Dazzle: Using Optimized Generative Adversarial Networks to Address Security Data Class Imbalance Issue

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ABSTRACT

Background: Machine learning techniques have been widely used and demonstrate promising performance in many software security tasks such as software vulnerability prediction. However, the class ratio within software vulnerability datasets is often highly imbalanced (since the percentage of observed vulnerability is usually very low). Goal: To help security practitioners address software security data class imbalanced issues and further help build better prediction models with resampled datasets. Method: We introduce an approach called Dazzle which is an optimized version of conditional Wasserstein Generative Adversarial Networks with gradient penalty (cWGAN-GP). Dazzle explores the architecture hyperparameters of cWGAN-GP with a novel optimizer called Bayesian Optimization. We use Dazzle to generate minority class samples to resample the original imbalanced training dataset. Results: We evaluate Dazzle with three software security datasets, i.e., Moodle vulnerable files, Ambari bug reports, and JavaScript function code. We show that Dazzle is practical to use and demonstrates promising improvement over existing state-of-the-art oversampling techniques such as SMOTE (e.g., with an average of about 60% improvement rate over SMOTE in recall among all datasets). Conclusion: Based on this study, we would suggest the use of optimized GANs as an alternative method for security vulnerability data class imbalanced issues.

KEYWORDS

Security Vulnerability Prediction, Class Imbalance, Hyperparameter Optimization, Generative Adversarial Networks.

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1 INTRODUCTION

Machine learning has been used for many security tasks; e.g. security vulnerability prediction [23]. A core problem with a security dataset is class imbalance; i.e., there may be very few instances of security events within many such datasets. For example, Figure 1 shows that components with known security vulnerabilities within Mozilla are very rare. As another example, as security bug reports can describe the critical security vulnerabilities in software products, Peters et al. [49] show that only 0.8% of bug reports are known to be security bug reports in their study.

When the target class is rare, it is challenging for a learner to distinguish the goal (security target) from other event [34]. There are many ways to handle the class imbalance. For example, SMOTE (i.e. Synthetic Minority Oversampling TEchnique) [13] is a highly-cited methods that oversamples the minority class by generating new samples. Specifically, SMOTE works by introducing new synthetic samples along with the line segments of k nearest minority class neighbors. However, SMOTE generates new samples via a simplistic linear interpolation between minority neighbors. Also, when generating new data in some local regions, SMOTE does not use knowledge from the whole minority class samples – which means its interpolations might not be helpful. Recently, SMOTE has been used extensively in software analytics in work published at top venues such as ICSE [1, 58], TSE [8], EMSE [33], etc.

SMOTE was first proposed in 2002, and this paper explores “can we do better than SMOTE?” For example, a new approach to generate samples for resampling purposes is GANs [25]; i.e. Generative Adversarial Networks. Unlike SMOTE’s issue with local inference, GANs oversampling can effectively learn the whole data characteristics and generate samples close to the distribution of original input data. Considering that GANs can achieve some impressive results in producing meaningful, realistic samples in prior studies (e.g., in

Figure 1: Mozilla code [47]. Only a few modules (seen in red) are vulnerable components.
domains such as computer vision [31, 63]), more security practitioners have adopted variants of GANs in many security tasks [5, 15, 30] (see Table 1).

One reason to prefer SMOTE over GANs is that the SMOTE is much easier to implement and apply. GANs have two parts: a generator model that generates new plausible examples and a discriminator model that checks if it can distinguish real from fake examples. However, training a useful and stable GANs can be a difficult task [52]. Here, stable means a balance between generator and discriminator with proper coordination. For example, if one model overpowers the other, neither can learn more even with more iterations. Some other challenges with training GANs include mode collapse (discussed in §2.5), in which situation the generator may not explore much of the possible solution space and thus fails to produce a variety of realistic outputs.

This empirical study tries to tame the GANs training problem as well as using GANs as a data oversampler with hyperparameter optimization on Wasserstein GAN (WGAN) [6, 7]. WGAN applies the Wasserstein distance metric instead of the cross-entropy loss used in the traditional discriminator. The advantage of the Wasserstein distance metric is that it measures the distributions of each data feature and determines how far apart the distributions are for real and fake data. Considering the complexity of tuning two components in the GANs architecture, we use a novel optimizer called Bayesian Optimization [54, 57]. Our Bayesian optimizer explores the hyper-parameter set of WGAN’s generator and discriminator and returns an optimal solution set towards the evaluation target. We refer to our proposed combination of GANs and Bayesian Optimization as “Dazzle”. The experiments of this paper evaluate Dazzle with three security datasets, i.e., Moodle vulnerable files, Ambare bug reports, and JavaScript function code dataset. The results show that we can achieve an average 60% improvement rate in recall across all datasets. We recommend using optimized GANs for security vulnerability dataset class rebalancing purposes based on this study.

As for the novelty and contribution of this work, we note that this paper is not the first work to apply Bayesian optimization to tune the GANs architecture. For example, prior work [17] has proposed using optimized GANs in the sign language classification. However, the main focus of this empirical study is to show that the idea of using optimized GANs is able to help solve some existing security tasks, and it is more promising than currently widely used SMOTE-based methods. We also note that this study cannot cover all security tasks as we show in Table 1, and we believe this would be an interesting future direction to explore.

The remainder of this paper is organized as follows. We discuss background and related work in Section 2 and our methodology in Section 3. We then report our experiment details in Section 4, including datasets, evaluation metrics, etc. Section 5 presents our experiment results. We discuss the threats of validity in Section 6 and provides a remark of addressing class imbalanced issues in Section 7 and then we conclude in Section 8.

