

Vulnerability Clustering and other Machine Learning Applications of Semantic Vulnerability Embeddings

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Abstract. Cyber-security vulnerabilities are usually published in form of short natural language descriptions (e.g., in form of MITRE’s CVE list) that over time are further manually enriched with labels such as those defined by the Common Vulnerability Scoring System (CVSS). In the Vulnerability AI (Analytics and Intelligence) project, we investigated different types of semantic vulnerability embeddings based on natural language processing (NLP) techniques to obtain a concise representation of the vulnerability space. We also evaluated their use as a foundation for machine learning applications that can support cyber-security researchers and analysts in risk assessment and other related activities. The particular applications we explored and briefly summarize in this report are clustering, classification, and visualization, as well as a new logic-based approach to evaluate theories about the vulnerability space.

1 Introduction

For the Vulnerabilities Equities Process (VEP) [36] and more generally for Cyber-Security Risk Assessment, it is important to keep an eye on the big picture of how the cyber-security vulnerability space is structured and how it is evolving over time. Furthermore, it should be possible to quickly place newly discovered vulnerabilities in the space and support subject matter experts with tools to visualize and navigate the space. In this report on the Vulnerability AI (Analytics and Intelligence) project, we discuss a fully data-driven approach that leverages machine learning (especially natural language processing, classification, and clustering) algorithms to serve as a foundation for such tools. Our approach is centered around the generation and evaluation of semantic vulnerability embeddings on which algorithms for visualization, clustering and classification can be built. It also serves as a basis for a novel capability for vulnerability space analysis using logical theories that we briefly explore.

2 Vulnerability Datasets and Labels

To employ and validate machine learning algorithms in the proper application context we have identified the National Vulnerability Database (NIST NVD)

[27] as the most suitable dataset. It is fed from MITRE’s CVE list [25], and with about 150K entries covering the years 1999 – 2021 the most comprehensive list of publicly disclosed cyber-security vulnerabilities.

From the NVD dataset, we extract the CVE-identifier (which identifies the vulnerability), the publication date, the natural language description of the vulnerability. We furthermore extract three types of labels: The Common Weakness Enumeration (CWE) [26] label that identifies the underlying software weaknesses (typically only one but sometimes multiple weaknesses are associated with a vulnerability) that the vulnerability exploits, and a reduced version of the Common Platform Enumeration (CPE) [24] label that identifies the vendor and product in which the vulnerability was observed. Furthermore, we extract the Common Vulnerability Scoring System (CVSS) [8] labels related to the most commonly used base metrics, which have components qualitatively summarizing the impact (e.g. the confidentiality, integrity, availability impact, and the potential change of scope) and the exploitability (e.g., attack complexity, attack vector, privilege/authentication requirement, and need for user interaction). Quantitative assessments on an ad-hoc scale 0 – 10 are also available and sometimes used for our visualizations, but as these are derived scores (and as we will discuss not reflected in empirical data), our machine learning algorithms operate directly on the qualitative features for better precision. We also distinguish between CVSS V2 and V3 labels,¹ but we will gloss over these details in this summary.

It is noteworthy that labels have been added by subject matter experts and are often incomplete and sometimes not very informative (e.g., in case of CWE labels). Our machine learning workflow is designed to take labeled and unlabeled data into account. While our workflow explores predictors/classifiers for all the label categories mentioned above and others such as the year/day of publication, we use the (qualitative) CVSS labels for validating our models and focus on these in this report. In the scope of the public dataset available to us for our analysis, we consider them as the most abstract and most relevant properties in the context of the VEP and other high-level risk assessment activities.

3 Methods and Algorithms

Our workflow, which is formally defined as a graph with high-level dataflow dependencies, includes a natural language processing (NLP) stage applied to vulnerability descriptions and a number of machine learning models for dimensionality reduction, clustering, classification, and visualization. The visualization

¹ To partly bridge the differences between CVSS V2 and V3, we enrich the V2 labels with additional components (about user interaction and obtaining privileges) available in the NVD. The main remaining differences from V2 to V3 (regarding the base metrics) are the generalization of access complexity to attack complexity, the introduction of a component flagging a change of scope (typically related to privileges) and the consideration of a physical attack vector. A smaller difference is that confidentiality, integrity, and availability labels (the CIA properties) use the categories “None”, “Low”, or “High” in V3 instead of “None”, “Partial”, and “Complete”.

is not only relevant for the end-user but also allows us to gain a better understanding of the dataset and potential limitations such as missing labels.

A simplified illustration of our basic workflow is shown in Fig.1. An extension of this workflow with more advanced capabilities will be discussed in Section 7. The workflow was developed and executed using JupyterFlow [35], a framework and an engine for interactive and parallel/distributed machine-learning workflows that we developed in an earlier DARPA project.

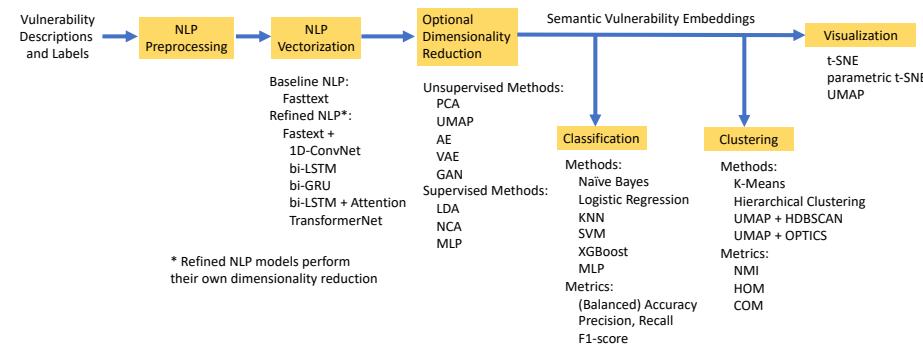


Fig. 1. Simplified Excerpt of the Vulnerability AI Workflow to Evaluate Semantic Vulnerability Embeddings and Algorithms for Classification, Clustering, and Visualization

Our NLP stage is based on Fasttext [4,15], which evolved from earlier work on representing the distributional semantics of natural language using vector-space embeddings (the most well-known being Word2Vec, see [11] for an introduction) that can be learned by training relatively simple neural networks on a large corpus of documents. The advantage of Fasttext is that by means of hashing techniques it can assign useful semantic embeddings to unknown terms (e.g. misspelled words or filenames containing pieces of natural language). For this project, we use a Fasttext model trained on Common Crawl [7] which represents a large part of the World Wide Web and hence also includes many terms and acronyms related to computer security, hardware/software platforms, and applications. Our preprocessing stage uses a number of heuristics to clean up and normalize the natural language descriptions of vulnerabilities. We also incorporate composite terms using various sources including a database of known products/applications. Similar to the Fasttext approach to sentence embeddings, the abstract vector-space representation of a vulnerability is the mean of all non-zero normalized (to the unit norm) embeddings of relevant components (i.e., words, acronyms, numbers, filenames, or composite terms that have not been discarded by our preprocessing) of the description (represented by 300-dimensional vectors). In the following, we refer to this as the baseline NLP model that because of its low complexity can be expected to have the highest generalization capability.

A more refined representation will play a role in our exploration of neural language models (in particular, convolutional networks, bidirectional GRU/LSTM networks, and transformer networks as they can be found in, e.g., [2]) that operate on the sequence of vectors representing the vulnerability description. Some of these refined NLP models are also equipped with a self-attention mechanism that can take advantage of the typical structure of CVE vulnerability descriptions to improve accuracy and other relevant metrics.

