



Killing Two Birds with One Stone: Malicious Package Detection in NPM and PyPI using a Single Model of Malicious Behavior Sequence

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Open-source software (OSS) supply chain enlarges the attack surface of a software system, which makes package registries attractive targets for attacks. Recently, multiple package registries have received intensified attacks with malicious packages. Of those package registries, NPM and PyPI are two of the most severe victims. Existing malicious package detectors are developed with features from a list of packages of the same ecosystem and deployed within the same ecosystem exclusively, which is infeasible to utilize the knowledge of a new malicious NPM package detected recently to detect the new malicious package in PyPI. Moreover, existing detectors lack support to model malicious behavior of OSS packages in a sequential way.

To address the two limitations, we propose a single detection model using malicious behavior sequence, named CEREBRO, to detect malicious packages in NPM and PyPI. We curate a feature set based on a high-level abstraction of malicious behavior to enable multi-lingual knowledge fusing. We organize extracted features into a behavior sequence to model sequential malicious behavior. We fine-tune the pre-trained language model to understand the semantics of malicious behavior. Extensive evaluation has demonstrated the effectiveness of CEREBRO over the state-of-the-art as well as the practically acceptable efficiency. CEREBRO has detected 683 and 799 new malicious packages in PyPI and NPM, and received 707 thank letters from the official PyPI and NPM teams.

CCS Concepts: • Security and privacy → Software security engineering; • Computing methodologies → Artificial intelligence; • Software and its engineering → Software libraries and repositories.

Additional Key Words and Phrases: malicious package detection, open source packages, behavior sequence modeling, large language models

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ACM 1557-7392/2024/11-ART

<https://doi.org/10.1145/3705304>

1 INTRODUCTION

As the adoption of open source software (OSS) continues to grow, the security concerns about OSS supply chain have attracted increased attention [20, 29, 42, 72, 77]. The frequency and impact of OSS supply chain attacks have reached unprecedented levels. According to Sonatype [74], there has been an astonishing average annual increase of 742% in OSS supply chain attacks over the past three years. According to Gartner’s prediction [22], 45% of organizations worldwide will have experienced OSS supply chain attacks by 2025. This alarming trend can be attributed to the expanded attack surface through the OSS supply chain. For example, installing an NPM package introduces an average of 79 transitively dependent packages and 39 maintainers which can be exploited; and some popular packages influence more than 100,000 packages and thus become attractive targets for attacks [96].

Problem. One of the OSS supply chain attacks is to inject malicious code into packages hosted in popular package registries. Package registries NPM and PyPI have been flooded with malicious packages, as revealed by recent reports [34, 45, 61, 71, 73]. For example, the PyPI team removed over 12,000 packages in 2022, which were mostly malware [34]; and the Sonatype team caught 422 malicious NPM packages and 58 malicious PyPI packages in December 2022 [73], mostly data exfiltration through typosquatting or dependency confusion attacks. An alarming incident occurred in December 2022 was the dependency confusion attack on PyTorch [66]. The attack exploited the fact that the nightly built version of PyTorch depended on a package named “torchtriton” from the PyTorch nightly package index. However, a malicious package with the same name was uploaded to PyPI. Since PyPI takes precedence over the PyTorch nightly package index, the malicious “torchtriton” was installed instead of the legitimate version. The prevalence of malicious packages in NPM and PyPI calls for practically effective malicious package detection system.

Existing Approaches. Several approaches have been proposed to detect malicious packages in NPM and PyPI. They can be classified into rule-based [12, 51, 80, 83, 87, 88, 94], unsupervised learning [21, 47, 58], and supervised learning approaches [15, 16, 43, 57, 70, 90]. Rule-based approaches often rely on predefined rules about package metadata (e.g., package name) and suspicious imports and method calls. They often incur high false positives, which is far from reaching practical demands [85]. Learning-based approaches capture malicious behavior as a set of discrete features. They overlook the sequential nature of malicious behavior which is usually composed of a sequence of suspicious activities, hindering the practical effectiveness. Moreover, except for [12, 51, 80], these approaches are designed and evaluated for one ecosystem (i.e., either NPM or PyPI). OSS Detect Backdoor [51] and Taylor et al. [80] adopt lightweight rules to support different ecosystems, while Duan et al. [12] use heavyweight rules that require both static and dynamic program analysis.

Limitations. We summarize two limitations that hinder the effectiveness of existing approaches. The first limitation is that the knowledge of malicious packages from different ecosystems is not sufficiently leveraged. Although there are evident clues of attackers transcribing malicious packages and spreading them across multiple ecosystems [65], there has been limited action in addressing this evolving threat landscape. Moreover, the NPM and PyPI teams do not publicly release the entire collection of malicious packages for preventing potential misuse or exploitation, and hence the publicly available datasets of malicious NPM and PyPI packages [12, 59] are small in size, which are significantly smaller than the reported ones [34, 73]. The malicious package detection may be less effective when the available malicious package data is limited. The second limitation is that sequential knowledge is missing in existing approaches. Malicious packages typically conduct a sequence of suspicious activities to achieve an attack. However, existing rule-based and learning-based approaches fail to consider the sequential nature of malicious behavior. Consequently, false positives and negatives may arise due to imprecise modeling.

Our Approach. To address these two limitations, the challenges become 1) *how to leverage the knowledge of malicious packages from different ecosystems in a unified way such that multi-lingual malicious package detection can be feasible*, and 2) *how to model malicious behavior in a sequential way such that maliciousness can be precisely*

captured. To that end, we propose a single model, named CEREBRO, to detect malicious packages in NPM and PyPI using malicious behavior sequences.

CEREBRO has three key components which are the feature extractor, behavior sequence generator, and maliciousness classifier. The feature extractor employs static analysis to extract a set of 16 features. We curate this feature set based on a high-level abstraction of malicious behavior, which is language independent. Thus, it enables multi-lingual knowledge fusing across NPM and PyPI, and solves the first challenge. Notably, CEREBRO is focused solely on static features and does not consider metadata or dynamic features, as it aims to strike a balance between effectiveness and efficiency.

The behavior sequence generator produces a behavior sequence of a package by organizing extracted features based on their likelihood of execution and their sequential order in execution, which solves the second challenge. We determine the execution likelihood according to the time phase of execution (i.e., install-time, import-time or run-time), and we determine the sequential order according to generated call graph.

The maliciousness classifier employs a fine-tuned language model [37, 50, 67] on the generated behavior sequence to determine whether a package is malicious or not. We transform the behavior sequence into a textual description to ease the semantic understanding of malicious behavior. We fine-tune the model on NPM and/or PyPI packages into a binary classifier.

Evaluation. To evaluate the effectiveness and efficiency of CEREBRO, we conduct extensive experiments on a dataset of 2,675 malicious and 7,391 benign NPM and PyPI packages. Our evaluation results have demonstrated that CEREBRO outperforms the state-of-the-art by an average of 10.0% in precision and 7.4% in recall in the mono-lingual scenario (i.e., train and test on the same ecosystem), and by 9.9% in precision and 8.9% in recall in the bi-lingual scenario (i.e., train on two ecosystems and test on one of the two ecosystems). CEREBRO takes an average of 10.5 seconds to analyze a package, which is practically efficient. Further, we conduct an ablation study to validate the contribution of behavior sequence.