## 2 BACKGROUND AND RELATED WORKS

### 2.1 Software Vulnerability Prediction

Software security vulnerabilities are critical issues that would impact software systems’ confidentiality, integrity, and availability. The exploitation of such vulnerabilities would result in tremendous financial loss. To mitigate these issues, many machine learning and data mining techniques are proposed to build vulnerability prediction models to aid security practitioners [23].

Prior works have demonstrated several ways to extract useful features to train vulnerability prediction models. For example, as software bug reports can describe security vulnerabilities in software products, prior researchers [32, 49, 65] proposed a way to adopt natural language text based text mining techniques to identify security-related keywords. Vulnerability prediction models are then built by using the frequency of security-related keywords as features. Source code is another widely used avenue to derive vulnerability prediction models. Each piece of code can be represented by text, metric, token, tree, or graph. For example, in the metric-based representation, a code fragment is represented by a vector of features, such as lines of code, number of functions, total external calls, etc. These metrics can be extracted automatically with existing source code analyzers or extractors, which become ideal available resources to train prediction models [19, 41, 62]. Metric-based representation is often used at the file/component fragment level.
2.2 Software Vulnerability Dataset Class Imbalance

Software bug report based [49] or source code metric based [45] prediction models mostly require a large amount of prior knowledge of vulnerabilities, which means many known vulnerable bug reports or codes are needed to train supervised machine learning models effectively. However, the imbalance between non-security bug reports and security bug reports or non-vulnerable code and vulnerable code brings significant challenges. When training machine learning prediction models with those class imbalanced datasets, the resulting models usually demonstrate a heavy bias towards the majority class. They tend to classify new data into the majority class, but they belong to the minority class. Such a phenomenon makes prediction models difficult to detect rare vulnerabilities (which are important) since models cannot effectively learn the decision boundary, resulting in poor performance.

Many prior studies have introduced various ways to tackle this issue, such as utilizing the "sampling" idea with the imbalanced data and they mainly fall into the following categories:

- UnderSampling to remove majority class instances;
- Oversampling to generate more of the minority class instances;
- Some hybrid of the first two methods.

How to choose an appropriate way to sample the datasets is based on the characteristics of the datasets. Machine learning researchers [27] advise that undersampling usually works better than oversampling if there are hundreds of minority instances in the datasets. When there are only a few dozen of minority instances, the oversampling approaches are superior to undersampling. In the case of large size training datasets, the hybrid methods would be preferred. The datasets we studied fall into the second category. Therefore, oversampling is a better choice.

2.3 SMOTE

A simple way to oversample data is to duplicate samples from the minority class in the training dataset before training a model. Samples from the training dataset are selected randomly with replacement. This method is called RandomOverSampler. It is referred to as a "naive" method because it assumes nothing about the data and provides no additional information to the model but barely balances the class distribution.

An improved way is synthesizing new samples with existing samples from the minority class. Synthetic Minority Oversampling Technique, also known as SMOTE [13], is an algorithm that oversamples the minority class by creating new synthetic samples. SMOTE works by selecting samples that are close in the feature space, drawing a line between the samples, and generating a new sample at a point along that line (as shown in Figure 2). Specifically, SMOTE calculates the k nearest neighbors for each minority class sample. Depending on the amount of oversampled instances required, one or more of the k-nearest neighbors are selected to create the synthetic samples. This amount is usually denoted by oversampling percentage (e.g., 50% by default). The next step is to create a synthetic sample connecting two minority samples randomly.

![Figure 2: An example of how SMOTE works. The blue dots denote the majority class samples and the orange dots denote the minority class samples. In SMOTE, a neighbour sample X2 is selected for sample X1 and a new synthetic sample X' (i.e., the red dot) is created as a linear interpolation.](image)

Algorithm 1: Pseudocode for SMOTE.

```
1 Function SMOTE (D_training, k, m, r);
2 Input: Training datasets - D_training,
3 Number of nearest neighbours - k,
4 Number of synthetic samples to create - m,
5 Distance metric parameter - r
6 Output: Resampled training datasets - D_resampled
7 while # of Minority samples < m do
8     x ← random minority class samples from D_training
9     neighbours ← k nearest neighbours of x
10    for n_i ∈ neighbours do
11        x_new ← interpolate(x, n_i)
12        Add x_new to D_resampled
13 return D_resampled
```

Algorithm 1 describes how SMOTE works. A random sample from the minority class is firstly chosen. Then k of the nearest neighbors of that example are found. For each selected neighbor, a synthetic example is created at a randomly selected point between the two samples in feature space. The approach is more effective than the naive duplicate oversampling because new synthetic samples from the minority class are created that are plausible and relatively close in feature space to existing samples from the minority class.

Table 2 also lists several variants of SMOTE, which are used as our baseline methods for comparison purposes. For example, ADASYN [29] (i.e., Adaptive Synthetic Sampling) is an improved version of SMOTE, which creates synthetic data according to the data density. The synthetic data generation would be inversely proportional to the density of the minority class. It means more synthetic data are created in regions of the feature space where the density of minority examples is low and fewer or none where the density is high. BorderlineSMOTE [28] involves selecting those
instances of the minority class that are misclassified. Unlike with the SMOTE, where the synthetic data are created randomly between the two data, BorderlineSMOTE only makes synthetic data along the decision boundary between the two classes. KMeansSMOTE [38] applies a KMeans clustering before to over-sample using SMOTE, and SVMSMOTE [48] uses an SVM algorithm to detect sample to use for generating new synthetic samples. SMOTETUNED [1] is an auto-tuning version of SMOTE that optimizes its parameters.