Dimensionality reduction techniques operating in the semantic space of vulnerability descriptions (obtained using our NLP pipeline) include unsupervised and supervised methods. Unsupervised methods are Principal Component Analysis (PCA, which is used as a baseline), Uniform Manifold Approximation and Projection (UMAP) [19], Autoencoders (AEs), Variational Autoencoders (VAEs) [16], and Generative Adversarial Networks (GANs) [12]. As supervised methods we employed Linear Discriminant Analysis (LDA), Neighborhood Component Analysis (NCA), and various types of Multi-Layer Perceptrons (MLPs).

A number of classification methods operating either directly on semantic embeddings or the reduced representation have been investigated. They include Naive Bayes Classifiers (baseline), k-Nearest Neighbor Classifiers, Logistic Regression, Support Vector Machines (SVM), Gradient-Boosted Decisions Trees (using the XGBoost [6] framework), and a family of Multi-Layer Perceptrons parameterized by complexity (number of hidden layers in the range 1 . . . 3). The purpose of classifiers in our workflow is twofold. First, they can be directly used as classifiers by the end-user, e.g., to label unknown or new vulnerabilities. Classifiers may also be viewed as a method to extract information from our semantic representation (e.g., in the form of CPE, CWE, CVSS or other properties). Second, and more important to us is that their evaluation provides us with metrics (e.g. accuracy) to assess the quality of our vector-space embeddings relative to the subject-matter-expert labeling. In this way, classifiers serve as an indirect evaluation tool for previous stages in the workflow, i.e., NLP and dimensionality reduction techniques.

Operating in the optionally reduced semantic space, we investigated a number of clustering algorithms, namely K-Means (baseline), Hierarchical Clustering (Ward’s method), and two different algorithms for Density-Based Clustering, namely Hierarchical Density-based Spatial Clustering of Applications with Noise (HDBSCAN) [18] and Ordering Points To Identify Cluster Structure (OPTICS) [1]. The latter two algorithms can achieve robustness to noise by using a partial clustering, which means that some vulnerabilities will not be included in clusters. The selection of these algorithms is dictated by the need to scale to a large dataset (in our case we have about 150K vulnerabilities). By operating in the dimensionality-reduced space scalability can be further improved with only a minor loss in precision.

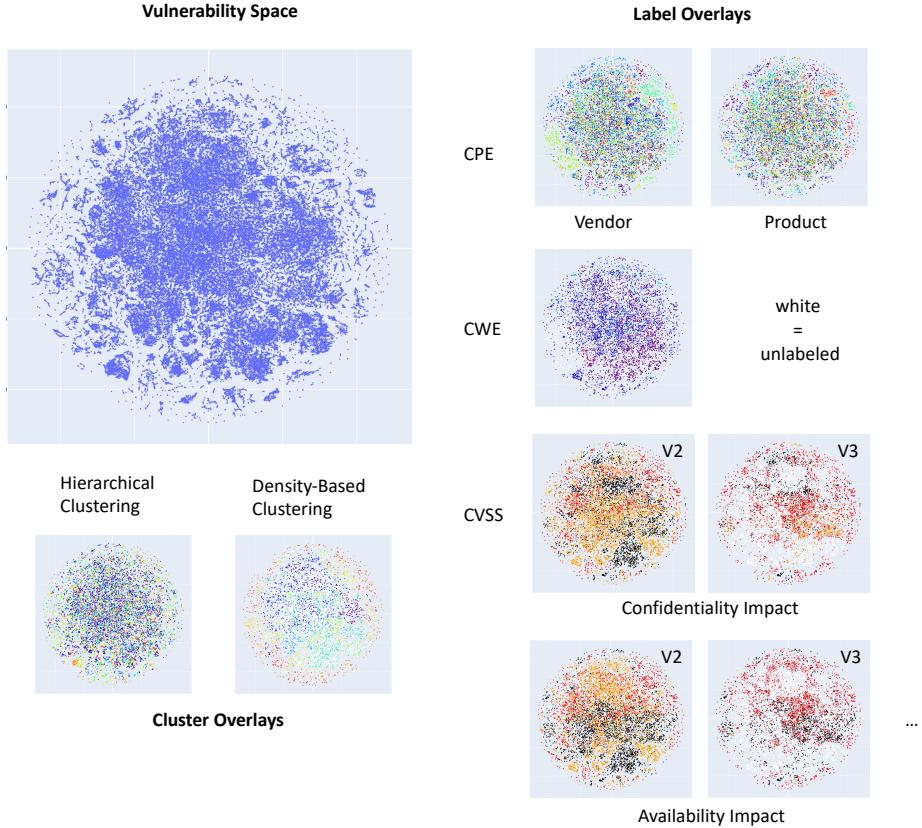


Fig. 2. The figure at the top left is a 2D t-SNE projection of all semantic vulnerability embeddings (up to 2020, about 150K) using our autoencoder-based representation. On the right, we show a subset of possible overlays using color-coded labels. At the bottom, we show clustering results as overlays for two algorithms. Clusterings and CWE labels are equipped with a hierarchical structure, which is captured by color similarity. We use the white color to denote absence of labels or no cluster assignment (in case of density-based clustering). In case of CVSS labels (we only show confidentiality and availability for illustration), we use black/orange/red to denote no/low/high impact.

4 Visualization Techniques

A number of algorithms for projections, i.e., 2D-visualizations of the vulnerability space, have been incorporated into our workflow. They include t-distributed Stochastic Neighbor Embedding (t-SNE) [33], a version of t-SNE parameterized by neural networks (parametric t-SNE) [32], and a version of Uniform Manifold Approximation and Projection (UMAP) [19]. All these algorithms try to map the high-dimensional space into lower dimensions while approximately preserving

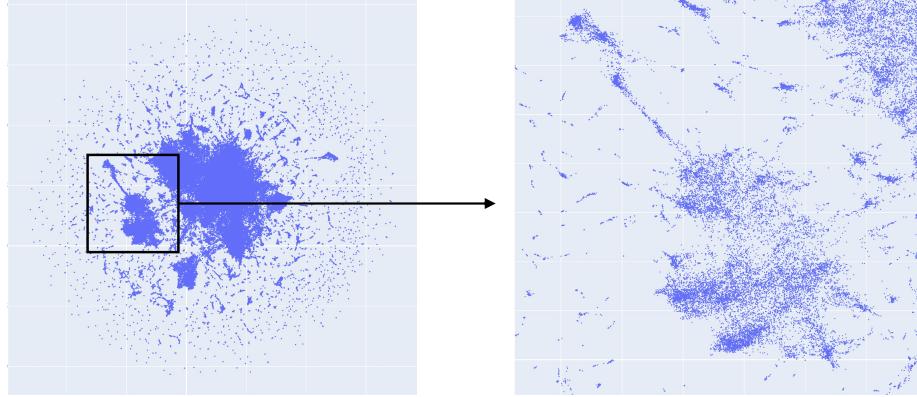


Fig. 3. An alternative 2D projection of the same vulnerability space as in Fig. 2 using UMAP. The large clusters on the left-hand side have multiple levels of finer cluster structure that becomes visible in the magnification (right-hand side).

the local distribution of the data. In our workflow, visualizations are automatically generated for all combinations of methods for projection, dimensionality reduction, and clustering. The visualizations (see Fig. 2 and 3) are interactive and hence allow the user to easily navigate the space of vulnerabilities (a form of semantic navigation). Additionally, we provide these visualizations for different subsets, e.g., organized by year, and with color-coded overlays, e.g., using CVSS, CWE, or CPE labels. It is noteworthy that unlabelled vulnerabilities are also placed in the same space making it easy for the user to put them in the context of known and/or better-understood vulnerabilities.