To evaluate the usefulness of CEREBRO in practice, we run CEREBRO on the newly-published packages in PyPI and NPM over 8 and 7 months. From 923,638 newly-published package versions, we detect 5,976 potentially malicious package versions. After our manual confirmation, we detect 683 malicious PyPI package versions and 799 malicious NPM package versions. We report these detected malicious package versions to the official PyPI and NPM teams. All these malicious package versions have been removed by the official teams. 775 of them have already been removed before our report, and hence we receive 707 thank letters for the remaining ones.

Contributions. Our work makes following contributions.

- We proposed and implemented a single model using malicious behavior sequence, named CEREBRO, to detect malicious packages in NPM and PyPI.
- We conducted extensive experiments to demonstrate the effectiveness and efficiency of CEREBRO.
- We detected 683 and 799 new malicious packages in PyPI and NPM, and received 707 thank letters from the official team of PyPI and NPM.

2 THREAT MODEL

We discuss the stakeholders and their activities involved in the development and distribution of OSS. Different from existing work [42], our threat model is particularly focused on the threats of using package registries, i.e., NPM [24] and PyPI [19]. NPM and PyPI are widely recognized as the primary package registries for hosting Python and JavaScript packages, respectively. To facilitate package management, PyPI is seamlessly integrated with the *pip* package manager, which is the default package manager for Python. Similarly, NPM is closely integrated with the *npm* package manager. As shown in Figure 1, Package Developers (PDs) develop and maintain packages, and use the package manager to upload their packages to the package registry. Registry Administrators (RAs) then vet the uploaded packages and determine whether they should be published. Once published, packages

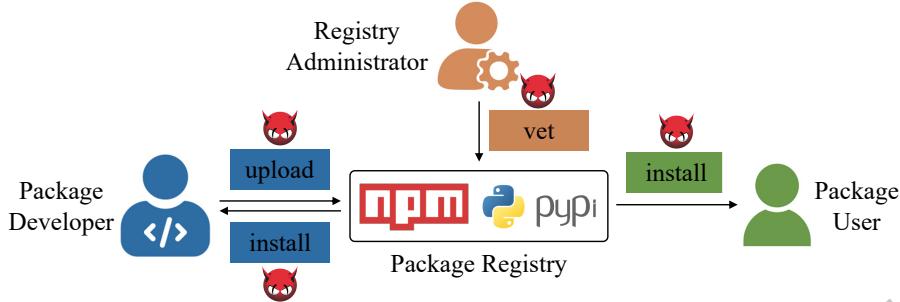


Fig. 1. Threats in the Package Registry Ecosystem

become publicly available on the package registry. Package Users (PUs) then leverage the package manager to conveniently download and install desired packages for use in their own projects. We analyze the threats in these package management steps, which involve three key stakeholders (i.e., PDs, RAs and PUs).

2.1 Threats in Developing Packages

The threats in developing packages allow the injection of malicious code into packages. We summarize two key threats.

Weak/Compromised Credentials. Various tools (e.g., version control systems and build systems) are used during the development of packages. Hence, account hijacking may happen due to weak credentials [39], or compromised credentials by exploiting vulnerabilities in these tools [30, 41]. As a result, attackers can gain access to PDs' accounts, and hence have the privilege to inject malicious code.

Weak Governance in Collaborative Development. Packages are collaboratively developed by OSS community with many PDs. However, the governance of PDs is weak. First, malicious contributors can fool the development team of an existing package. They may first pretend to be benign to gain trust by committing useful features and then secretly commit malicious code, or submit pull requests that fix bugs or add useful features but also include additional malicious code [23]. Second, benign PDs of an existing package may add malicious PDs into the team [75] or become malicious PDs by social engineering tactics, or the ownership is transferred to malicious PDs [8]. As a result, malicious PDs have the full right to inject malicious code and publish malicious packages. Third, instead of infecting existing packages, attackers may first publish a benign and useful package, wait until it is used, and then update it to include malicious code [56], or launch squatting attacks to inject malicious code into a new package whose name is similar to a popular and benign package [87].

2.2 Threats in Vetting Packages

The threats in vetting packages allow malicious packages to be publicly available to PUs. We summarize two key threats.

Ineffective/Insufficient Package Vetting. A vetting system is often employed by RAs to first automatically identify suspicious packages and then manually triage them. However, the vetting system lacks effectiveness, which allows malicious packages to evade detection and be published. This is evidenced by the recent report from Snyk [10], which has documented around 6,800 malicious packages on PyPI and NPM since the beginning of 2023. One major contributing factor is the overwhelming flood of suspicious packages and the limited resources and budgets for RAs. For example, PyPI had one person on-call to hold back weekend malware rush [9]. A recent interview with PyPI's RAs also confirms this dilemma [85]. Consequently, the manual triage in the vetting system is not sufficient, allowing malicious packages to bypass the system.

Insecure Governance of RAs. As package registries are often maintained by the OSS community, not all RAs can be blindly trusted. Attackers can disguise themselves as trustworthy developers to gain RAs’ trust; and they may employ social engineering tactics to gain control of RAs’ accounts. As a result, such malicious RAs have the right to grant and publish malicious packages to registries.

2.3 Threats in Using Packages

The threats in using packages allow malicious behaviors to be potentially triggered. We summarize two key threats.

Weak Awareness of Security. When PUs (including application developers and package developers) input the package name, the package manager searches and retrieves the corresponding package from the package registry. Unfortunately, this process is susceptible to various attacks. Attackers often exploit techniques such as typosquatting [80], combosquatting [87] and dependency confusion [4] to deceive PUs into mistakenly installing malicious packages. Attackers may also employ search engine optimization (SEO) poisoning or phishing techniques [35] to advertise their packages on package registries, increasing the risk of unintended installation.

Weakness in Automated Dependency Resolution. Package managers employ automated dependency resolution algorithms to select package versions when updating package versions and installing transitive dependencies. As a result, malicious package versions can be silently installed. This places a long-standing burden on PUs, as they must consistently monitor potential compromises among package updates [96].

3 PRELIMINARY AND MOTIVATION

We present preliminary information on triggering malicious behavior, and then show two motivating examples.

3.1 Triggering Malicious Behavior

Once malicious code is present in an application’s OSS supply chain (i.e., its direct and transitive dependencies) in NPM and PyPI, malicious behavior can be triggered in three scenarios.

Install-Time Execution. Malicious code is often contained in install scripts that are automatically executed during package installation [59]. For PyPI packages, *pip* automatically executes the *setup.py* script present at the root of the package during installation. This script is responsible for performing any necessary preparation or configuration required for the installation. Similarly, NPM introduces a mechanism that utilizes *scripts* property in the package *.json* [11]. This property allows developers to specify certain keys, such as *preinstall* and *postinstall*, to indicate the paths of scripts to be automatically executed. In this scenario, attackers inject the malicious payload into install scripts. The malicious payload is executed without requiring any additional action as long as the infected package is installed. This scenario provides attackers with the highest probability of successfully carrying out attacks.

Import-Time Execution. Malicious code can also be executed when a package module is imported. This is achieved in Python/JavaScript by injecting malicious code into the initialization file *__init__.py*/*index.js*, which is executed by default when the interpreter executes *import/require* statements. Further, the interpreter continues to load the imported module file and execute the code at the global scope. The code at the global scope typically refers to statements that exist outside any method or class declaration. For the ease of presentation, we refer to the code at the global scope as the implicit “main” method. Attackers take advantage of this module import mechanism by injecting malicious code into this implicit “main” method.