### 2.4 GANs

Compared with SMOTE, GANs is a new emerging technique, and in this work, we explore the merits of GANs over SMOTE. Generative Adversarial Networks (GANs) [25] are a neural network architecture that has a set of two models used to produce synthetic data. The GANs model architecture (see Figure 3) typically involves two submodels, i.e., a generator and a discriminator. The generator model generates new plausible examples in the problem domain, while the discriminator model distinguishes whether the new generated examples by generator are real or fake, from the perspective of the domain. Both of the models are trained in a min-max zero-sum game since the generator tries to produce synthetic instances of data that reliably trick the discriminator, while the discriminator tries to distinguish between real and fake data.

The two models, the generator and discriminator, are trained together. The generator generates a batch of samples, and these, along with real examples from the domain, are provided to the discriminator and classified as real or fake. The discriminator is then updated to get better at discriminating real and fake samples in the next round, and importantly, the generator is updated based on how well or not, the generated samples fooled the discriminator. When training begins, the generator produces obviously fake data, and the discriminator quickly learns to tell that it’s fake. Finally, if generator training goes well, the discriminator gets worse at telling the difference between real and fake. It starts to classify fake data as real, and its accuracy decreases. Both the generator and the discriminator are neural networks. The generator output is connected directly to the discriminator input. Through backpropagation, the discriminator’s classification provides a signal that the generator uses to update its weights. In fact, a really good generative model may be able to generate new examples that are not just plausible, but indistinguishable from real examples from the problem domain.

The loss function of GANs is shown as follows:

\[
\min_{G} \max_{D} V(D, G) = E_{x} [\log (D(x))] + E_{z} [\log (1 - D(G(z)))]
\]  

where \(D(x)\) is the discriminator’s estimate of the probability that real data instance \(x\) is real, \(E_{x}\) is the expected value over all real data instance. \(G(z)\) is the generator’s output when given noise \(z\) and \(D(G(z))\) is the discriminator’s estimate of the probability that a fake instance is real. \(E_{z}\) is the expected value over all random inputs to the generator. The goal of discriminator is to bring \(D(G(Z))\) closer to 0, while the goal of generator is to bring it closer to 1. If the generator outputs a probability of 0.5, then this means the discriminator is unable to make a right decision whether the instance is real or fake.

### Algorithm 2: Pseudocode for a simple GANs as an oversampler.

```
1 Function simpleGAN (D_{training}, G):
2   Input : Training datasets - D_{training},
3       Discriminator - D, Generator - G
4   Output: Resampled training datasets - D_{resampled}
5   for epoch \( \in \) number of epochs do
6       Sample a mini-batch of real data, train as true
7       sample a mini-batch of fake data from Generator G, train as false
8       Update the gradient of Discriminator D
9       /* Train Discriminator */
10      Sample a mini-batch of fake data from Generator G, which should be classified as true
11      Update the gradient of Generator G
12      /* Train Generator */
13     Generate new data \(X_{new}\) with Generator G
14     Add \(X_{new}\) to \(D_{resampled}\)
15   return \(D_{resampled}\)
```
GANs are rapidly evolving fields, delivering promising results in generating realistic examples across a range of problem domains, most notably in tasks such as synthesizing images from text description [67], image compression [2], image classification [69], etc. In the security domain, prior work indicates that GANs would be an ideal technique to train a classification model to explore unforeseen data threats with generated data. Table 1 lists recent work that use GANs as data oversampler (used in a way similar to Algorithm 2). Those works motivate our study; however, we also note that they hardly introduce any way to optimize their GANs architecture as we do in this study.

2.5 Challenges with traditional GANs

Although GANs have achieved notable success in multiple domains, GANs also face several challenges which may cause issues such as unstable training [31, 52].

Nash Equilibrium. Nash Equilibrium (NE) [46] is a notion in game theory where two players come to a joint strategy in which each player select a best response (i.e., a strategy that yields the best payoff against the strategies chosen by the other player). In the context of GANs, the generator and discriminator represent the two players, which work in an adversarial way against each other. The generator and discriminator train themselves simultaneously for NE. When both generator and discriminator update their cost function independently without coordination, it is hard to achieve NE.

Vanishing Gradient. Vanishing gradient occurs when one part of GANs is more powerful than the other part. For example, if the generator model is very poor, then the discriminator can easily distinguish between real and fake samples. This further causes the probability of the generated samples being real from generator close to zero, i.e., gradients of \( \log(1 - D(G(z))) \) will be very small. Therefore, discriminator fails to provide gradients and the generator will stop updating.

Mode Collapse. Model collapse is one of the most crucial issues with GANs training, which means the output samples from generator lacks of variety (i.e., producing same outputs). If the generator starts to produce the same output, an ideal strategy for the discriminator is to reject the output. However, if the discriminator gets stuck in local minima and does not find the strategy, then the generator tends to find the same output that seems most plausible to the discriminator.

2.6 Attempts to Address the Challenges

Prior work indicates that Wasserstein GAN (WGAN) [6, 7] is designed to prevent vanishing gradients. In WGAN, the discriminator does not classify input instances, but it outputs an exact score for each instance. WGAN does not use a threshold to decide whether an instance is real or fake but tries to make the score bigger than fake instances. WGAN also alleviates mode collapse since it prevents the discriminator from getting stuck in local minima. In this case, the generator has to try new samples since the discriminator would reject the same sample. For the Nash equilibrium problem (i.e., non-converge), prior work [18] suggests an exhaustive hyper-parameter and architecture search, and hence this work. We will discuss WGAN and architecture optimization in detail in the next subsections.