To analyze historical patterns of vulnerabilities and their dynamics we also implemented a visualization feature that allows us to use clustering algorithms to depict the evolution of CVE clusters over time (using annual granularity). This is complementary to our visualization of the entire vulnerability space over time (see Fig. 4), as it allows reducing the complexity by focusing on single clusters and temporal patterns. To avoid information overload, we currently use a simple heuristics showing the top-n largest clusters, but other heuristics taking into account the trend may be worthwhile to investigate in future work. In general, the temporal patterns can be quite informative (see Fig. 5), e.g., some vulnerability clusters lead to a single peak in the number of CVE incidents and then simply disappear, while some clusters are continuously growing or slowly declining. Other vulnerability clusters have more complex patterns, e.g. a smaller peak followed by a much higher peak, which could indicate that the core problem was not properly extinguished or it might have been generalized or transferred into other contexts.

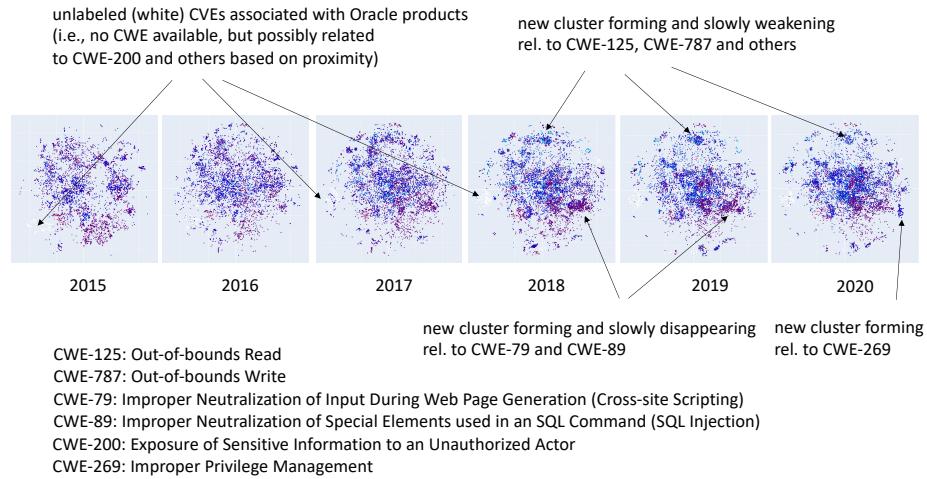


Fig. 4. A visualization of the vulnerability space evolving over time (with CWE overlay). We can easily see how the overall structure of the space is changing over the entire period and how smaller clusters emerge, morph, and sometimes disappear over time. Most of the CWEs referenced in this figure are still on MITRE’s list [21] of the top 25 most dangerous software weaknesses for 2021. Many vulnerabilities are not equipped with CWE labels (white color), but their placement in the space allows us to narrow down the likely candidates (even without using classification algorithms). Newly discovered vulnerabilities can be treated in a similar way.

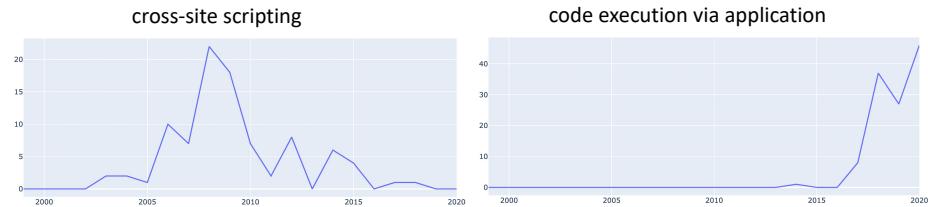


Fig. 5. A more fine-grained quantitative trend analysis is possible by utilizing the results of clustering algorithms. In this figure, we show the number of occurrences of vulnerabilities over time in two sample clusters, one related to certain types of cross-site scripting vulnerabilities and another one related to types of remote code execution facilitated by an application. While the former class of vulnerabilities seems to have disappeared (or became too small to be measured), the latter class can be expected to remain a (possibly growing) problem.

5 Evaluation using Baseline NLP Model

For the evaluation of algorithms, our base dataset which currently covers the years 1999 – 2020 will be split into a training (90%) and validation set (10%). The partial data from 2021 that is already available in the CVE/NVD database has not been utilized yet and could serve as an additional validation set in future work. To partly compensate for concept drift, we suggest that all data should be incorporated into operational models (periodic retraining of all stages) once the validation is completed.

We first evaluated the quality of the semantic vulnerability embeddings generated by the baseline NLP model using classification algorithms as a validation tool. The main classification metrics we used are accuracy, balanced accuracy (which corrects for class imbalance), precision, recall, and the F1-score. Balanced accuracy is a useful tool to compare the power of the classifier w.r.t. different types of labels, but less important for the end-user if we assume that the distribution of new data will be somewhat representative of the distribution of our dataset. In reality, one would expect some drift over time, and it would be worthwhile to quantify this in future work, and possibly develop techniques (e.g., temporal weighting) to take it into account, but a challenge would be the additional model complexity and the possibility of overfitting to very recent data.

The semantic embeddings are either the 300-dimensional vectors from the baseline NLP model or dimensionality-reduced semantic embeddings generated by one of the following models. To utilize the Euclidean norm, all NLP vectors will be normalized to the unit norm before the reduction is performed.

Our baseline model is Principal Component Analysis (PCA) which has the advantage of being computationally efficient and as a linear model maximally preserves the properties of the NLP vector space, e.g., its compositional structure [20] which often allows us to interpret addition as a form of feature conjunction.

Another dimensionality-reduction technique is UMAP, which has already been mentioned as a projection technique for our 2D visualizations. Here we use it for the reduction of our NLP vectors to smaller dimensions while approximately preserving the local distribution of the data (and hence its manifold structure). An advantage of UMAP over t-SNE is that it is computationally more efficient for high-dimensional target spaces.

Our Autoencoder (AE) model uses an encoder with two hidden layers (500 and 2000 units) and a symmetrically structured decoder with relu-activation, dropout-regularization, trained with mean-squared-error loss using Adam (10000 epochs with batch size 1000). Our Variational Autoencoder (VAE) model uses a similar structure but it is a generative probabilistic model with normal distribution on the latent variables (code space).

Our Generative Adversarial Network (GAN) model uses a slightly more complex generator based on a normal input distribution (three hidden layers with 2000, 500, and 500 units) and a discriminator with three hidden layers (1000 units each). The loss is defined by binary cross-entropy to distinguish real from fake vulnerabilities (real vulnerabilities being those from our dataset). Interleaved training of generator and discriminator is performed as usual (10000 epochs

with batch size 100). To enable the use of our GAN for dimensionality reduction we also train an inverter (a network with three hidden layers of 2000, 500, and 2000 units) using Adam with mean-squared-error loss (for 5000 epochs).

For comparison, we also employed two supervised classical dimensionality reduction techniques, namely Linear Discriminant Analysis (LDA) and Neighborhood Component Analysis (NCA). While performing better than the (unsupervised) PCA, neither of these can match the performance of our unsupervised autoencoder-based models, which are highly non-linear in nature, and hence seem more suitable to capture the complexity of the semantic vulnerability space. As generative models, VAEs and GANs have their own advantages, which can be useful for certain applications (e.g., to sample from the vulnerability space for applications such as those discussed in Section 7), but in our specific workflow aiming at classification and clustering their performance was inferior even compared with our baseline PCA.