Run-Time Execution. Malicious code can also be executed at run-time during the normal control flow of applications. This is achieved by including the malicious code in a legitimate method that is unlikely to raise suspicion while hoping that the infected method will be invoked by applications. This scenario provides the

Table 1. Feature Types used in Existing Literature

Feature Type	Description	Example Literature
Metadata Feature	Package name, package size, uploader profile, etc	Zimmermann et al. [96], Taylor et al. [80], Vu et al. [87], Zahan et al. [94]
Syntactic Feature	Elements and structures within the source code	Liang et al. [90], Vu et al. [84], Vu et al. [86], Ladisa et al. [43]
Semantic Feature	Features that have explicit semantic meanings	Garrett et al. [21], Fang et al. [14]
Implicit Feature	Implicit features vectorized from program dependence graph, abstract syntax trees, etc	Ohm et al. [58]
Dynamic Feature	Features captured during runtime execution	Duan et al. [12], Ohm et al. [60]
Hybrid Feature	Mixture of the single feature types	Liang et al. [47], Duan et al. [12], Sejfia et al. [70], Ohm et al. [57]

Table 2. Feature Set to Model Malicious Behavior (● = Supported, ○ = Unsupported)

Dimension	Feature Description	CEREBRO	AMALFI[70]	MALOSS[12]	PPD[47]	Garrett et al.[21]	Ohm et al.[57]	Fang et al.[14]
Metadata	M1: suspicious package name	○	○	●	●	○	●	○
	M2: suspicious maintainer	○	○	●	●	○	○	○
	M3: malicious dependencies	○	○	●	○	○	○	○
	M4: abnormal publish time	○	●	●	○	○	○	○
	M5: contain package install script	○	●	●	●	○	●	○
	M6: contain executable file	○	●	●	○	○	○	○
Information Reading	R1: import operating system module	●	●	○	○	○	○	●
	R2: use operating system module call	●	○	●	●	○	○	●
	R3: import file system module	●	●	○	○	○	●	●
	R4: use file system module call	●	○	●	●	●	○	●
	R5: read sensitive information	●	●	●	●	○	●	●
Data Transmission	D1: import network module	●	●	○	○	○	●	●
	D2: use network module call	●	○	●	●	●	○	●
	D3: use URL	●	○	●	●	○	●	●
Encoding	E1: import encoding module	●	●	○	○	○	○	●
	E2: use encoding module call	●	○	○	●	○	●	●
	E3: use base64 string	●	○	○	●	○	●	○
	E4: use long string	●	○	○	●	○	○	○
Payload Execution	P1: import process module	●	●	○	○	○	●	●
	P2: use process module call	●	○	●	○	●	○	●
	P3: use bash script	●	○	○	●	○	○	○
	P4: evaluate code at run-time	●	●	●	○	●	●	○
Dynamic	/	○	○	●	○	○	○	○

largest attack surface, as attackers can inject malicious code into any package method. However, it achieves the lowest probability of successfully carrying out attacks, as the infected method has a low chance of being called.

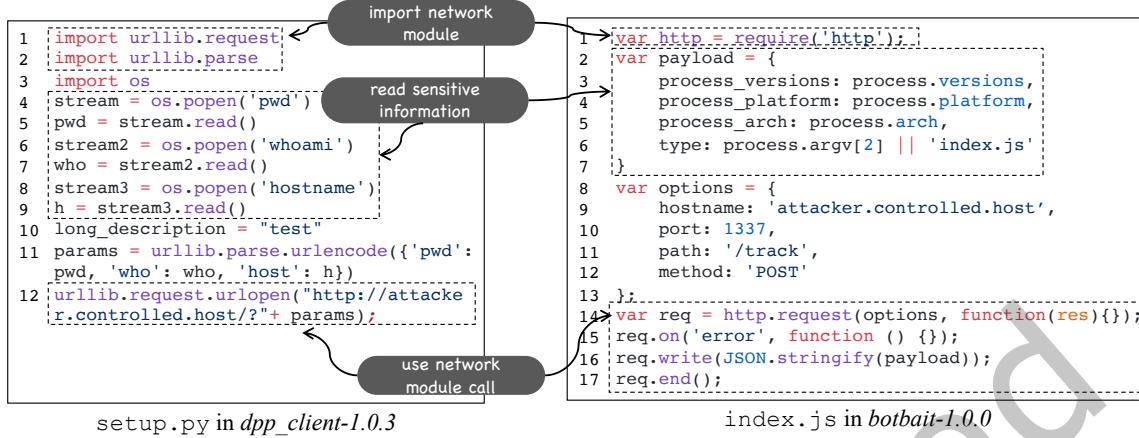


Fig. 2. Malicious Packages from PyPI and NPM that Share Similar Malicious Behavior

3.2 Literature Survey on Malicious PyPI and NPM Package Features

We conducted a comprehensive literature survey to understand malicious features in PyPI and NPM packages. We searched for related academic papers on Google Scholar using the keywords “malicious”, “PyPI” and “NPM”. We also employed a snowballing process to include referenced and cited papers. In total, we obtained 16 papers including long technical papers and short papers. We categorized the features used in those papers into six types, i.e., Metadata Feature, Syntactic Feature, Semantic Feature, Implicit Feature, Dynamic Feature, and Hybrid Feature, presented in Table 1. Additionally, we conducted a deeper comparison with the related literature focusing on Semantic and Hybrid Features. We excluded Metadata Features due to their lack of generalizability and adaptability to different package registries with varying metadata. Syntactic and Implicit Features were excluded because their results are often uninterpretable. Dynamic Features were also excluded due to their significant computational overhead and time-consuming nature.

Based on above literature, we summarize the malicious features into six dimensions based on a high-level abstraction of malicious behavior, i.e., metadata, information reading, data transmission, encoding, and payload execution, which is presented in Table 2. We can observe the existing approaches have varying implementation on the metadata and semantic features. Metadata, information reading and data transmission are the most frequently mentioned dimensions, followed by encoding and payload execution.

3.3 Motivating Examples

Example 1: Malicious Packages from PyPI and NPM Share Similar Malicious Behavior. Figure 2 shows the snippets of malicious PyPI package *dpp_client-1.0.3* and NPM package *botbait-1.0.0*, which are taken from Backstabber’s Knife Collection dataset [59]. The package *dpp_client-1.0.3* gathers sensitive information, including current working directory, user name and hostname, via executing CLI commands (e.g., *pwd*, *whoami* and *hostname*) in *setup.py* (Lines 4 to 9). Similarly, the package *botbait-1.0.0* collects sensitive information about process’s version, platform and architecture in *index.js* (Lines 2 to 7). Both packages send the sensitive information to remote servers using different libraries, i.e., *requests* in *setup.py* (Line 12) and *http* in *index.js* (Lines 14 to 17). Although being implemented in different languages with distinct syntax, these packages exhibit similar malicious behavior, involving the read of sensitive information and the calling of network operations. Sonatype also found that some malicious PyPI and NPM packages shared the same author, contained the identical malicious code, and used the same offending URL to fetch content from the remote [71].