2.7 cWGAN-GP

Traditional GANs is motivated to minimize the distance between the actual and predicted probability distributions for real and generated samples. Typically, there are two metrics to measure the similarity between two probability distributions, the Kullback-Leibler divergence and the Jensen-Shannon divergence.

Kullback-Leibler divergence [37], also known as KL divergence, is a metric to measure relative entropy between two probability distributions over the same variable. Consider distributions \( P \) and \( Q \) of a continuous random variable, the KL divergence is computed as an integral as follows:

\[
KL(P||Q) = \int p(x) \log \left( \frac{p(x)}{q(x)} \right) dx
\]  

where \( p(x) \) and \( q(x) \) are the probability density functions of distribution \( P \) and \( Q \), respectively. The lower the KL divergence value, the closer the two distributions are to each other.

An extension to KL divergence is the Jensen-Shannon divergence [21], also known as JS divergence. Compared with KL divergence, this metric is a symmetric version, which means calculating the divergence for distribution \( P \) and \( Q \) will result in the same score as from distribution \( Q \) and \( P \). Define the quantity \( M = (P + Q) / 2 \), JS divergence is formulated as follows:

\[
JS(P||Q) = \frac{1}{2} KL(P||M) + \frac{1}{2} KL(Q||M)
\]

Besides symmetric, JS divergence is also a smoothed and normalized version, and the square root of this score which referred as Jensen-Shannon distance is commonly used.

The JS divergence scores provides ways to calculate scores for cross-entropy which is commonly used as a loss function in classification models such as the discriminator in GANs. However, researchers notice that such loss function does not necessarily correlate with the sample quality and therefore does not guarantee the convergence between generator and discriminator to an equilibrium [24]. Wasserstein GAN [6, 7] improves traditional GANs' optimization goal based on Wasserstein distance, which is formulated as follows:

\[
W(P, Q) = \inf_{\gamma \sim \pi} \mathbb{E}_{(x, y) \sim \gamma} [\|x - y\|]
\]

where \( \pi(P, Q) \) is the set of all possible joint distributions in which \( P \) and \( Q \) are combined. For each possible joint distribution \( \gamma \), a real sample \( x \) and a generated sample \( y \) can be sampled, and the sample distance \( \|x - y\| \) is calculated, so that the expected value \( \mathbb{E}_{(x, y) \sim \gamma} [\|x - y\|] \) of the sample to the distance under the joint distribution \( \gamma \) can be calculated. This expected value can be taken to the lower bound in all possible joint distributions and defined as the Wasserstein distance of the two distributions. This distance is helpful when facing two distributions with non-overlapping, in which case JS divergence fails to provide a useful gradient.

WGAN with Gradient Penalty (WGAN-GP) further suggests to add a gradient penalty to address the concern of Lipschitz constraint. With the gradient penalty, the norm of the gradient is limited to a

\[
\|D_{\theta}(z)\|_{l_2} \leq 1
\]
value of 1 to satisfy the 1-Lipschitz continuous condition. This is helpful to build a “worse” discriminator, but provide more gradient information that helps to train a better generator. In short, the use of gradient penalty helps enhance the training stability and reduce the mode collapse of the networks.

Moreover, we adopt an extension to WGAN-GP, which is called conditional WGAN-GP. In this method, both the generator and discriminator add data category information, with which the optimization function of WGAN-GP is a maximal and minimal game with this condition.

2.8 Bayesian Optimization

Since training a new GANs model can be difficulty, this works checks if that process can be automated with hyperparameter optimization. Typically a hyperparameter has a known effect on a model in the general sense, but it is not clear how to best set a hyperparameter for a given dataset. Hyperparameter optimization or hyperparameter tuning is a technique that explores a range of hyperparameters and search for the optimal solution for a task. Bayesian optimization [54, 57] is a widely-used hyperparameter optimization technique that keeps track of past evaluation results. The principle of Bayesian optimization is using those results to build a probability model of objective function, and map hyperparameters to a probability of a score on the objective function, and therefore use it to select the most promising hyperparameters to evaluate in the true objective function. This method is also called Sequential Model-Based Optimization (SMBO).

The probability representation of the objective function is called surrogate function or response surface because it is a high-dimensional mapping of hyperparameters to the probability of a score on the objective function. The surrogate function is much easier to optimize than the objective function and Bayesian methods work by finding the next set of hyperparameters to evaluate the actual objective function by selecting hyperparameters that perform best on the surrogate function. This method continually updates the surrogate probability model after each evaluation of the objective function.

Several prior works have combined Bayesian optimization with GANs in tasks from other domains [16][17], and this work shares the similar underlying idea with previous studies and adopts this combination in selected security tasks.

3 METHODOLOGY

3.1 Dazzle: Optimized cWGAN-GP

In designing the network architecture of cWGAN-GP, another concern emerges as how to select the hyperparameters of the structure. GANs models might be highly sensitive to the hyperparameter selection. Prior work on DCGANs [50] introduced a deep convolutional generative adversarial networks that made several modifications to the model hyperparameters of CNN architecture to address the architectural topology constraints and made the GANs’ training more stable. For example, that work

(1) replaced pooling layers with strided convolutions and fractional-strided convolutions;
(2) used batch normalization for generator & discriminator;
(3) used ReLU activation in generator;

(4) used LeakyReLU activation in discriminator.

Inspired by this work, we hypothesize that GANs would benefit from an automatic optimized architecture. We mean proper hyperparameter selection would help with GANs training to converge and further achieve better performance. In our case as using GANs as data oversampler, if we indicate a not well-designed GANs as GANs A and a well-designed GANs as GANs B, then if we build classification model with training data from GANs B, then the prediction performance is better than the models built from data with GANs A.

