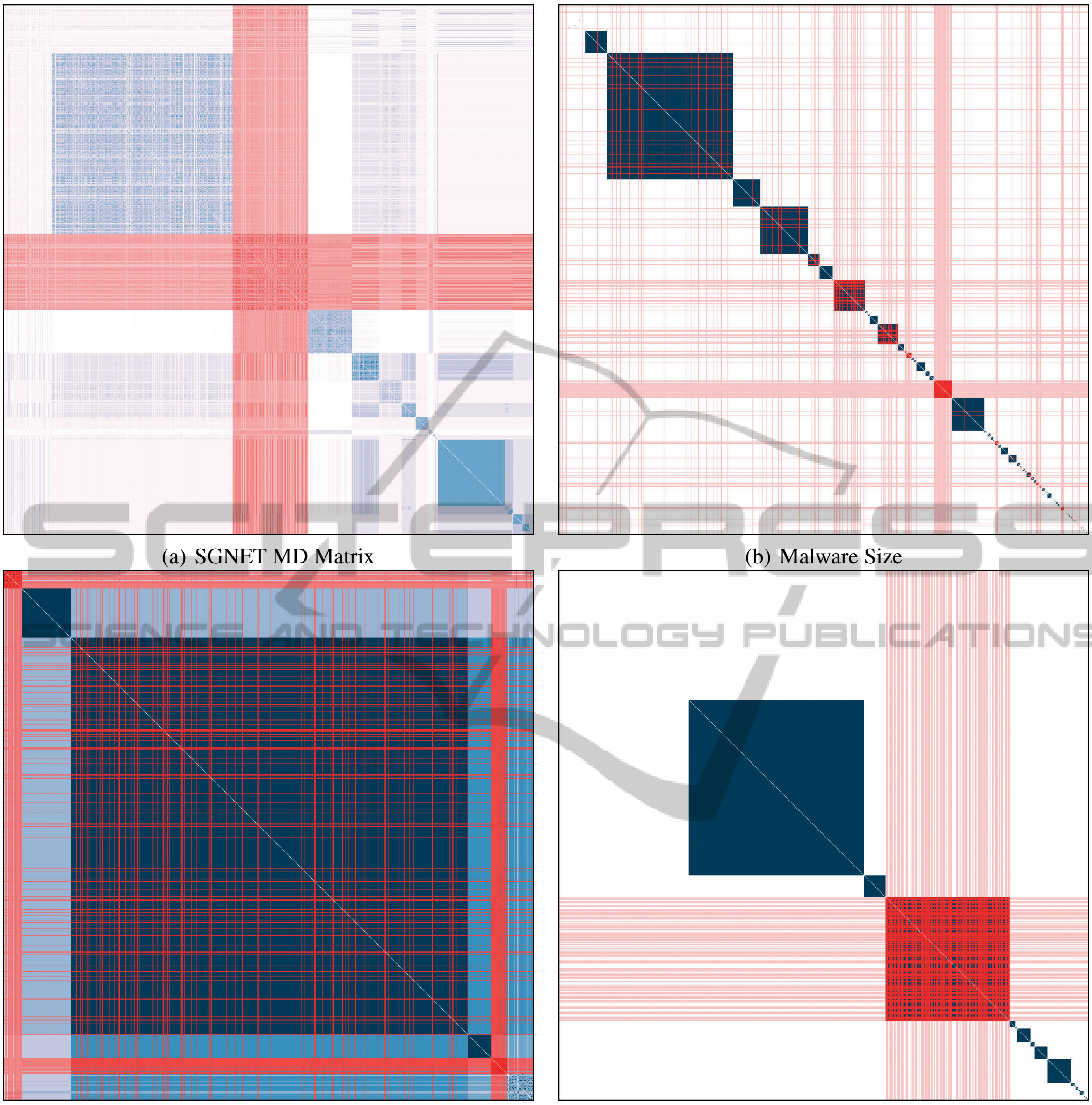
Scenario (S2): The null clusters could easily be selected and focussed on. Re-sampling and sorting enabled easy assessment. No significant substructures were identified in HARMUR or SGNET, thus they could be safely removed. The datasets were then re-sampled to increase their resolution.

Scenario (S3): Brushing a cluster quickly revealed those attributes which were involved in its formation (highlighted rows and columns which were tightly bunched) and those attributes which were not (highlighted rows and columns which were scattered). This is shown in Figure 4. Salient off-diagonal blocks could be brushed to highlight the corresponding clusters simultaneously and examine the similarities between them. In all the datasets darker clusters were generally easier to explain than lighter clusters.

Small clusters were difficult to select without zooming. We applied the following strategy to deal with this problem: we assessed and removed the largest clusters, then re-sampled to increase the resolution and repeated the process.