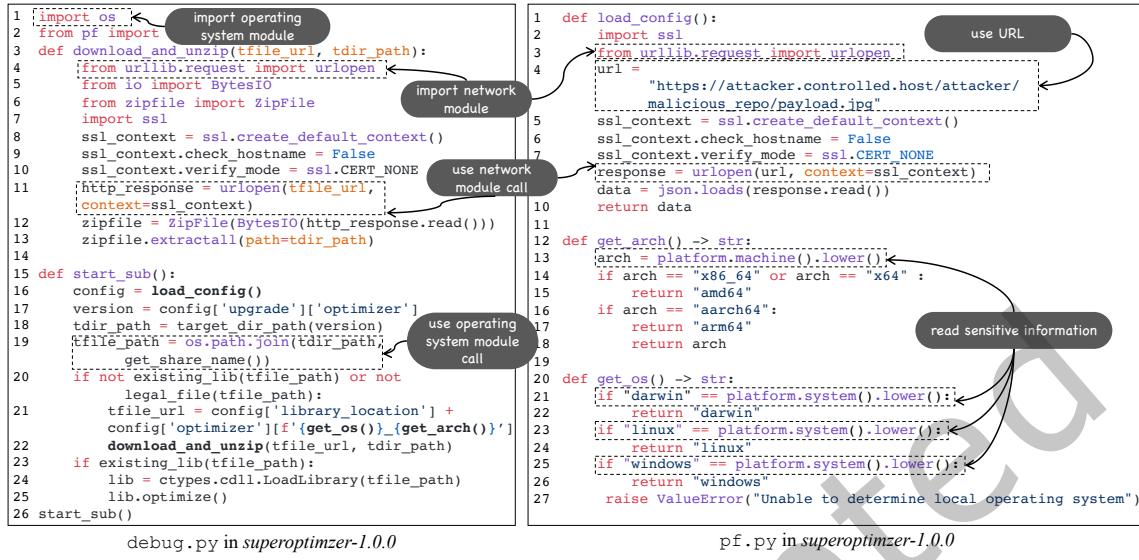


Fig. 3. A Malicious Package from PyPI with a Malicious Behavior Sequence

Therefore, this opens up new opportunities for fusing the knowledge of malicious packages from different ecosystems at a high-level abstraction and for designing a unified detection system that supports different ecosystems. Such a unified detection system can partially address the challenge of limited dataset of malicious packages. It can also allow us to identify unknown malicious packages that may have already been encountered in other package registries.

Example 2: A Malicious Package Has a Malicious Behavior Sequence. Figure 3 shows the snippet of a malicious PyPI package *superoptimizer-1.0.0*. The malicious behavior sequence is located in *debug.py* and *pf.py*, and is triggered upon the import of *debug.py*. When *debug.py* is imported, the method *start_sub* is invoked in *debug.py* (Line 26). In *start_sub*, there are several inter-procedural calls that carry out the attack, i.e., *load_config* (Line 16), *get_os* (Line 21), *get_arch* (Line 21) and *download_and_unzip* (Line 22). In *load_config* (Lines 1 to 10 in *pf.py*), two suspicious activities, including using URL and using network call, download the payload (in a json format) from a remote server to config. Then, config is parsed to obtain version, *tdir_path* and *tfile_path* (Lines 17 to 19 in *debug.py*). In *get_os* (Lines 20 to 27 in *pf.py*) and *get_arch* (Lines 12 to 18 in *pf.py*), sensitive information about the underlying operating system and architecture is read. Then, a target URL *tfile_url* is obtained by concatenating *config['library_location']* and *config['optimizer']* (Line 21 in *debug.py*). Finally, in *download_and_unzip* (Lines 3 to 13 in *debug.py*), a network call is used to download the payload from *tfile_url*. We can observe that the malicious behavior is often composed of a sequence of suspicious activities.

Therefore, the modeling of malicious behavior sequence plays a crucial role in the accuracy of malicious package detection system. However, the state-of-the-art detection systems model malicious behavior as discrete features, and do not consider the sequential nature of malicious behavior.

4 METHODOLOGY

We first introduce the overview of our approach, then elaborate each step of our approach in detail, and finally present the implementation of our approach.

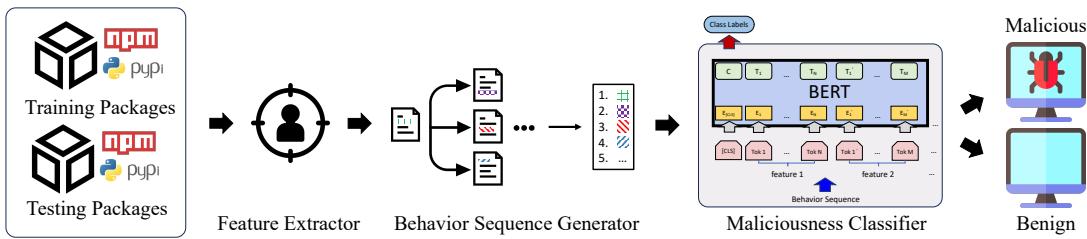


Fig. 4. An Approach Overview of CEREBRO for Detecting Malicious NPM and PyPI Packages

4.1 Approach Overview

The goal of our approach is to support the analysis of NPM and PyPI packages with a unified model by leveraging the bi-lingual knowledge of malicious packages from NPM and PyPI as well as their sequential malicious behavior knowledge. To achieve this, we propose CEREBRO, a system designed to detect malicious packages in NPM and PyPI ecosystems. The approach overview of CEREBRO is shown in Figure 4. Overall, it consists of three key components, i.e., feature extractor (see Section 4.2), behavior sequence generator (see Section 4.3), and maliciousness classifier (see Section 4.4).

In the offline training phase, CEREBRO takes inputs as a set of malicious and benign NPM and PyPI packages, uses feature extractor and behavior sequence generator to prepare the fine-tuning inputs, and fine-tunes a maliciousness classifier as the output. Similarly, in the online prediction phase, CEREBRO takes an NPM or PyPI package as the input, uses feature extractor and behavior sequence generator to prepare the prediction input, and uses the maliciousness classifier to determine whether the package is malicious or benign.

Specifically, the feature extractor component extracts features from each source code file via static analysis. It enables bi-lingual knowledge fusing across NPM and PyPI through a set of language-independent features derived from a high-level abstraction of malicious behavior. Then, the behavior sequence generator component generates behavior sequence for each package based on extracted features. It captures the sequential relation among extracted features by call graph traversal. Finally, the maliciousness classifier component fine-tunes a pre-trained language model with behavior sequences into a binary classifier for malicious package detection.

Our malicious package detection system addresses the threats in Section 2 as it trusts none of the stakeholders and prevents malicious packages from being published into package registries and thus from being used as well.

4.2 Feature Extractor

The details of our features are presented in Table 2. Each feature has a corresponding ID and a textual description (e.g., R5: read sensitive information). We use common words to describe the feature to make use of the full capability of the language model in the maliciousness classifier (see Section 4.4). Due to space limitation, we compare our feature set with only state-of-the-art rule-based approach MALOSS [12], unsupervised approaches Garrett et al.'s work [21] and PPD [47], and supervised approaches AMALFI [70] and Ohm et al.'s work [57]. Notice that different approaches may have different implementations for a rule. For example, MALOSS considers a package name suspicious if it is similar to popular ones in the same registry, or if it is the same as popular packages in different registries, but with different authors. Differently, PPD determines a suspicious package name simply based on the package name's Levenshtein distance.

Metadata. The metadata includes package name (M1), maintainers (M2), dependencies (M3), publish time (M4), and the existence of specific file types (M5 and M6). These metadata features only provide the abstraction for appearance characteristics without looking into code-level behavior. Besides, analyzing metadata features relies on assumptions that may not hold in some circumstances. For example, information about popular packages may not exist universally in different package registries, or it is difficult to identify suspicious maintainers as prior

knowledge. In order to make CEREBRO more universally applicable, CEREBRO does not leverage any metadata feature, but only uses features that can be extracted from code. In this way, CEREBRO operates independently of specific registry characteristics and enhances its capability to detect malicious behavior across different package registry sources.