However, hyperparameter optimization is not a trivial work, especially when facing a complex system such as neural networks. The tuning process is more challenging since there are more hyperparameter with neural networks, and what’s the most important, even one iteration of evaluation would be time consuming. Traditional hyperparameter optimization techniques such as “random search” or “grid search” either suffer from not ideal performance or would be costly expensive. To address this concern, we propose a method called Dazzle that adopts a novel optimizer called Bayesian optimization that fine-tunes both generator model and discriminator model.

Figure 4: An example of the Bayesian optimization process. Bayesian optimization incorporates prior belief about objective function and updates the prior with samples drawn from objective function to get a posterior that better approximates objective function. The model used for approximating the objective function is called surrogate function. Bayesian optimization also uses an acquisition function that directs sampling to areas where an improvement over the current best observation is more likely. Note that the Bayesian optimization we use come from the HyperOpt [9] library, in which the optimization algorithm is based on Tree of Parzen Estimators (TPE).
Table 3: Hyperparameter selection ranges chosen to optimize in Dazzle.

| Hyperparameter                      | Range       |
|-------------------------------------|-------------|
| Batch Size                          | 16, 32, 64, 128 |
| Learning Rate for Generator         | 0.0005, 0.001, 0.005, 0.01, 0.05, 0.1 |
| Learning Rate for Discriminator     | 0.0005, 0.001, 0.005, 0.01, 0.05, 0.1 |
| Optimizer for Generator             | Adadelta, Adagrad, Adam, Adamax, NAdam, RMSprop, SGD |
| Optimizer for Discriminator         | Adadelta, Adagrad, Adam, Adamax, NAdam, RMSprop, SGD |
| Activation Function for Generator   | elu, relu, selu, sigmoid, softmax, tanh, hard_sigmoid, softplus, leakyRelu |
| Activation Function for Discriminator| elu, relu, selu, sigmoid, softmax, tanh, hard_sigmoid, softplus, leakyRelu |
| No. of Epochs                       | True, False |
| Generator Layer Normalization       | quniform(5, 20, 1) |
| Discriminator Layer Normalization   | True, False |

* Note: quniform(low, high, q) is a function returns a value like round(uniform(low, high)/q) * q, while uniform(low, high) returns a value uniformly between low and high. We also note that we do not tune the number of layers but with a fixed number (e.g., 4) in our study, and we find that such architecture suffices to achieve good performance on considered datasets.

Algorithm 3: Pseudocode of Dazzle’s training process.

1. **Function** Dazzle(D\textsubscript{Training}, D\textsubscript{Validation}, D, G, θ, F).
2. Input: D\textsubscript{Training} \textbullet{} D\textsubscript{Validation}.
3. D\textsubscript{Training} \textbullet{} D\textsubscript{Validation}.
4. D, G, θ, F.
5. **Output:** Optimal resampled training dataset D\textsubscript{resampled}\textsubscript{optimal}.
6. Optimal hyperparameter set θ\textsubscript{optimal}.
7. for iteration, ∈ number of Bayesian Optimization iterations do
8. Select a hyperparameter set θ\textsubscript{optimal} ∈ θ.
9. Train D and G with θ\textsubscript{optimal}.
10. Generate new resampled training dataset D\textsubscript{resampled}.
11. Build classifier with D\textsubscript{resampled} and evaluate with D\textsubscript{validation}.
12. Compute loss with target function F.
13. Rank all optimization iterations by loss with smallest on the top.
14. return D\textsubscript{resampled}\textsubscript{optimal} and θ\textsubscript{optimal}.

Dazzle’s training process is on the training dataset and validation dataset. During each iteration of Bayesian optimization, Dazzle selects a hyperparameters for discriminator and generator from Table 3, and generates new minority samples. These samples are used to resample the original dataset (and to build the classifier). Each time, the classifier is only evaluated with validation dataset. With the optimization goal, the loss is computed. Finally, we rank all the optimization iterations by loss with smallest on the top of the rank, and select the trained classifier from that iteration as the optimized classifier. Moreover, we choose 30 iterations for Bayesian optimization and repeat the whole experiment process 10 times.

Algorithm 3 lists the optimization steps of Dazzle. Note that our task with the security datasets is a binary classification problem. In Dazzle, we choose g-measure as our optimization goal (i.e., the target to increase). G-measure is the harmonic mean of recall and the complement of false positive rate. We choose g-measure based on the following considerations. For an imbalanced dataset where there is a skew in class distribution, we have two competing goals:

- We focus on minimizing false negatives, i.e., increase recall;
- We prefer not to predict too many non-security samples as security samples, i.e., reduce false positive rate.

Therefore, g-measure is ideal for chasing both goals.

Table 4: Statistics of security datasets used in this study. Note that the security target column indicate the number of vulnerable files, security bug reports, and JavaScript function code, respectively.

| Dataset                  | Security Target | Total | Imbalance Rate (%) | No. of Features |
|--------------------------|-----------------|-------|--------------------|-----------------|
| Moodle Vulnerable Files  | 24              | 2,942 | 0.8                | 13              |
| Ambari Bug Reports       | 29              | 1,000 | 2.9                | 101             |
| JavaScript Function Code | 1,496           | 12,125 | 12.3              | 36              |

4 EXPERIMENTAL EVALUATION

4.1 Datasets

Our evaluations are experimented on datasets that are widely studied in prior work. Moodle [62] is an open source learning management system, and the data source for Moodle vulnerabilities is the National Vulnerabilities Database (NVD), from with a variety of vulnerabilities are covered, such as code injection, path disclosure, XSS, etc. A total of 24 vulnerable files are included in this dataset. Ambari [49] is an open source project of Apache that aims to provide, manage and monitor Apache Hadoop cluster. Bug reports with BUG or IMPROVEMENT label from the JIRA bug tracking system are selected, and then the selected bug reports are further classified with scripts or manually into six high impact bugs (i.e., Surprise, Dormant, Blocking, Security, Performance, and Breakage bugs). All the target bug reports in the Ambari dataset all belong to Security bug reports (i.e., bug reports of the type Security). The JavaScript [19] function code dataset extracts data from Node Security Platform and the Snyk Vulnerability Database, and used static source code metrics as predictor features. Table 4 shows a list and description of the datasets used in this study. As we can observe from the table, all datasets suffer from different levels of class imbalanced issues.