In the 419SCAM dataset we discovered a near one-to-one correspondence between telephone numbers and MD clusters. In the SGNET dataset we discovered an MD cluster with light, but uniform colouring, which is very unusual. Brushing revealed that the most prominent feature was the MD5 hash of the malware samples; i.e. the samples in the cluster were all identical. The colouring had been *brightened* by the other attributes, which were not uniform.

Scenario (S4): As mentioned above, darker clusters could generally be explained without the need for focussing. In the SGNET dataset it was useful to focus on a small set of similar clusters, rather than a single cluster. This was easy to achieve with our prototype.



(a) SGNET MD Matrix

(b) Malware Size

(c) Executable Sections

(d) Operation Summary

Figure 4: The *MD* and *Malware Size* matrices are visually distinct due to their generating similarity functions. The *Malware Size* and *Execution Sections* matrices are clearly less relevant than the *Operation Summary* matrix for the formation of the brushed cluster.

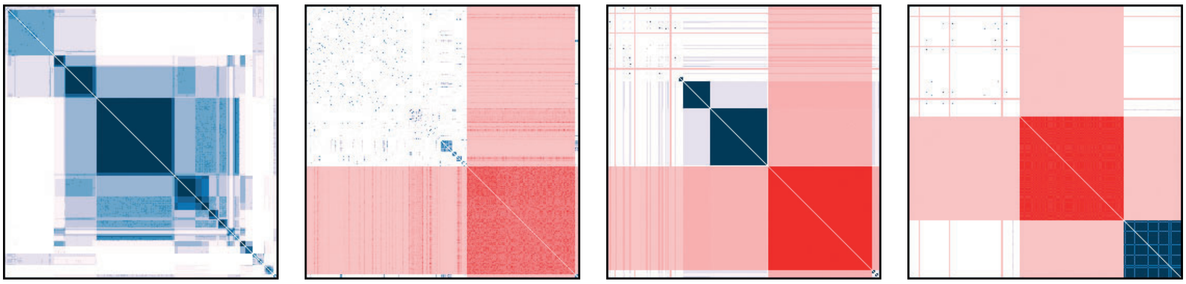
Focussing on the fourth largest HARMUR cluster, we were able to identify a strong sub-cluster, which could probably be separated from the other entities in the cluster. A set of missing values led to its inclusion in the larger cluster (see Figure 5).

We examined 3 clusters with multiple telephone numbers in the 419SCAM dataset. Sorting and brushing revealed that the telephone numbers defined cluster sub-structures. The other attributes were responsible for holding the clusters together.

The temporal attribute in the 419SCAM dataset became useful when examining the internals of clusters. However, it was difficult to use, since the clusters in this matrix were not sorted by date.

5 DISCUSSION

The goal of our prototype was to support the exploration of clusters generated by the TRIAGE framework. We chose a common, similarity-based representation for all attributes; the matrix. The cho-



(a) HARMUR MD Matrix (b) Domain Name (c) Creation Date (d) Registrar

Figure 5: A zoomed view of the fourth cluster in the HARMUR dataset. A salient subcluster is visible. Highlighting reveals a group of similar domain names registered on the same day using the same address. Some missing values in the *Creation Date* and *Registrar* led to linkage of this cluster with a larger group of entities.

sen representation is not dependent on attribute type, enabling a homogeneous presentation of a heterogeneous set of attributes. With the help of brushing and linking we were able to coordinate the matrix displays. Panning, zooming and filtering enabled detailed exploration of multi-dimensional clusters for datasets of up to around 20 attributes.

At present, we support datasets of up to around 10 000 entities. While this is a comparatively small amount of raw data, the matrices generated each contain around $10\,000^2$ entries. Handling the problem thus becomes challenging despite the small size of the raw data. In addition, the high complexity of the clustering algorithms prohibits the consideration of much larger datasets.

We could successfully carry out the usage scenarios defined above. However, they did reveal two weaknesses in our prototype. Firstly, matrices containing many small clusters were difficult to explore, since the clusters only occupied small amounts of screen space. Secondly, the matrices were not always an ideal representation. The user should have access to more appropriate representations of temporal attributes. This problem could also be solved by introducing other seriation methods (e.g. sort in ascending order). In addition, we noticed that for certain similarity functions (e.g. simple matching) the matrices could be replaced with simpler representations. However, the representation of the attributes would then no longer be heterogeneous.

The requirement for sampling is potentially a major limitation of our work. For every dataset with n entities, there is a minimum percentage p of entities which is required in a uniform sample to reproduce the distribution of the original dataset. The percentage of entities required is entirely dataset dependent, so we cannot actually specify a maximum dataset size for our system. If $p \times n$ is much larger than the sample size, then our approach will not work.