Information Reading. Attackers often attempt to read sensitive information (R5), including personal information (e.g., account details, passwords, crypto wallets and credit card information) as well as machine-related information (e.g., run-time environment and machine name). They either steal such information, or use such information to carry out the attack. Besides, to effectively read sensitive information, attackers often leverage utility libraries provided by operating system and file system. To detect such behavior, we focus on identifying the utilization of these libraries in the package, including module imports (R1 and R3) and method calls (R2 and R4).

Data Transmission. Attackers often manipulate malicious packages to enable data transmission, either by downloading payloads or sending sensitive information. In order to detect such behavior, we consider the import of network modules (D1) and the use of network-related method calls (D2) as suspicious indicators. Moreover, we identify string literals written in a URL format as an additional suspicious behavior (D3). By examining the package code, we search for strings that adhere to the format of a URL. This indicates the presence of potential data transmission activities, such as communication with external servers or services.

Encoding. Attackers often leverage encoding methods to obfuscate the malicious characteristics of their code, making it less noticeable and harder to detect. Therefore, we identify suspicious behavior related to the import of encoding modules (E1) and the presence of encoding calls within the code (E2). Besides, we also heuristically detect the use of base64 strings (E3) and the use of long strings (E4), which are known to be used in obfuscating or hiding malicious code [5].

Payload Execution. One of the goals of attackers is to execute the payload downloaded to the malicious package. This suspicious behavior encompasses the import of process modules (P1) and the use of process-related function calls (P2). For example, the call to Popen in the subprocess module in Python is considered as suspicious, as it allows the execution of arbitrary commands. The presence of such calls raises concerns about potential payload execution within the package. It could either be benign or malicious in our context. Further, we also identify suspicious behavior related to the use of bash scripts (P3). By analyzing the package code, we match patterns of commands, including `python <file>.py` and `wget https://url`. The detection of these patterns suggests the potential execution of commands or scripts that may facilitate payload execution. Moreover, we identify run-time code evaluation (P4) such as eval as a suspicious behavior as it may execute the downloaded payload.

Dynamic. Dynamic features are collected by executing a package, which is heavyweight. Only MALOSS [12] leverages these features, and we do not report the detailed list of dynamic features in Table 2. We do not consider dynamic features to strike a balance between effectiveness and efficiency.

The four abstraction dimensions, information reading, data transmission, encoding, and payload execution, are often used in combination to launch attacks. For example, attackers first read sensitive information and then send it through data transmission, or attackers first use data transmission to download payload, and then execute the payload. Encoding is leveraged to further hide the previous malicious behavior.

After introducing the feature set, we introduce how to extract these features. Generally, our feature extractor parses the abstract syntax tree (AST) of each source code file in a package to match patterns of features. Formally, the extracted feature instances are denoted as \mathcal{F} . Each feature instance f in \mathcal{F} is denoted as a 3-tuple $\langle m, l, id \rangle$, where m and l respectively denote the method and the line number where the feature instance is extracted, and id denotes the ID of the feature.

1.<debug.py, 1, R1>	7.<pf.py, 8, D2>	11.<debug.py, 1, R1>	7.<pf.py, 23, R5>
2.<debug.py, 4, D1>	8.<pf.py, 13, R5>	2.<pf.py, 3, D1>	8.<pf.py, 25, R5>
3.<debug.py, 11, D2>	9.<pf.py, 21, R5>	3.<pf.py, 4, D3>	9.<pf.py, 13, R5>
4.<debug.py, 19, R2>	10.<pf.py, 23, R5>	4.<pf.py, 8, D2>	10.<debug.py, 4, D1>
5.<pf.py, 3, D1>	11.<pf.py, 25, R5>	5.<debug.py, 19, R2>	11.<debug.py, 11, D2>
6.<pf.py, 4, D3>		6.<pf.py, 21, R5>	

(a) Feature Instances

(b) Behavior Sequence

Fig. 5. Extracted Feature Instances and Generated Behavior Sequence for the Package in Figure 3

Example 4.1. Figure 5(a) presents the extracted feature instances for the two source code files in Figure 3. For the ease of understanding, we use the source code file name instead of the method name in the extracted feature instances.

4.3 Behavior Sequence Generator

Our behavior sequence generator has three steps to organize the extracted feature instances into a behavior sequence based on their likelihood of execution and their sequential order in execution. The first step prioritizes the methods in a package according to the three triggering scenarios introduced in Section 3.1, which is used to determine the execution likelihood of a feature instance. The second step constructs the call graph of a package, which is used to determine the execution order of a feature instance. The last step generates the behavior sequence of a package by querying sub call graphs in the order of prioritized methods and traversing them.

Prioritizing Methods. We first abstract the entire package into a collection of methods. The code at the global scope of each source code file is modeled into an implicit “main” method. Then, we identify and prioritize the methods based on their triggering scenarios. As discussed in Section 3.1, there are three triggering scenarios, i.e., install-time, import-time and run-time execution. Overall, methods that are executed at install-time have high priority, followed by methods executed at import-time. Methods that are executed at run-time have low priority.

For methods executed at install-time, they are the implicit “main” methods of `setup.py` or script files specified in the `scripts` property of `package.json` by `preinstall`, `install` and `postinstall`. For methods executed at import-time, they consist of the implicit “main” methods in `__init__.py`, `index.js` and the imported module files. For methods executed at run-time, they encompass all publicly accessible methods, excluding private methods. In order to identify these methods, we need to exclude any method marked as private. In Python, a method is considered private when its name is prefixed with a double underscore (“`__`”). In JavaScript, private methods are indicated by a hash (“`#`”) prefix before the method name[64].

When this step finishes, we obtain a prioritized method list, denoted as \mathcal{M} . Notice that the methods under the same triggering scenario are ranked in alphabet order by their names.

Constructing Call Graph. We employ static analysis techniques to construct the call graph of a package, which serves as the foundation for subsequent analysis. Specifically, we denote the call graph \mathcal{G} as a 2-tuple $\langle \mathcal{M}, \mathcal{E} \rangle$, where \mathcal{M} denotes the prioritized list of methods in the previous step, and \mathcal{E} denotes the total set of calling edges. Each calling edge e in \mathcal{E} is denoted as a 3-tuple $\langle m_a, l, m_b \rangle$, which means that there is a method call at line l in method m_a that calls method m_b .

Generating Behavior Sequence. We iterate each method r in \mathcal{M} (i.e., in the order of execution likelihood), and query \mathcal{G} to get a sub call graph with its root being method r . We start from visiting r , and traverse the sub call graph in the order of execution to generate the behavior sequence.

During the sub call graph traversal, when a method m is visited, we retrieve the feature instances extracted from m (denoted as \mathcal{F}_m) and obtain the calling edges starting from m (denoted as \mathcal{E}_m). Then, we enqueue \mathcal{F}_m and \mathcal{E}_m together into a queue in the order of their line numbers. In other words, given $f \in \mathcal{F}_m$ and $e \in \mathcal{E}_m$, we compare $e.l$ and $f.l$ to determine their execution order. Next, we dequeue elements from the queue. If the

```
start entry superoptimizer/_init__.py, ..., end of entry, start entry superoptimizer/debug.py, import
operating system module, import network module, use URL, use network module call, use operating
system module call, use sensitive information, use sensitive information, use sensitive information, use
sensitive information, import network module, use network module call, end of entry, start entry ...
```

Fig. 6. Textual Description of the Behavior Sequence Generated for the Package in Figure 3

dequeued element is a feature instance f , we append f into the behavior sequence \mathcal{S} ; and if the dequeued element is a calling edge e , we start to recursively visit the called method $e.m_b$. This makes CEREBRO to preserve the sequential information through inter-procedural analysis, ensuring that the generated behavior sequence reflects the execution order.