4.2 Machine Learning Algorithms

We apply five machine learning algorithms, namely K-Nearest Neighbours (KNN), Logistic Regression (LR), Decision Tree (DT),
Random Forest (RF) and Support Vector Machine (SVM) in our experiment. We choose them since they are widely used in previous literatures in different classification tasks in security [61] or other domains such as defect prediction [40]. We implement these algorithms with open source tool called Scikit-learn. In order to reduce the influence of model hyperparameters to our evaluation results, we adopt default settings from Scikit-learn. We do not claim that the list of algorithms that we use is complete, but we note that these algorithms are enough for our study purpose.

4.3 Evaluation Metrics

For the performance of the classification models, the confusion matrix is used, where TP, TN, FP and FN indicate true positive, true negative, false positive and false negative, respectively. We report the results of recall (pd), false positive rate (pf), f-measure and g-measure as we defined in Table 5. Note that precision and accuracy in the table are not endorsed in our study, since both of these metrics can be inaccurate for datasets where the positive class is rare case. For example, Menzies et al. [44] argue that when the target class is less than 10%, the precision results become more a function of the random number generator used to divide data (for testing purposes). G-measure is a composite metric, which is the harmonic mean of recall and the complement of false positive rate. A higher g-measure indicates higher recall and lower false positive rate. As we discuss before, this metric is also our optimization target in Dazzle. We also report f-measure for completeness purpose.

Table 5: Performance evaluation metrics. Definitions of recall (pd), false positive rate (pf), precision (pre), accuracy (acc), f-measure (f1) and g-measure (g-score).

| Metric      | Expression                                      |
|-------------|-------------------------------------------------|
| Recall (pd) | \( \frac{TP}{TP+FN} \)                        |
| False Positive Rate (pf) | \( \frac{FP}{TP+FP} \) |
| Precision (pre) | \( \frac{TP}{TP+FP} \) |
| Accuracy (acc) | \( \frac{TP+TN}{TP+TN+FP+FN} \) |
| F-Measure (f1) | \( \frac{2\cdot prec \cdot recall}{prec + recall} \) |
| G-Measure (g-score) | \( \frac{2\cdot prec \cdot recall}{prec + recall + 2\cdot recall} \) |

4.4 Experiment Rigs

Our datasets are split in a stratified way into two parts with a ratio of 8:2 where the latter part is used as testing set. We further split the former part into training set and validation set with the same ratio. Therefore, the final ratio between the actual training, validation, and testing part is 6.4: 1.6: 2 of the whole dataset. The training part is only used for training classifiers with selected hyperparameter set, and the validation part is used to evaluate the classifiers during optimization iterations towards optimization goal. Then the selected optimized models are evaluated on the testing dataset.

Lastly, our implementation of Bayesian Optimization is based on the tool called Hyperopt [10], which is one of the most cited hyperparameter optimizer in the literature at this time of writing. The implementation of SMOTE and its variants are based on the open-source imbalanced-learn toolbox [39] while SMOTUNED is implemented according to Agrawal et al.’s study [1]. SMOTUNED has three available parameters:

- Number of neighbours \( k \) with range \([1, 20]\).
- Minkowski distance \( r \) with range \([1, 6]\).
- Number of synthetic samples \( m \) to create with range \([50, 500]\).

5 RESULTS

Our study answers the following research questions:

| RQ1. Will GANs based oversampling better than SMOTE based oversampling? |
|---------------------------------------------------------------------|

For each treatment in our study, we use default learners for fair comparison. Table 6 lists all the evaluations results of metrics defined in Table 5 for all three datasets. In these results, the None treatment indicate the training process with original dataset without any oversampling techniques, after which different oversamplers such as RandomOversampler and variants of SMOTE are presented. The cWGAN-GP treatment is GANs based oversampler with optimization. In order to configure the architecture of cWGAN-GP, we randomly select parameter set from Table 3 during each run.

As we can observe from the table, the original dataset without oversampling performs badly across all datasets, even with different machine learning algorithms. The results are no surprise as we consider the percentage of security relevant class samples in Table 4. For moodle and Ambari dataset, the positive class samples are less than 3% of the whole datasets, it is hard for machine learning algorithms to learn the traits with so few samples. As a result, none of the learners can detect any true positive during the testing phase.

Naive oversampler such as the RandomOversampler shows some advantages for some learners, for example Logistic Regression and SVM, but fails for others. SMOTE and its variants demonstrate better results than RandomOversampler, but the advantage is not obvious. Previous state-of-the-art SMOTUNED works best among all SMOTE based oversampling techniques.

cWGAN-GP is the GANs version oversampler, and there are two observations from the results:

- cWGAN-GP achieves nearly tied performance with SMOTUNED in important metric such as recall, but we note that the latter is an optimized version which requires more effort and configuration.
- Unlike other oversamplers, cWGAN-GP does not fail totally in some certain machine learning algorithms. For example, the SVMSMOTE does not detect any true positive with LR and RF in Moodle dataset, and even 4 out of 5 learners fails in Ambari dataset. This phenomenon indicates that cWGAN-GP is more practical to use in general cases.