We also investigated a number of hybrid models combining aspects of autoencoders (information-bottleneck architecture) and multi-layer perceptrons (MLP) for supervised dimensionality reduction that we first applied to Common Weakness Enumeration (CWE) labels. There are two primary flavors of MLP models that we refer to as functional and relational models. The functional model generates a label prediction as output, whereas the relational model incorporates the label as an additional input and predicts if it is related to the main input. The relational models are clearly more general (and in one variation can take into account the hierarchical structure of CWEs), but it turned out that the functional models yield better accuracy, suggesting that the relational nature of the CVE/CWE associations and their hierarchical structure does not carry sufficient information to support a more complex model. We also investigated two orthogonal flavors of MLPs (classification and regression MLPs, where the regression model tries to be more semantically accurate by mapping CWEs into a semantic space induced by their natural language descriptions). Again, it turned out that the simpler classification-based model gave superior performance.

Since our objective is to amplify VEP-relevant properties, we next applied the functional and classification-based MLP (simply referred to as MLP in the following) to CVSS labels (specifically V2) to obtain a dimensionality-reduced representation of all CVEs with good performance (of the subsequent workflow) not only on V2 but also on V3-labels (an example of transfer learning). This is quite fortunate because V3 labels are only available for the last few years and expected to be even more prevalent in the future. Our hypothesis that the CWE labels could be used for transfer learning and hence improve the classification performance for CVSS labels was not confirmed, most likely to the quality and limited information content of CWE annotations (a few general classes of CWEs dominate the dataset, despite of the elaborate and fine-grained CWE taxonomy).

To compare the relative performance of the dimensionality reduction techniques we use relatively simple classifiers including a family of MLPs (with up to 3 hidden layers), but also a number of classical ML algorithms, in particular, Naive Bayes, Logistic Regression, k -Nearest Neighbor Classifiers (varying k be-

tween 1 and 100), Support Vector Machines (using RBF kernels) and Gradient-Boosted Decisions Trees (using XGBoost [6]). While the classical algorithms cannot achieve the performance of MLP classifiers in this application, they are in most cases simpler models and have their own advantages (e.g. in terms of explainability). In our relative performance evaluation, they turned out to be useful tools to better understand the quality/complexity of our embeddings. For example, the semantic vulnerability representation (reduced or not) seems to be too complex to be interpreted by linear models and SVMs with useful results.

In summary, our evaluation shows that autoencoder-based representations (in particular, the Autoencoder Model) yield superior performance in terms of accuracy among all unsupervised dimensionality reduction techniques, while the MLP-based model shows the best performance for classification and supervised dimensionality reduction.

After the NLP stage, (optional) dimensionality reduction, and (optional) classification, the next stage in our workflow is clustering which is inherently unsupervised and requires another set of metrics. To properly incorporate the distribution of the dataset, information-theoretic metrics should be used [28]. A common metric is Normalized Mutual Information (NMI), which is symmetric and measures the relationship (degree of coincidence) between predicted clusters and clusters generated by ground truth (in our case approximated by labels). Two other import information-theoretic metrics are homogeneity (HOM) and completeness (COM). The former measures how uniform the predicted clusters are (in the sense that ideally all elements should have the same label), whereas the latter measures how well the labels are represented by the predicted clusters (ideally, elements with the same label should be assigned to the same cluster). For many reasons, most importantly the fact that all clustering algorithms are based on heuristics to achieve computational feasibility and are parameterized to bias/constrain their results, ideal conditions are typically not achievable (see also [17]), so that our main objective with these metrics is to compare the performance of different semantic representations and clustering algorithms relative to each other. In our analysis, algorithms are typically parameterized to generate fine-grained clusters (several thousand) to provide a high degree of detail. Hence, homogeneity plays the most important role and is increased at the expense of completeness. As a summary measure, we use NMI with normalization by arithmetic averaging. It is identical to the V-measure [28] (or validity measure), which is defined as the harmonic mean of homogeneity and completeness, quite similar to the F1-score, which is the harmonic mean of precision and recall. It has been shown to have many properties that make it a useful (albeit not perfect) measure to compare algorithms independent of the size of the data set and the number/size of clusters.

These and other classical metrics are applied to the evaluation of the four clustering algorithms employed in our workflow. First, we have K-Means, which is simple and intuitive but severely limits the shape to clusters (convexity assumption). Then there is Hierarchical Clustering, which performs bottom-up agglomerative clustering by recursively merging pairs of clusters starting from

singletons using simple heuristics (we use Ward’s method to take into account variance). The method is quite intuitive and has the additional advantage that as a by-product a meaningful hierarchy is generated. Finally, there is the class of density-based algorithms of which we employed HDBSCAN [18] and OPTICS [1]. Both identify clusters based on high-density regions (without convexity limitations) of the data distribution but use different heuristics to determine what constitutes a cluster. Both algorithms can deal with noise by avoiding the creation of new clusters unless a certain minimum cluster size is reached. To compensate for unsatisfactory performance in high-dimensional spaces (even with only 10 or 20 dimensions), we combine the density-based algorithms with an additional dimensionality-reduction step which uses UMAP to reduce the dimension by a factor of two before the clustering algorithm is applied.

Our analysis based on CVSS labels (V2 and V3) shows that while Hierarchical Clustering shows performance similar to K-Means in our application, the improvement by density-based algorithms in all information-theoretic metrics (NMI, HOM, COM) clearly stands out across many comparable parameter settings and underlying models. We hypothesize that this at least is partly due to their capability to deal with noise, which in our context is a combination of noise in the natural language descriptions and labels. Another contributing factor may be that density-based algorithms can more reliably identify lower-dimensional manifolds of arbitrary shapes that are created by similar vulnerabilities. We also observed that OPTICS shows consistently better performance (NMI, HOM, COM) than HDBSCAN for most models in our baseline NLP workflow (supervised and unsupervised).²

For dimensionality reduction recall that our NLP representation of vulnerabilities has 300 dimensions, but to obtain models with high generalization potential (and as a way to increase robustness to concept drift) it is desirable to reduce the dimension as much as possible as long performance does not suffer substantially. We experimented with 10 and 20 dimensions and found that 20 dimensions result in notably better performance than 10, but higher dimensions do not yield improvements that are worthwhile the additional model complexity (which also affects runtime). Sample performance results for MLP classifiers and two clustering algorithms can be found in the appendix (Figs.9 and 10).

6 Evaluation using Refined NLP Models

Up to this point, the evaluation of our algorithms was based on 300-dimensional vector-space embeddings generated by the NLP stage of our workflow with an optional dimensionality reduction to 10 or 20 dimensions. Recall, that in our

² Interestingly, this is also the case of our MLP-based representation but not the case for our transformer-based models (see next section), where OPTICS scores better than HDBSCAN on HOM but worse on COM and NMI. This indicates a different tradeoff that might be caused by higher bias baked into the transformer-based representations. In fact, a closer examination shows that this is the case for both of our attention-based models, but not for the other refined NLP models.

baseline NLP model, the vector-space embeddings were defined simply as a mean of all non-zero normalized embeddings of the relevant components (i.e., words, acronyms, numbers, filenames, or composite terms) of the vulnerability description. This means that we have effectively employed a multiset abstraction of vulnerability descriptions which cannot take into account their sequential structure, e.g., natural language grammar or the typical organization of the vulnerability descriptions, which usually consist of multiple sentences providing an increasing level of detail. In this section, we discuss an extension of our workflow with a number of supervised NLP models that directly operate on the sequence of vectors corresponding to the components of the vulnerability description with the idea to learn and exploit the high-level structure of these descriptions in our dataset. It was not a priori clear if better performance (that can actually generalize) can be achieved due to the higher model complexity, but our evaluation shows that this is indeed the case.