Example 4.2. Figure 5(b) presents the generated behavior sequence when the implicit “main” method of debug.py is visited. Notice that this implicit “main” method is executed when debug.py is imported. We can see that the extracted feature instances in Figure 5(a) are organized according to their execution order in the two source code files in Figure 3.

4.4 Maliciousness Classifier

The maliciousness classifier leverages pre-trained language models to have a semantic representation of the behavior sequence from a package and then classify it as either malicious or benign. We adopt BERT [37], RoBERTa [50] and the encoder in T5 [67] as they are widely-used. Specifically, we first transform \mathcal{S} into a textual description \mathcal{D} to facilitate the bi-lingual knowledge fusing as well as to ease the semantic understanding of behavior sequence. Then, by feeding textual descriptions of malicious and benign packages, we fine-tune the pre-trained language model into a binary classifier that fits for our task of malicious package detection in NPM and PyPI.

Transforming Behavior Sequence into Textual Description. We iterate each feature instance f in \mathcal{S} , and append the corresponding feature description (as shown in Table 2) into the textual description \mathcal{D} . When transforming the part of the behavior sequence that is generated from a method, we insert two short descriptions, namely *start entry <file_name>* and *end of entry*, to mark the beginning and end of the feature instances originating from the same method. Consequently, we obtain a textual description for a package where the sequence of feature descriptions are concatenated through commas. As the pre-trained language model is exposed to massive textual data during pre-training, it is enabled to understand the semantics of certain security-related terms (e.g., “network”, “URL” and “base64”). Hence, by using common words, the maliciousness classifier can benefit from the knowledge acquired by the pre-trained language model.

Example 4.3. Figure 6 depicts the textual description of the behavior sequence of the package in Figure 3. To differentiate the descriptions generated from different methods, we highlight them with different colors. The green part corresponds to the behavior executed in the implicit “main” method in superoptimizer/__init__.py at import-time. The blue part corresponds to the behavior executed in the implicit “main” method in superoptimizer/debug.py when debug.py is imported, which is the textual description of the behavior sequence in Figure 5(b).

Fine-Tuning Pre-Trained Language Models. We append a fully connected layer and a softmax layer to each pre-trained language model’s architecture, and adopt the cross-entropy loss function to fine-tune the models into binary classifiers. We feed the model with textual descriptions of both malicious and benign packages from PyPI and NPM, enabling the classifier to learn bi-lingual knowledge. The position embedding module and self-attention mechanism in the pre-trained language model allow it to capture the sequential behavior knowledge.

Table 3. Statistics of the Dataset

Package Registry	Malicious			Benign		
	# Packages	Aver. Files #	Aver. KLOC #	# Packages	Aver. Files #	Aver. KLOC #
PyPI	887	5.6	0.987	2,398	75.3	19.492
NPM	1,788	4.4	1.642	4,993	214.3	9.256
Mixed	2,675	4.8	1.425	7,391	53.4	12.577

4.5 Implementation

We have implemented CEREBRO in 3.7K lines of Python code. To extract features, we employ tree-sitter [81] to transform Python and JavaScript code into an AST representation, and identify suspicious behavior by matching the syntactic structures using AST queries provided by tree-sitter. To prioritize methods, we also use tree-sitter to parse each source code. To generate call graph, we leverage PyCG [69] for Python and Jelly [17, 52, 53, 55] for JavaScript. During the fine-tuning process, we employ the Adam optimizer with a learning rate of 1e-6 and a batch size of 1. The model is trained for 3 epochs to ensure optimal learning and performance.

5 EVALUATION

We first present the evaluation setup, and then report the evaluation results of research questions.

5.1 Evaluation Setup

Research Questions. We design our evaluation to answer the following four research questions.

- **RQ1 Effectiveness Evaluation:** How is the effectiveness of CEREBRO, compared with the state-of-the-art malicious package detection approaches?
- **RQ2 Efficiency Evaluation:** How is the performance overhead of CEREBRO?
- **RQ3 Dataset Scale Evaluation:** How does the scale of the dataset affect the effectiveness of CEREBRO?
- **RQ4 Ablation Study:** How behavior sequence contributes to the effectiveness of CEREBRO?
- **RQ5 Usefulness Evaluation:** How useful is CEREBRO in real-world detection on PyPI and NPM?

Dataset Collection. We constructed the dataset as follows. For malicious packages, we collected malicious samples from three sources. We collected 438 malicious PyPI packages and 1,788 malicious NPM packages from Backstabber’s Knife Collection [59]. We added 88 malicious PyPI packages from MALOSS’s dataset [12]. We also sampled 361 packages out of a total of 5,874 packages from pypi_malregistry [89], with a confidence level of 95% and a margin of error of 5%. For benign packages, we collected 2,398 benign PyPI packages from Vu et al.’s dataset [85]. Following the procedure in prior work [57, 85], we selected the 5,000 most depended upon packages in the NPM registry as the dataset of benign NPM packages. However, we successfully downloaded 4,993 of them. In total, we curated a dataset of PyPI and NPM packages with 2,314 malicious packages and 7,391 benign packages, as listed in Table 3 where *Mixed* denotes the summation across PyPI and NPM. We also provide the average file count and average thousand lines of code (KLOC) for each package.

RQ Setup. For RQ1, we aim to compare the effectiveness of CEREBRO with state-of-the-art approaches. Specifically, we selected AMALFI [70], SAP [43] and MPHUNTER [90] as the state-of-the-art learning-based approaches, and OSS Detect Backdoor [51] and Bandit4Mal [83] as the state-of-the-art rule-based approaches. We adopted the same configuration used in the original paper [43, 70, 90]. For OSS Detect Backdoor and Bandit4Mal, we set the threshold of 3 alerts to distinguish malicious and benign packages, which was observed as the optimal threshold by Vu et al. [85]. We did not compare with MALOSS [12] as it used dynamic features and thus failed to run on many packages. We also did not compare with Malware Checks [88] as the PyPI team removed it recently. We split the dataset into training and testing dataset by 9:1. We measured the precision and recall of all

the approaches with 10-fold cross-validation on the testing datasets. We compared these approaches in three detection scenarios, i.e., mono-lingual scenario (i.e., train and test on the same ecosystem), cross-lingual scenario (i.e., train on one ecosystem and test on the other), and bi-lingual scenario (i.e., train on two ecosystems and test on one of the two ecosystems). We trained CEREBRO with BERT [37], RoBERTa [50] and T5 [67] on the PyPI, NPM and Mixed training datasets, denoted by CEREBRO *BERT*, CEREBRO *RoBERTa* and CEREBRO *T5*. We also trained AMALFI with decision tree (AMALFI_{DT}), naive bayes (AMALFI_{NB}) and SVM (AMALFI_{SVM}) on the same training datasets. We only evaluate SAP in both mono-lingual and bi-lingual scenarios, and MPHUNTER in the mono-lingual scenario for PyPI packages, as their do not support adaptation to other scenarios.