We have to point out that the false positive rate metric is not suggested to indicate which method is better than others. For example, in Table 6, for the Random Forest results of Moodle vulnerable files dataset, several treatments have achieve zero false positive rate (therefore highlighted in blue color), however, their recall results are also zero. Thus, these treatments are not recommended.

Since Dazzle optimizes GANs with the goal of increasing g-measure, which is the harmonic mean of recall and the complement
Table 6: Median performance results (converted to range 0 - 100) from 10 repeats. Best performances are highlighted.

| Metric   | Treatment             | Moodle Vulnerable Files | Ambari Bug Report | JavaScript Function Code |
|----------|-----------------------|-------------------------|-------------------|-------------------------|
|          |                       | KNN | LR | DT | RF | SVM | KNN | LR | DT | RF | SVM | KNN | LR | DT | RF | SVM |
|          | None                  | 0   | 0  | 0  | 0  | 0   | 0   | 0  | 14 | 0  | 0   | 63  | 0  | 68 | 68 | 11 |
| Recall   | RandomOversampler     | 0   | 100| 0  | 0  | 100 | 0   | 0  | 57 | 57 | 0  | 42  | 72  | 65 | 76 | 73 | 22 |
|          | SMOTE                 | 40  | 100| 20 | 0  | 100 | 0   | 0  | 100| 42 | 42 | 0  | 76  | 65 | 78 | 77 | 22 |
|          | ADASYN                | 60  | 100| 0  | 0  | 100 | 0   | 0  | 100| 57 | 57 | 0  | 78  | 49 | 76 | 77 | 29 |
|          | BorderlineSMOTE       | 40  | 60 | 0  | 0  | 60  | 0   | 0  | 100| 0  | 14 | 0  | 75  | 49 | 76 | 76 | 30 |
|          | SVMSMOTE              | 40  | 60 | 0  | 0  | 40  | 0   | 0  | 0  | 28 | 0  | 74  | 58 | 79 | 76 | 25 |
|          | SMOTUNED              | 60  | 100| 60 | 60 | 100 | 0   | 0  | 57 | 57 | 28 | 57  | 81  | 100| 80 | 83 | 100|
|          | cWGAN-GP              | 80  | 60 | 60 | 80 | 80  | 0   | 28 | 57 | 57 | 43 | 57  | 79  | 79 | 83 | 78 | 49 |
|          | Dazzle                | 100 | 80 | 100| 100| 80  | 85  | 71 | 71 | 57 | 57 | 86  | 84 | 83 | 83 | 78 |

| Function Code | None | RandomOversampler | SMOTE | ADASYN | BorderlineSMOTE | SVMSMOTE | SMOTUNED | cWGAN-GP | Dazzle |
|---------------|------|-------------------|-------|--------|-----------------|----------|----------|----------|--------|
| JavaScript    | 2    | 39                | 1     | 0      | 22              | 0        | 3        | 3        | 0      | 7     | 6    | 43   | 6    | 3    |
| Moodle        | 57   | 33                | 0     | 87     | 0               | 71       | 71       | 0        | 58     | 81    | 61   | 84   | 83   |
| G-Measure     | 69   | 74                | 0     | 0      | 85              | 0        | 7        | 71       | 59     | 82    | 56   | 84   | 85   |
| F-Measure     | 56   | 68                | 0     | 0      | 72              | 0        | 3        | 0        | 24     | 82    | 55   | 84   | 84   |

of false positive rate. Therefore, when the g-measure is increased, there would be three cases: 1) recall increased, FPR decreased; 2) recall increased, FPR increased; and 3) recall decreased, FPR decreased. Our results would fall into these three groups. When we notice that some improvements in recall come at the cost of increments in false positive rate, while the ideal false positive rate is zero. We say that the trade-off between the increments of recall and false positive rate is still acceptable, especially in mission-critical security tasks, as we do not want to miss any security relevant target samples in the detection. Such a “price” indicates more extra effort to read more source code or bug reports for security practitioners, and it is the price of software quality assurance.

**RQ2. Will Dazzle (optimized GAN) work even better?**

We optimize Dazzle with the goal of g-measure, which ideally with high recall and lower false positive rate. As we can observe from the result table, Dazzle works even better than cWGAN-GP. Benefit from optimizing, Dazzle achieves an average of improvement rate of 30%, 62% and 17% over cWGAN-GP in recall, respectively. This is explainable, as the “default” (with randomly selection in our case) hyperparameters for GANs might bring in issues in Section 3, hence is not one-size-fits-all across all scenarios and should be deprecated. We would recommend exploring and developing specialized tools for certain local domain.

**Answer**

cWGAN-GP is more practical to use in the general cases, as it is not sensitive to certain machine learning algorithms.

**Answer**

Dazzle (the optimized version) shows even better performance than cWGAN-GP across all studied datasets.
As shown in RQ1, Dazzle achieves promising improvement over baseline treatments in performance with 30 iterations of optimization trails. Table 7 lists the average runtime of each treatment of all machine learning algorithms. Considering the complexity of optimizing the architecture of neural networks, Dazzle is not surprisingly takes the most runtime cost. However, considering the mission-critical nature of the security tasks we are addressing, we would comment that the trade-off between performance and runtime is still worth. The experiment is carried out with CPU resources only, and with the help of GPU or parallel computing, Dazzle could be configured to be more practical to use.