Indeed, as the precision of the vulnerability clusters depends on the underlying NLP model, it makes sense to advance our baseline model by taking into account more information from the available labels in the dataset. To this end, we studied a number of supervised NLP models, in particular convolutional networks and bidirectional LSTMs (Long Short-Term Memory) and bidirectional GRU (Gated Recurrent Unit) networks, which have found many applications in text classification (see, e.g., [2] for a survey covering these models). In addition, we investigated neural network models utilizing a self-attention mechanism to focus on particular parts on the vulnerability description in a context-dependent manner. In particular, we implemented a version of bidirectional LSTMs with a simple notion of attention (similar to [37]) and a simplified version of the more recently developed transformer model [34] for NLP that in our setting will be applied to a classification problem rather than a transformation/translation problem that the more general model is targeting.

In summary, the following NLP models, all based on neural networks, were implemented and evaluated: 1D-convolutional networks, bidirectional LSTM networks (single layer of LSTM with global pooling), bidirectional GRU networks (single layer of GRU with global pooling), bidirectional LSTMs with simple dot-product attention, and transformer networks (simplified version suitable for classification). The main features of the latter are the more powerful notion of multi-head attention and the use of positional text encodings (which eliminate the need for recurrent or convolutional structure). All models were trained as classifiers with CWE and CVSS V2 labels, and are designed to perform their own dimensionality reduction (information-bottleneck architecture).

All these models are then employed for supervised dimensionality reduction (in the context of our larger workflow), and we found that the accuracy of CVSS classifiers and the quality of clusters (based on information-theoretic metrics) is indeed further improving. We focused on the NLP models supervised using CVSS labels, as these are the most abstract properties that are also used for cluster validation. Our analysis shows that the transformer model (without fine-tuning) shows the best tradeoff between generalization capability and classification ac-

curacy (and related information-theoretic metrics for clustering). It also yields better performance than our MLP-based model (the best supervised model built on our baseline NLP). We also evaluated variations of all models to retrain (fine-tune) word embeddings, which naturally leads to much higher model complexity and has not resulted in additional performance improvements.

The autoencoder model (for our baseline NLP) shows lower performance but it still remains relevant. As a fully unsupervised model, it is not biased by the subject-matter-expert CVSS labels and hence might have advantages for certain applications. In addition, we hypothesize that due to its lower complexity it may be less prone to concept drift, which is a separate issue that would be worthwhile to investigate in the future. In summary, we consider both the unsupervised autoencoder-based model as well as the supervised transformer-based model as the best-performing models arising from our investigation. For a comparison of sample performance results for these two types of models, we again refer to the appendix (Figs.9 and 10).

7 Evaluating Theories about the Vulnerability Space

In the following section, we discuss another application of our semantic vulnerability representations, that has the potential to further enlarge the toolbox for security risk assessment. Inspired by discussions with the Vulnerability AI team members, we implemented an experimental capability to test arbitrary logical theories in the context of our vulnerability dataset. It utilizes SRI’s Probabilistic Approximate Logic (PALO) framework to integrate logic and machine learning [29]. PALO was developed in a previous DARPA project in a biological context (network modeling) [30], and is now for the first time being applied in the security domain. Its implementation in SRI’s Logical Imagination Engine (LIME) uses a general form of Bayesian inference to synthesize probabilistic models under logical constraints (representing, e.g., domain knowledge or hypotheses). This tool may allow us to shed some light on certain hypotheses about the structure of the vulnerability space (e.g., regarding compositionality, see below) and more generally provide a (probabilistic) relational and hence graph-theoretic perspective with new types of visualizations and new ways to look at interesting subspaces. The experimental integration of PALO/LIME into the Vulnerability AI workflow is illustrated in Fig. 6.

For the Vulnerability AI project, we added support to deal with very large relations over the vulnerability space and visualize them partially as graphs (using graphml as a description language) with informative labels making them easy to navigate for the user. As a first test case, we applied our tool to a logical theory of compositionality that tries to exploit the (partially) compositional structure of the underlying NLP models [20]. The specific question (that was posed in a meeting with Galois) is if our NLP-based models have learned a compositional structure that can be in any way related to (or some approximation of) the composition of vulnerabilities in the real world as it plays a role in vulnerability chaining. To simplify the problem (and the formalization) we focused on a bi-

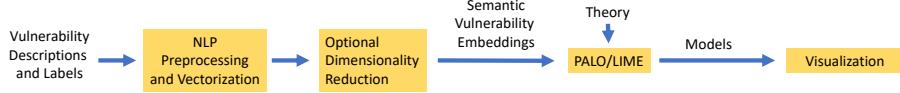


Fig. 6. Extension of the Vulnerability AI Workflow with PALO/LIME for Evaluating Theories about the Vulnerability Space

nary notion of compositionality that is reflexive and symmetric (i.e., formally a similarity relation) but usually not transitive. Reflexivity in our probabilistic approximately logic means that similar vulnerabilities are considered composable, the justification being that even a single vulnerability could be used multiple times in a single attack (self-composability), but many variations of this axiomatization are clearly possible and could be explored in the future. One of the axioms in our theory relates this hypothesized notion of vulnerability compositionality to composability in the NLP-sense, that for simplicity we approximate by the mean of the semantic vulnerability vectors, which has a very intuitive representation in the vulnerability space. More details about the theory can be found in Fig. 11.

We then conducted a systematic exploration of the models of our vulnerability composition theory. To this end, we selected three models as base models for our analysis, namely Principal Component Analysis (PCA), Autoencoders (AE), and transformer networks. The PCA-based models are of interest here, because as a linear transformation PCA will maximally preserve the compositional structure of the NLP space, while the other models can be expected to distort that structure due to their non-linear nature. Nevertheless, a visual inspection shows that all three base models lead to interesting graphs that focus on different subsets of the larger vulnerability space. In our preliminary analysis of these graphs (see Fig. 13 for a sample) we observed that highly connected (and hence in our theory highly composable) vulnerabilities are often associated with features such as "remote code execution" that can be critical steps of larger vulnerability chains. The nodes in their neighborhood often represent vulnerabilities that arise in a similar context and hence may be candidates for compositions, but on the other hand the information in the vulnerability descriptions is not sufficient to verify composability. Hence, the graphs resulting from this basic theory must be interpreted with a grain of salt and can at best be seen as an idea generator that requires additional filtering by a subject matter expert.

With about 150K nodes, the full graph of the vulnerability space is expected to be huge and impossible to visualize, but the inference and computation time is reasonable (several hours per model utilizing a state-of-the-art GPU) and the resulting small subgraphs (with up to 1000 nodes) are easy to navigate and to interpret thanks to the use of automatic layout algorithms and graph analysis tools for visualization. While these preliminary results show that our experimen-

tal tool scales up to the high complexity needed to explore theories about the vulnerability space, it is not clear if the particular logical theory based (only) on NLP compositionality is general/restrictive enough to be of practical interest. Hence, it would be worthwhile to consider alternative theories of composability in future work, e.g., by incorporating axioms about CWE, CVSS, or CPE labels from our dataset or by incorporating other datasets, features, or risk metrics into the theory. Another pragmatic approach is to develop an inductive theory of composability. It could start with empirical data about observed vulnerability chains (which is still needs to be collected) and utilize semantic vulnerability embeddings (and related similarity or equivalence relations) to extend this notion to new vulnerabilities and in this way derive new likely candidates for compositions.