For **RQ2**, we measured the time overhead of CEREBRO in offline training and online prediction. For **RQ3**, we evaluated the effectiveness of CEREBRO across different dataset scales. We incrementally increased the proportion of our training dataset from 10% to 100% in 10% steps. We trained CEREBRO and AMALFI_{DT} in the bi-lingual scenario using these varying dataset proportions. The trained models were then tested using the same testing dataset across all scales. The average F1-Score over 10-fold cross-validation was used to measure overall effectiveness.

For **RQ4**, we created three ablated versions of CEREBRO and compared their effectiveness with the original version of CEREBRO using the same dataset in **RQ1**. Specifically, to evaluate the impact of sequential behavior, we created “CEREBRO w/o Seq” by removing behavior sequence generator and feeding textual descriptions directly into maliciousness classifier. To evaluate the impact of textual description transformation, we created “CEREBRO w/o Text” by removing textual description transformation in maliciousness classifier. To evaluate the impact of pre-trained language models, we created “CEREBRO w/ DT” by removing behavior sequence generator and feeding features as a vector into the decision tree.

For **RQ5**, we ran CEREBRO using the BERT model against the newly published packages in PyPI and NPM for over nine months. This monitoring process started on March 03 2023 for PyPI and April 01 2023 for NPM, and ended at October 30 2023. CEREBRO analyzed 599,493 PyPI package versions and 324,145 NPM package versions. We manually confirmed the potentially malicious package versions flagged by CEREBRO. Specifically, two authors manually assessed the maliciousness of the packages in the dimension of static characteristics, dynamic behaviors and third-party detection tools. Two authors conducted a manual assessment to determine the maliciousness of the packages. This process covered comprehending the source code, inspecting the dynamic behaviors, and referencing detection results from third-party detection tools (e.g., virustotal [82]). The two authors are postgraduate and undergraduate students with security/malware background. The human inspection was conducted daily, costing one hour each day, over a period of ten months. The average number of reviewed packages daily was 30. All packages confirmed by two authors as malicious were reported to the official PyPI and NPM teams, all of which were accepted by the two registries. Further, by adding the confirmed malicious and benign packages into the original training datasets (i.e., incremental learning), we retrained CEREBRO using the BERT model to evaluate whether CEREBRO could learn from new data to improve its effectiveness. We also analyzed the malicious intentions and triggering scenarios of the new malicious packages.

$$\begin{aligned} \text{Pre.} &= \frac{|MP_{tool} \cap MP_{test}|}{|MP_{tool}|} \\ \text{Rec.} &= \frac{|MP_{tool} \cap MP_{test}|}{|MP_{test}|} \\ F1 - Score &= \frac{2 \times \text{Pre.} \times \text{Rec.}}{\text{Pre.} + \text{Rec.}} \end{aligned} \quad (1)$$

Evaluation Metric. The precision (Pre.), recall (Rec.) used in **RQ1**, **RQ4**, **RQ5** and F1-Score used in **RQ3** are defined in Equation 1. Specifically, MP_{tool} denotes the set of malicious packages predicted by tools (e.g., CEREBRO), and MP_{test} denotes the set of true malicious packages in the testing dataset. Precision is calculated

Table 4. Evaluation Result in Mono-Lingual Scenario for Learning-based Approaches

Train	Test	CEREBRO <i>BERT</i>		CEREBRO <i>RoBERTa</i>		CEREBRO <i>T5</i>		AMALFI _{DT}		AMALFI _{INB}		AMALFI _{SVM}		SAP		MPHUNTER		
		Pre.	Rec.	Pre.	Rec.	Pre.	Rec.	Pre.	Rec.	Pre.	Rec.	Pre.	Rec.	Pre.	Rec.	Pre.	Rec.	
PyPI	PyPI	95.8%	89.4%	96.0%		91.7%	93.4%	70.9%	81.9%	83.9%	59.5%	7.5%	30.3%	30.9%	83.9%	61.5%	21.8%	85.4%
NPM	NPM	98.2%	91.8%	98.5%		92.9%	98.9%	91.0%	92.7%	86.0%	92.1%	77.1%	10.2%	26.7%	90.5%	35.4%	–	–

Table 5. Evaluation Result in Mono-Lingual Scenario for Rule-Based Approaches

Test	OSS Detect Backdoor		Bandit4Mal	
	Pre.	Rec.	Pre.	Rec.
PyPI	19.9%	60.4%	24.9%	74.4%
NPM	41.1%	85.1%	–	–

by the proportion of true positives (i.e., $MP_{tool} \cap MP_{test}$) in the predicted malicious packages (i.e., MP_{tool}), and recall is calculated by the proportion of true positives (i.e., $MP_{tool} \cap MP_{test}$) in the ground truth (i.e., MP_{test}).

5.2 Effectiveness Evaluation (RQ1)

Mono-Lingual Scenario. The result of learning-based approaches in mono-lingual scenario is reported in Table 4 and the result of rule-based approaches is reported in Table 5. Overall, CEREBRO *RoBERTa* outperforms all the other approaches. In PyPI, CEREBRO *RoBERTa* achieves a precision of 96.0% and a recall of 91.7%. It achieves the best result, with slight advantages compared with CEREBRO *BERT* and CEREBRO *T5*. It outperforms the state-of-the-art SAP by 12.1% in precision, and MPHUNTER by 6.3% in recall. In NPM, CEREBRO *RoBERTa* achieves a precision of 98.5% and a recall of 92.9%. It outperforms CEREBRO *T5* with a 1.9% higher recall and a 0.4% lower precision, and CEREBRO *BERT* with a 0.3% higher precision and 1.1% higher recall. It outperforms the state-of-the-art AMALFI_{DT} by 5.8% in precision and 6.9% in recall. The two rule-based approaches have low precision and recall.

Cross-Lingual Scenario. The result of cross-lingual scenario is presented in Table 6. When the model is trained on NPM packages and tested on PyPI packages, CEREBRO *RoBERTa* obtains a highest precision of 75.1%. However, CEREBRO *T5* achieves a more balanced performance with a precision of 65.2% and a recall of 63.4%. Although AMALFI_{SVM} has better recall, CEREBRO *T5* significantly surpasses it in precision, resulting in an overall F1-Score advantage of 13.3%. When the model is trained on PyPI packages and tested on NPM packages, CEREBRO *RoBERTa* obtains a highest precision of 46.5%, and a recall of 92.7%. Although AMALFI_{SVM} has better recall, CEREBRO *RoBERTa* significantly surpasses it in precision, resulting in a F1-Score advantage of 17.7%. This result potentially owes to our well-abstracted feature set. Notice that CEREBRO in the cross-lingual scenario achieves a lower precision and recall than in the mono-lingual scenario, which indicates that some malicious behaviors might be not common, and thus bi-lingual knowledge fusing is necessary.

Bi-Lingual Scenario. The result of bi-lingual scenario is shown in Table 7. Overall, CEREBRO *RoBERTa* outperforms all the other approaches in PyPI and NPM packages. For testing PyPI packages using the model trained on mixed packages, CEREBRO *BERT* obtains a precision of 95.0% and a recall of 92.0%, and CEREBRO *RoBERTa* obtains a precision of 96.1% and a recall of 90.9%. They achieve very similar results, with CEREBRO *RoBERTa* outperforming CEREBRO *BERT* by 1.1% in precision, while CEREBRO *BERT* surpasses CEREBRO *RoBERTa* by the same margin in recall. Comparing with the state-of-the-art, CEREBRO *RoBERTa* outperform AMALFI_{DT} by 12.9% in precision and 9.8% in recall. For testing NPM packages using the model trained on mixed packages, CEREBRO *RoBERTa* achieves a precision of 98.9% and a recall of 93.9%. It outperforms CEREBRO *BERT* by 0.2% in precision and 0.9% in recall, and surpasses CEREBRO *T5* by 1.9% in recall. Comparing with the state-of-the-art, CEREBRO *RoBERTa* outperforms AMALFI_{DT} by 6.8% in precision 8.1% in recall. Although AMALFI_{SVM} outperforms CEREBRO in recall by 0.7%, it suffers from a very low precision of 28.8%.