It is worth noting that the TRIAGE approach is conceptually close to subspace clustering in high-dimensional data (Vidal, 2011). Subspace clustering is an extension of traditional clustering techniques that seeks to find clusters in different subspaces within a dataset. In high-dimensional data, many attributes are often irrelevant and can mask existing clusters by adding noise. Subspace clustering algorithms localise the search for relevant attributes, which allows them to find clusters that exist in multiple, possibly overlapping subspaces (Kriegel et al., 2009; Parsons et al., 2004). A possible direction for future work is to include overviews of attribute relationships, such as the correlation view in GAP (Wu et al., 2010). This could facilitate the application of our technique to datasets with more attributes by including interactions to filter and group attributes. It would also enable explicit support for data subspace exploration tasks, which are important in subspace clustering applications.

As mentioned in Section 2 user studies such as those by Ghoniem et al. and Keller et al. and which compare matrices to node-link diagrams are generally focused on information retrieval tasks (Ghoniem et al., 2005; Keller et al., 2006). To the best of our knowledge there are no studies which examine the exploratory tasks we have presented in matrices. We see this as a promising avenue for future work.

6 CONCLUSIONS

We presented a linked, matrix-based visualisation prototype for the appraisal and interpretation of clusters delivered by the TRIAGE framework. A key challenge we addressed was to assist the user in effectively interpreting clusterings delivered by the framework. Our prototype used matrices to provide a consistent visual metaphor across multiple heterogeneous attributes. With the help of coarse seriation, a compact overview was generated for user appraisal of overall clustering results. Zooming and filtering capabilities combined with brushing and linking allow the detailed exploration of clusters to understand how and why they were formed. A fine seriation functionality enables users to gain an understanding of cluster substructures. Finally, a sampling mechanism enables the fluid exploration of large data sets at multiple levels of detail.

Our design was guided by four usage scenarios, which were used to demonstrate and assess the prototype. The usage scenarios were carried out successfully with real-world datasets from the cyber-security domain. However, they did reveal some weaknesses in our approach.

Our prototype was developed for the TRIAGE approach to cluster analysis. It is generic enough to be used with similar clustering pipelines.

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REFERENCES

Abello, J. and van Ham, F. (2004). Matrix zoom: A visual interface to semi-external graphs. In *IEEE Symposium on Information Visualization*, pages 183–190.

Behrisch, M., Davey, J., Fischer, F., Thonnard, O., Schreck, T., Keim, D., and Kohlhammer, J. (2014). Visual analysis of sets of heterogeneous matrices using projection-based distance functions and semantic zoom: Visual analysis of sets of heterogeneous matrices. *Computer Graphics Forum*, 33(3):411–420.

Beliakov, G., Pradera, A., and Calvo, T. (2007). *Aggregation Functions: A Guide for Practitioners*, volume 221. Springer Berlin Heidelberg, Berlin and Heidelberg.

Bertin, J. and Berg, W. J. (2010). *Semiology of graphics: Diagrams, networks, maps*. ESRI Press and Distributed by Ingram Publisher Services, Redlands and Calif, 1st ed edition.

Bremm, S., Schreck, T., Boba, P., Held, S., and Hamacher, K. (2010). Computing and visually analyzing mutual information in molecular co-evolution. *BMC Bioinformatics*, 11(1):330.

Choquet, G. (1954). Theory of capacities. *Annales de l'institut Fourier*, 5:131–295.

Ellis, G. and Dix, A. (2002). Density control through random sampling: an architectural perspective. In *Sixth International Conference on Information Visualisation*, pages 82–90.

Ellis, G. and Dix, A. (2007). A taxonomy of clutter reduction for information visualisation. *IEEE transactions on visualization and computer graphics*, 13(6):1216–1223.

Everitt, B. S., Landau, S., Leese, M., and Stahl, D. (2011). *Cluster Analysis*. John Wiley & Sons.

Fischer, F., Davey, J., Fuchs, J., Thonnard, O., Kohlhammer, J., and Keim, D. A. (2014). A visual analytics field experiment to evaluate alternative visualizations for cyber security applications. In *EuroVis Workshop on Visual Analytics*, pages 43–47, Swansea, UK. Eurographics Association.

Ghoniem, M., Fekete, J.-D., and Castagliola, P. (2005). On the readability of graphs using node-link and matrix-based representations: a controlled experiment and statistical analysis. *Information Visualization*, 4(2):114–135.

Gower, J. C. (1971). A general coefficient of similarity and some of its properties. *Biometrics*, 27(4):857.

Henry, N. and Fekete, J. (2006). MatrixExplorer: a dual-representation system to explore social networks. *IEEE Transactions on Visualization and Computer Graphics*, 12(5):677–684.