Finally, we should remind ourselves that the basic compositionality theory only served as a test case for our experimental tool. We expect that the tool can be applied to a wide range of relational and quantitative theories that test other hypotheses or highlight hidden structures/patterns in the vulnerability space that are not apparent in our more abstract cloud-based or cluster-based visualizations.

8 Related Work

The core of our work is concerned with the unsupervised learning of semantic vulnerability embeddings, which can serve as a basis for visualization, clustering, and classification models for quite different types of applications. We have also investigated the use of supervised methods to learn vulnerability embeddings that are naturally biased by the training labels (in this report we focused on CVSS labels but we also explored the use of CWE labels). Not surprisingly the latter models yield better performance for tasks related to those labels, which will be useful, e.g., to improve clustering performance in an application (e.g., in the context of the VEP) where high-level properties such as those related to CVSS labels play an important role.

In the following, we discuss some related work that utilizes NLP techniques to extract information from vulnerability descriptions. In particular, the named entity recognition/extraction (NER) problem has attracted considerable interest in the cyber-security research given the large number of unstructured textual information sources that are relevant in that domain. While our work focusses on the representation of vulnerabilities and their classification (which is also a form of information extraction), there is an overlap with NER and similarity in the types of models employed that we briefly discuss using a few very recent works. For a more complete review, we refer to [9].

For example, the top-level objective of [3] is to translate vulnerability descriptions from the NVD into interaction rules for MulVAL (a network security analyzer based on Datalog). The main problem in this context is attack-entity extraction (a form of NER), i.e. the extraction of specific attack-related entities (operating system, attack vector, attack technique, impact, etc.) from the vulnerability description. To this end, the authors use Word2Vec (a predeces-

sor of Fasttext). Instead of using a pretrained model, they specifically train a Word2Vec model on the NVD descriptions, and show that its performance is superior to pretrained ELMo and BERT models for this particular task, which is not too surprising, but might also mean that the Word2Vec model is fit to the particular dataset which is quite small for training a language model. Clusters of Word2Vec embeddings typically contain instances belonging to the same entity (e.g., operating system). Attack-entity extraction is then performed by feeding the word embeddings for the description into a bidirectional LSTM classifier. To enable supervised learning, the vulnerability descriptions were labeled manually by a large number of students. Different from our work, embeddings are only used at the level of words rather than for vulnerabilities, and it is not clear how well the models would generalize to new vulnerabilities/descriptions (which might be less important for this particular application). On the other hand, some aspects of this approach (e.g., the need to complete missing information) might actually benefit from clustering at the level of vulnerabilities, that is by taking into account the bigger picture that we focus on in our work.

In other recent work [10], the authors are exploring general models for NER in the cyber-security domain. As a starting point, they use the popular bidirectional LSTM model with a Conditional Random Field layer (bi-LSTM-CRF) [13] and investigate two extensions, multi-head attention and the use of domain-specific dictionaries (providing additional input to the network to improve performance for rare entities). The advantages of using an attention mechanism are clearly demonstrated by improved precision (which is independent of the improvement due to dictionaries). We also observed improvements by using dot-product attention in the context of simpler bidirectional LSTM classifiers, but finally identified the transformer-based classification model that is inherently based on attention (and in this way completely avoids the need for recurrent networks) as providing the best performance tradeoffs for our application. An interesting question remains how well our semantic vulnerability representation that is not trained for NER would perform for related classification tasks and if it could provide any other benefits (e.g., due to the highly compressed semantic representation).

Another line of work is the use of NLP techniques to better quantify exploitability risk, and hence address one of the shortcomings of CVSS. The CVSS base metrics provide only a very limited static picture, and a dynamic data-driven approach to assess exploitability is clearly more appropriate for the VEP and other risk assessment activities. While CVSS temporal metrics have been defined to address this problem, their adoption seems to be much more limited. Exploitability was already investigated in the early work [5], where an SVM was trained to predict exploitability based on the very limited data sources available at that time (CVE and OSVDB, using data up to 2007). This work nicely illustrates the large discrepancy between predicted exploitability (based on empirical data) and the CVSS exploitability score, which is another reason why it is not used in our work. A more recent promising approach is to build parsimonious probabilistic models of exploitability as in [14], which introduced the Exploit Prediction Scoring System (EPSS). In addition to features based on keyphrases

extracted from CVE/NVD descriptions (a simple form of NLP), the authors incorporate various exploit databases (covering proof-of-concept and weaponized exploits) to determine the probability that a vulnerability will be exploited after publication and propose regularized logistic regression (Elastic Net Model) as a predictive model, which seems quite appropriate given the still relatively limited amount of data available about exploits. Utilizing a broader set of additional data sources, the recent work [31] addresses a similar problem with a notion of expected exploitability and develops neural-network-based models to predict exploitability with particular focus on addressing label noise. All these approaches (which use simple forms of NLP not based on semantic embeddings) suggest that our semantic vulnerability representations (possibly refined by utilizing additional data sources) could serve as a unifying basis for similar approaches and offer potential improvements. Indeed, as stated in [31] this direction has been briefly explored but seems challenging and is left for future work: “Overall, our result reveals that creating higher level, semantic, NLP features for exploit prediction is a challenging problem, and requires solutions beyond using off-the-shelf tools. We leave this problem to future work.”

9 Conclusions and Directions for Future Work

For the Vulnerabilities Equities Process (VEP) a big picture view of the vulnerability space can be immensely useful. The big picture allows the expert to understand the structure of the space and how it is evolving over time at an aggregate level and through the use of clustering techniques recognize important trends that may influence the risk assessment of new vulnerabilities that are being discovered. On a smaller scale, newly discovered vulnerabilities can be put into context of existing vulnerabilities simply by allowing the user to navigate the semantic vulnerability space. Classification algorithms such as those investigated in our work can exploit vector-space embeddings to label newly discovered vulnerabilities, but may also be used to label existing vulnerabilities in the dataset that have not been labeled due to limited resources. Classifiers and visualizations of the semantic space may also be used to find problems with the existing annotations, e.g., mislabeling or other inconsistencies.

In addition to the informal use of our semantic vector-space embeddings and their use as part of classification and clustering algorithms, there are other interesting applications. One application that we briefly explored (and which can be further generalized as discussed below) is the representation of vulnerabilities and their relations in the context of theories that need to be tested. Other applications that we did not investigate include the support of semantic search algorithms to find similar vulnerabilities and the pruning of a search space of vulnerabilities in the context of symbolic formal methods, e.g., to check or refute certain logical properties. Semantic vulnerability embeddings and their associated notion of similarity (or equivalence in case of clustering) can also be used to extend empirical data about vulnerabilities to anticipate new risks. A security

analyst, for example, may utilize our embeddings and clusterings to explore and anticipate candidates for new vulnerability chains based on existing ones.

In the remainder of this section, we will briefly discuss directions for possible future work. First of all, there is simply the further evolution of our models by integrating with additional data sources. One limitation of the CVE/NVD dataset is the small amount of detail about the vulnerability represented in the description. Additional information may come from evaluating security blogs or even source code repositories that are partly referenced in the CVE/NVD entries. To process larger security-related documents, enhanced NLP models (including NER, as discussed under related work) and domain-specific training (on a large corpus, e.g., blogs, research papers) would be worthwhile to explore.

Another dimension that would be important to add to our models is empirical risk, which ideally should be regarded as a dynamic and context-dependent notion. One key aspect, empirical exploitability, is tracked by a number of commercial efforts, and we have already discussed the work on the Exploit Prediction Scoring System [14] and on Expected Exploitability [31], two notions that could be potentially predicted more accurately by utilizing semantic vulnerability embeddings (ideally enriched by taking into account commercial data sources) as a unifying foundation.