Lastly, we believe that there are several directions that can be explored after this work. For example, we would like to try more security tasks to check and endorse the merits of the proposed methods in other cases. Secondly, we would plan to compare with other baselines such as recent improvements on SMOTE and methods other than oversampling. Thirdly, we would like to perform more analysis of the new samples generated by the proposed method to get a better understanding of the methods.

6 THREATS TO VALIDITY

6.1 Evaluation Bias
In our work, we choose some commonly used metrics for evaluation purpose and set g-measure as our optimization target. We do not use some other metrics because relevant information is not available to us or we think they are not suitable enough to this specific task (e.g., precision). In addition, we use equal weight in recall and specificity in the definition of g-measure, which is widely adopted in existing literature. We agree that it is important for these two elements to be re-weighted for different tasks, and this can be further explored as one of our future directions. Our implementation is flexible and we can adjust to proper metrics or balances with minor code modification.

6.2 Parameter Bias
We have to note that default hyperparameter values have been used for the baseline machine learning algorithms, which means that the performance results reported in Table 6 might be suboptimal for baseline methods. To some degree, this also might have the effect of magnifying the advantages of the proposed method. Previous studies have also indicated that it is a good practice to avoid using default settings of machine learning algorithms [36] [56] [59]. In the case if those hyperparameters have been tuned, the conclusions from the proposed method might be different.

6.3 Learner Bias
Research into automatic classifiers is a large and active field. While different machine learning algorithms have been developed to solve different classification problem tasks. Any data mining study, such

| Table 7: Runtime of oversampling treatments in minutes for each dataset. Note that “<” means the runtime is close but less than the given results. |
|-----------------------------------------------|
| Treatment          | Moodle Vulnerable Files | Ambgro Bug Report | JavaScript Vulnerability |
| RandomOversampler  | < 1                      | < 1               | < 1                      |
| SMOTE              | < 1                      | < 1               | < 1                      |
| ADASYN             | < 1                      | < 1               | < 1                      |
| BorderlineSMOTE    | < 1                      | < 1               | < 1                      |
| SVMSMOTE           | < 1                      | < 1               | < 1                      |
| SMOTUNED           | < 3                      | < 2               | < 5                      |
| cWGAN-GP           | < 5                      | < 5               | < 5                      |
| Dazzle             | < 25                     | < 25              | < 30                     |

as this paper, can only use a small subset of the known classification algorithms. For this work, we select machine learning algorithms that are commonly used in classification tasks.

6.4 Input Bias
Our results come from the space of hyperparameter optimization explored in this paper. In theory, other ranges might lead to other results. That said, our goal here is not to offer the best optimization but to argue that optimized GANs architecture is better than current state-of-the-art oversampler in addressing class imbalance. For those purposes, we would argue that our current results suffice.

6.5 Dataset Bias
This empirical study demonstrates the effectiveness of the proposed method in security vulnerability/bug report datasets. However, the internal difference between studied datasets and datasets from other security tasks (e.g., in Table 1) or from other domains cannot be ignored. Therefore, there is no guarantee that the findings in this study would still hold in other datasets.

7 OTHER NOTES ON CLASS IMBALANCE

Class-imbalance learning [43] refers to methods to handle class imbalance issues. Data oversampling is not the only effective way to address data imbalance issues. Other approaches can mainly fall into the following categorizations according the the problem space:

Data Sampling level. Apart from data oversampling, data undersampling [35, 42] is another alternative way to deal with class imbalance from the data level. In data undersampling, we can remove some instances from majority class. Generally, this method is suggested when there is large number of training instances. However, data undersampling might suffer from information loss due to removal of majority class instances.

Model Training level. Many prior work propose various ways to train efficient models with class imbalanced datasets. For example, bagging ensemble [22] is a technique that divides the original training datasets into several subsets of same size, while each subset is used to train a single classifier, and then the method aggregates individual classifiers into an ensemble classifier. This method is well-known for its simplicity and good generalization ability. Some other work [56] applies hyperparameter optimization on both data pre-processors and machine learning models to explore optimal
When the target class is rare, as it is often within security datasets, prior researchers in software engineering often use SMOTE (or its variants, see Table 2) as a solution. SMOTE is an oversampling technique in addressing security dataset imbalance issues. It is not fair to offer all data imbalance solutions extensively. It is not fair to offer a general conclusion that one technique outperforms other techniques in all tasks. Rather, the focus of this work is to explore the merits of optimized generative adversarial network as an data over-sampling technique in addressing security dataset imbalance issues.

A hybrid combination of above mentioned approaches (including this work) might work even better, and we would like to explore as an interesting future direction.

8 CONCLUSION

When the target class is rare, as it is often within security datasets, it is hard for a machine learning algorithm to distinguish the goal (security target) from others (the normal events). To address such class imbalance issue, prior researchers in software engineering often use SMOTE (or its variants, see Table 2) as a solution. SMOTE was first proposed in 2002, nearly two decades ago. This paper seeks a better method than SMOTE.

One recent alternative to SMOTE is the Generative Adversarial Networks. This architecture contains two components (the generator and the discriminator) that “fight it out” to generate new examples. The experience has been that it is hard to balance these two components manually, so we experimented with addressing that problem with automatic hyperparameter optimization. The empirical study shows that GANs with hyperparameter optimization outperforms prior SMOTE (and its variants) and standard GANs (without optimization). For example, Dazzle can achieve an average of about 60% improvement rate over SMOTE in recall on studied dataset among different classifiers. Based on this study, we recommend using GANs with hyperparameter optimization (and not off-the-shelf default settings) to train a good security vulnerability prediction model (from the view of data oversampling). More generally, we suggest using hyperparameter optimization in other tasks in SE community.

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