Henry, N., Fekete, J.-D., and McGuffin, M. J. (2007). NodeTrix: a hybrid visualization of social networks. *IEEE Transactions on Visualization and Computer Graphics*, 13(6):1302–1309.

Holten, D. and van Wijk, J. J. (2010). Evaluation of cluster identification performance for different PCP variants. *Computer Graphics Forum*, 29(3):793–802.

Isacenkova, J., Thonnard, O., Costin, A., Balzarotti, D., and Francillon, A. (2013). Inside the SCAM jungle: A closer look at 419 scam email operations. In *2013 IEEE Security and Privacy Workshops (SPW)*, pages 143–150.

Kaufman, L. and Rousseeuw, P. J. (2009). *Finding Groups in Data: An Introduction to Cluster Analysis*. John Wiley & Sons.

Keller, R., Eckert, C. M., and Clarkson, P. J. (2006). Matrices or node-link diagrams: which visual representation is better for visualising connectivity models? *Information Visualization*, 5(1):62–76.

Kriegel, H.-P., Kröger, P., and Zimek, A. (2009). Clustering high-dimensional data: A survey on subspace clustering, pattern-based clustering, and correlation clustering. *ACM Trans. Knowl. Discov. Data*, 3(1):1:1–1:58.

Leita, C. and Cova, M. (2011). HARMUR: Storing and analyzing historic data on malicious domains. In Kirda, E. and Holz, T., editors, *Proceedings of the First Workshop on Building Analysis Datasets and Gathering Experience Returns for Security (BADGERS)*, pages 46–53.

Leita, C. and Dacier, M. (2008). SGNET: A worldwide deployable framework to support the analysis of malware threat models. In *2008 Seventh European Dependable Computing Conference EDCC*, pages 99–109.

Lex, A., Streit, M., Partl, C., Kashofer, K., and Schmalstieg, D. (2010). Comparative analysis of multidimensional, quantitative data. *IEEE Transactions on Visualization and Computer Graphics*, 16(6):1027–1035.

Li, J., Martens, J.-B., and van Wijk, Jarke J (2008). Judging correlation from scatterplots and parallel coordinate plots. *Information Visualization*, 9(1):13–30.

Mueller, C., Martin, B., and Lumsdaine, A. (2007a). A comparison of vertex ordering algorithms for large graph visualization. In *Asia-Pacific Symposium on Visualisation 2007*, pages 141–148.

Mueller, C., Martin, B., and Lumsdaine, A. (2007b). Interpreting large visual similarity matrices. In *Asia-Pacific Symposium on Visualisation 2007*, pages 149–152.

Parsons, L., Haque, E., and Liu, H. (2004). Subspace clustering for high dimensional data: A review. *SIGKDD Explor. Newsl.*, 6(1):90–105.

Rao, R. and Card, S. K. (1995). Exploring large tables with the table lens. In *Conference Companion on Human Factors in Computing Systems*, CHI '95, pages 403–404, New York, NY, USA. ACM.

Shneiderman, B. (1996). The eyes have it: a task by data type taxonomy for information visualizations. In *1996 IEEE Symposium on Visual Languages*, pages 336–343.

Spenke, M., Beilken, C., and Berlage, T. (1996). FOCUS: The interactive table for product comparison and selection. In *Proceedings of the 9th Annual ACM Symposium on User Interface Software and Technology*, UIST '96, pages 41–50, New York, NY, USA. ACM.

Strehl, A. and Ghosh, J. (2003). Relationship-based clustering and visualization for high-dimensional data mining. *INFORMS Journal on Computing*, 15(2):208–230.

Thonnard, O., Mees, W., and Dacier, M. (2010). On a multicriteria clustering approach for attack attribution. *ACM SIGKDD Explorations Newsletter*, 12(1):11.

Vidal, R. (2011). Subspace clustering. *IEEE Signal Processing Magazine*, 28(2):52–68.

Ware, C. (2013). *Information Visualization: Perception for Design*. Morgan Kaufmann Publishers, Waltham and MA, third edition.

Wong, P. C., Mackey, P., Foote, H., and May, R. (2013). Visual matrix clustering of social networks. *Computer Graphics and Applications, IEEE*, 33(4):88–96.

Wu, H.-M., Tien, Y.-J., and Chun-houh Chen (2010). GAP: A graphical environment for matrix visualization and cluster analysis. *Computational Statistics & Data Analysis*, 54(3):767–778.

Yager, R. R. (1988). On ordered weighted averaging aggregation operators in multicriteria decisionmaking. *IEEE Transactions on Systems, Man, and Cybernetics*, 18(1):183–190.