A remaining limitation of our current machine learning workflow is that we are focusing on the lowest level of the MITRE cyber-security abstraction hierarchy where the most amount of data is available, namely at the level of specific vulnerabilities, i.e., MITRE’s Common Vulnerability Enumeration (CVE), but for many other applications such as monitoring, forensics, and defense, the larger context of vulnerabilities is important, which would require taking into account higher levels of abstraction, e.g., the Common Weakness Enumeration (CWE) [26] (which we already used in some of our classifiers), the Common Attack Pattern Enumeration and Classification (CAPEC) [23], and the Framework for Adversarial Tactics, Techniques & Common Knowledge (ATT&CK) [22]. While moving to higher levels of abstraction is very challenging due to the limited amount of empirical data, new modeling techniques that integrate state-of-the-art machine learning with logical (in particular relational) modeling may help to overcome the current limitations through the use of formal theories (as a representation of domain knowledge or hypotheses) as a natural counterpart to the input data.

One possible approach to address these issues is to further generalize our work to incorporate logical theories based on Probabilistic Approximate Logic (PALO) [29] that we already applied to test a theory of vulnerability composition. This approach has been originally developed in the DARPA Rapid Threat Assessment project [30] and our preliminary experiments show that it is applicable to our vulnerability dataset as well. Based on these foundations, a natural future direction is to develop a tool that allows us to bridge multiple levels of abstractions and test virtually arbitrary logical theories and hypotheses related to cyber-security risks by combining multiple sources of information. Such a tool should also have the capability to generate relational/graphical models as a new

way of visualizing/explaining different subsets of vulnerabilities in the context of other entities and relations referenced by flexible user-defined theories.

Acknowledgments We gratefully acknowledge contributions from the entire Vulnerability AI team, in particular Pat Lincoln, Steven Cheung, and Vinod Yegneswaran for the idea to explore vulnerability clustering, for helping to select the proper datasets, and for pointers to related work. We are also grateful for feedback from Galois, in particular John Launchbury for the idea to investigate the relationship between vulnerability composition and composition in vector-space NLP models. Finally, we would like to thank Carolyn Talcott for contributing many ideas, especially in the context of PALO/LIME and the overall machine learning workflow.

A Other Visualizations and Results for Selected Models

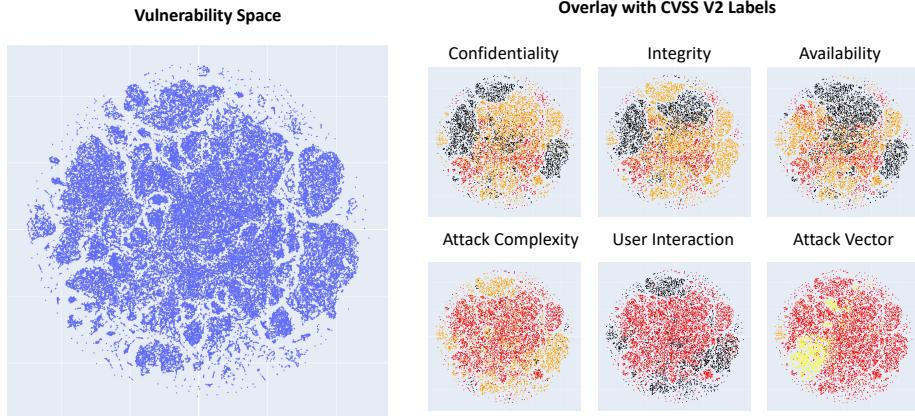


Fig. 7. On the left, we see a 2D t-SNE projection of the vulnerability space using transformer-based embeddings. It is instructive to compare it with the representation based on the autoencoder model in Fig. 2. The supervised nature of the model leads to a visibly more pronounced cluster structure and a slightly better fit with the CVSS labels (shown on the right-hand side using a subset of the CVSS V2 labels). We use red to denote higher risk categories, orange for medium risk, followed by yellow and black for lower or no risk. In the case of user interaction, red means it is not required. In the case of the attack vector, red, orange, and yellow means network, adjacent network, and local network, respectively.

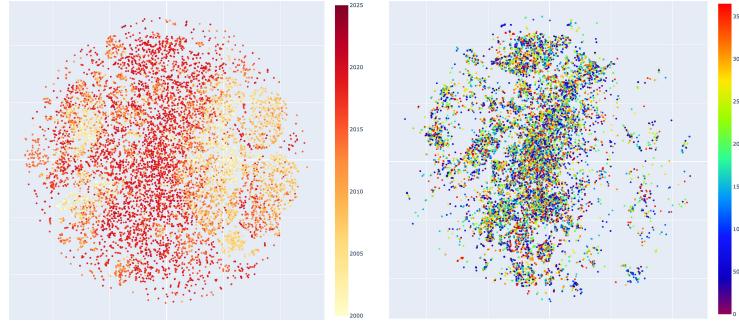


Fig. 8. On the left, we see a 2D t-SNE projection of the vulnerability space (in fact, a random sample) using transformer-based embeddings color-coded by the year of publication. It is quite noticeable that the vulnerabilities from the same year are often clustered together (partly caused by temporal clustering of similar technologies and attacks). To look at a finer temporal resolution, on the right-hand side, we show the vulnerabilities for 2020 color-coded by day of the year. It may be less obvious, but there is a slight tendency for similar vulnerabilities to be published on the same day (mini-clusters), which can be often explained by related vulnerabilities arriving in small batches (e.g., because of a common underlying weakness).

Results for 20-dimensional, autoencoder-based representation (unsupervised)

	AV	AC	PR	UI	S	C	I	A
1	0.88	0.94	0.80	0.90	0.95	0.80	0.81	0.86
2	0.88	0.94	0.81	0.90	0.95	0.81	0.82	0.86
3	0.88	0.91	0.80	0.90	0.94	0.80	0.81	0.85
Accuracy								
	AV	AC	PR	UI	S	C	I	A
1	0.87	0.92	0.78	0.89	0.94	0.79	0.81	0.85
2	0.88	0.93	0.80	0.90	0.95	0.81	0.81	0.86
3	0.87	0.91	0.79	0.90	0.94	0.80	0.81	0.85
F1-Score								

Results for 20-dimensional, transformer-based representation (supervised by V2)

	AV	AC	PR	UI	S	C	I	A
1	0.88	0.95	0.83	0.92	0.96	0.85	0.86	0.88
2	0.88	0.94	0.83	0.92	0.96	0.84	0.85	0.87
3	0.87	0.93	0.81	0.91	0.94	0.83	0.84	0.86
Accuracy								
	AV	AC	PR	UI	S	C	I	A
1	0.88	0.94	0.82	0.92	0.96	0.84	0.86	0.88
2	0.88	0.94	0.82	0.92	0.96	0.84	0.85	0.87
3	0.87	0.93	0.81	0.91	0.94	0.83	0.84	0.85
F1-Score								

Fig. 9. Sample Results for MLP Classifiers w.r.t. CVSS V3 Labels. Comparing two underlying models (autoencoder and transformer networks) the improvement in performance is quite notable in almost all labels. The CVSS V3 labels are: attack vector (AV), attack complexity (AC), privilege requirement (PR), user interaction (UI), change of scope (S), confidentiality (C), integrity (I), and availability(A). The first column denotes the number of hidden layers, and we can see that one or two hidden layers are optimal (depending of the type of underlying model).

Results for 20-dimensional, autoencoder-based representation (unsupervised)

	AV	AC	PR	UI	S	C	I	A
NMI	0.12	0.05	0.12	0.12	0.08	0.16	0.17	0.14
HOM	0.75	0.69	0.67	0.76	0.79	0.73	0.74	0.75
COM	0.07	0.02	0.07	0.06	0.04	0.09	0.10	0.07
Hierarchical Clustering								
	AV	AC	PR	UI	S	C	I	A
NMI	0.15	0.06	0.15	0.14	0.10	0.19	0.20	0.16
HOM	0.86	0.84	0.80	0.85	0.88	0.84	0.85	0.87
COM	0.08	0.03	0.08	0.08	0.05	0.11	0.11	0.09
Density-Based Clustering (OPTICS)								

Results for 20-dimensional, transformer-based representation (supervised by V2)

	AV	AC	PR	UI	S	C	I	A
NMI	0.13	0.05	0.13	0.13	0.09	0.18	0.19	0.15
HOM	0.79	0.77	0.71	0.85	0.89	0.80	0.83	0.81
COM	0.07	0.03	0.07	0.07	0.05	0.10	0.11	0.08
Hierarchical Clustering								
	AV	AC	PR	UI	S	C	I	A
NMI	0.15	0.07	0.16	0.15	0.11	0.20	0.21	0.16
HOM	0.87	0.88	0.83	0.92	0.94	0.88	0.90	0.90
COM	0.08	0.03	0.09	0.08	0.06	0.11	0.12	0.09
Density-Based Clustering (OPTICS)								

Fig. 10. Sample Results for Clustering w.r.t. CVSS V3 Labels. The first column in the tables denotes the information-theoretic evaluation measure. Comparing two underlying models (autoencoder and transformer networks), the improvement in performance again is quite notable in almost all labels (abbreviations as in Fig. 9). Orthogonal improvements are possible due to the type of clustering algorithm. Here we compare hierarchical clustering and OPTICS as a representative of density-based clustering (which has the advantage of allowing partial clustering).

B Testing a Theory of Vulnerability Composition

```

predicate("vul","Space",pred_class="mlp",complexity=2)
predicate("co","Space","Space",pred_class="ntn",complexity=20)

function("first","Pair","Space",definition=lambda d:d[:,dim])
function("second","Pair","Space",definition=lambda d:d[:,dim:])

sort Space .
sort Vul .
sort Pair .
sort VulPair .

subsort Vul < Space .
subsort VulPair < Pair .

op first : Pair -> Space .
op second : Pair -> Space .

op vul : Space -> Bool .
op co : Space Space -> Bool .
op plus : Space Space -> Space .

predicate("vul","Space",pred_class="mlp",complexity=2)
predicate("co","Space","Space",pred_class="ntn",complexity=20)

function("first","Pair","Space",definition=lambda d:d[:,dim])
function("second","Pair","Space",definition=lambda d:d[:,dim:])

function("plus","Space","Space","Space",definition=lambda d0,d1:(d0+d1)/2)

axiom("forall [vx : Vul] co('vx','vx)",lbound=0.9)
axiom("forall [x : Space] not co('x','x)",lbound=0.5)
axiom("forall [x y : Space] not co('x','y)",lbound=0.5)
axiom("forall [vx vy : Vul] not co('vx','vy)",lbound=0.5)
axiom("forall [x y : Space] co('x','y') implies co('y','x')",lbound=0.9)
axiom("forall [x : Space] not vul('x')",lbound=0.5)
axiom("forall [vx : Vul] vul('vx')",lbound=0.9)
axiom("forall [vx vy : Vul] vul(plus('vx','vy')) implies co('vx','vy')",lbound=0.9)
axiom("forall [x y : Space] co('x','y') implies vul('x')",lbound=0.9)
axiom("forall [x y : Space] co('x','y') implies vul('y')",lbound=0.9)

```

Fig. 11. This figure shows the signature (left-hand side) and the axioms (right-hand side) of a simple test theory of compositionality used in our experiments with PALO/LIME. The space of potential vulnerabilities and known vulnerabilities are represented by sorts `Space` and `Vul`, respectively. Vulnerabilities that may exist (known or unknown) are (probabilistically) modeled as a learnable unary predicate (from the MLP family) and the binary composability relation `co` is a learnable relation (from the family of Neural Tensor Networks). A key axiom relates `co` and `plus`, which is defined as an average to approximate our NLP composition. All axioms are equipped with roughly estimated probabilistic lower bounds (to be concretized by the engine), as they clearly cannot be satisfied together in a classical sense. The models synthesized by our LIME engine approximately satisfy all these constraints (see Fig. 12). Somewhat surprisingly, the best models in terms of respecting the axioms are those generated using a transformer-based representation of vulnerabilities.

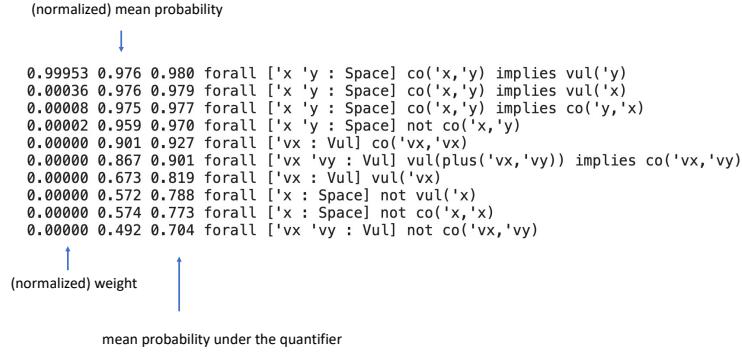


Fig. 12. Sample model generated by LIME utilizing a transformer-based representation. The normalized mean probability is given for each axiom of the theory. Other models synthesized by the engine may lead to slightly different tradeoffs between the axioms. Hence, multiple models are generated in our parallel workflow.

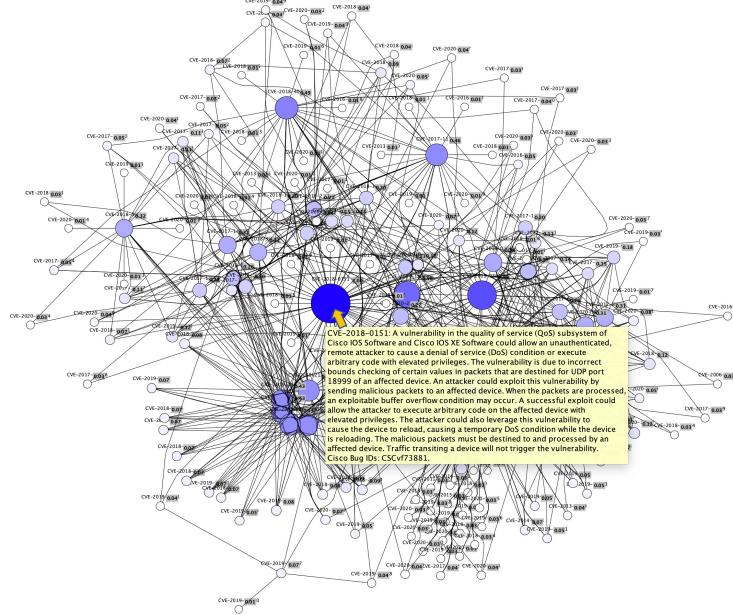


Fig. 13. Partial graph of the composability relation (focussing on highest probability edges) associated with the model in Fig. 12. The size of nodes highlights the number of connected edges (one possible centrality measure). In many cases, we found that nodes with high centrality are particularly suitable to be composed. In this figure, the highlighted node enables remote code execution, which can be potentially combined with many other vulnerabilities.

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