Comparing Bi-lingual with Mono-lingual. Comparing the effectiveness of CEREBRO in bi-lingual and mono-lingual scenarios, we observe that CEREBRO *BERT*, CEREBRO *RoBERTa*, and CEREBRO *T5* trained on mixed

Table 6. Evaluation Result in Cross-Lingual Scenario

Train	Test	CEREBRO <i>BERT</i>		CEREBRO <i>RoBERTa</i>		CEREBRO <i>T5</i>		AMALFI <i>DFT</i>		AMALFI <i>NB</i>		AMALFI <i>SVM</i>	
		Pre.	Rec.	Pre.	Rec.	Pre.	Rec.	Pre.	Rec.	Pre.	Rec.	Pre.	Rec.
NPM	PyPI	72.0%	49.1%	75.1%	44.1%	65.2%	63.4%	72.0%	18.0%	42.0%	31.5%	38.4%	76.0%
PyPI	NPM	41.9%	93.0%	46.5%	92.7%	37.5%	90.9%	14.4%	4.7%	48.8%	5.2%	28.8%	94.6%

Table 7. Evaluation Result in Bi-Lingual Scenario

Train	Test	CEREBRO <i>BERT</i>		CEREBRO <i>RoBERTa</i>		CEREBRO <i>T5</i>		AMALFI <i>DFT</i>		AMALFI <i>NB</i>		AMALFI <i>SVM</i>		SAP	
		Pre.	Rec.	Pre.	Rec.	Pre.	Rec.	Pre.	Rec.	Pre.	Rec.	Pre.	Rec.	Pre.	Rec.
Mixed	PyPI	95.0%	92.0%	96.1%	90.9%	94.6%	69.6%	83.2%	81.1%	42.0%	35.6%	45.1%	37.2%	80.2%	60.2%
	NPM	98.7%	93.0%	98.9%	93.9%	98.9%	92.0%	92.1%	85.8%	93.9%	76.6%	28.8%	94.6%	90.4%	39.5%

packages outperform their mono-lingual counterparts. For detecting malicious PyPI packages, the bi-lingual model of CEREBRO achieves an average precision increase of 0.2% and an average recall increase of 0.2%. For NPM packages, the bi-lingual model achieves an average precision increase of 0.3% and an average recall increase of 1.1%. These results indicate that our bi-lingual knowledge fusion is useful.

When comparing the performance of CEREBRO *BERT* and CEREBRO *RoBERTa*, we observe that CEREBRO *RoBERTa* generally outperforms CEREBRO *BERT* in most scenarios. This advantage can be attributed to RoBERTa's use of more advanced training strategies, including dynamic masking, larger batch sizes, and an increased number of training steps, which enable the model to learn more efficiently. However, in cross-lingual and bi-lingual tasks, CEREBRO *BERT* achieves higher or comparable recall compared to CEREBRO *RoBERTa*. Further analysis reveals that for malicious packages detected by CEREBRO *BERT* but missed by CEREBRO *RoBERTa*, the sequences tend to be longer. This suggests that CEREBRO *RoBERTa* may be less effective at capturing long-range dependencies within longer sequences, which are essential for recognizing complex malicious patterns. A potential explanation for this discrepancy lies in the pre-training tasks of the two models: RoBERTa does not include the Next Sentence Prediction (NSP) task during its training, while BERT does. The inclusion of NSP in BERT's training may enhance its ability to comprehend long-context relationships, making it better at detecting certain malicious packages that RoBERTa misses.

Summary. CEREBRO *RoBERTa* outperforms the state-of-the-art by averagely 10.0% in precision and 7.4% in recall in the mono-lingual scenario, and averagely 9.9% in precision and 8.9% in recall in the bi-lingual scenario. CEREBRO learns bi-lingual knowledge from two package registries, which contributes to an average increase of 0.3% in precision and 0.7% in recall.

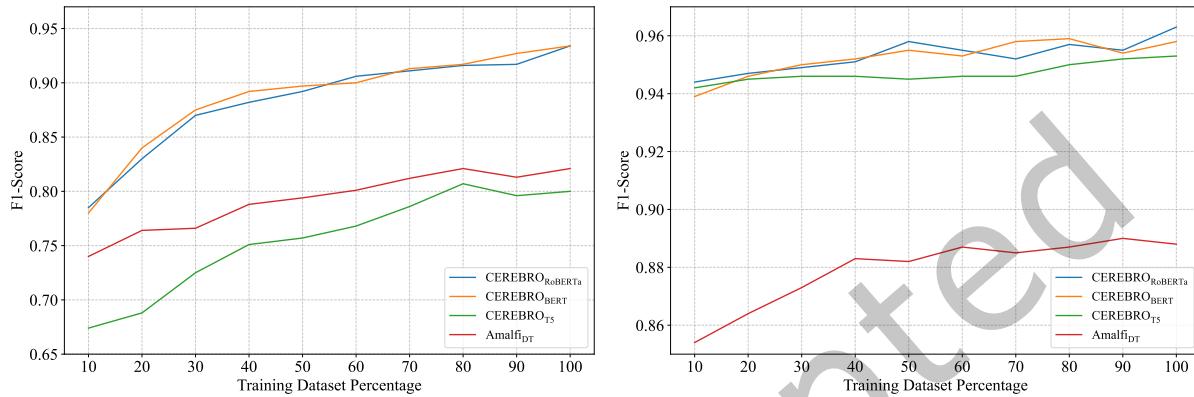
5.3 Efficiency Evaluation (RQ2)

We measure the time overhead of CEREBRO for training and prediction, including all components described in Section 4. CEREBRO is trained on a machine with an Intel Xeon(R) Silver 4314 CPU at 2.40GHz, 128G of RAM and an NVIDIA GeForce RTX 3090. The same machine is employed for predictions. Table 8 presents the efficiency results. To train CEREBRO with packages from a single package registry, it takes around 14.1 hours for PyPI packages and 25.2 hours for NPM packages. To equip CEREBRO with bi-lingual knowledge using the mixed packages, the training time is proportional to the scale of the dataset, which amounts to 39.3 hours. Moreover, the average prediction time for a package is similar for BERT, RoBERTa, or T5 trained on PyPI, NPM and mixed packages, which is respectively 11.552, 10.030 and 10.527 seconds.

Summary. CEREBRO takes less than two days to train the model; and CEREBRO takes an average of 10.5 seconds to predict whether a package is malicious, which is acceptable.

Table 8. Efficiency Evaluation Results

Training Data	Training Time (h)	Average Prediction Time (s)			
		Feature Extractor	Behavior Sequence Generator	Maliciousness Classifier	Total
PyPI	14.1	3.737	7.807	0.008	11.552
NPM	25.2	2.412	7.611	0.007	10.030
Mixed	39.3	2.856	7.664	0.007	10.527



(a) PyPI Packages as the Testing Dataset

(b) NPM Packages as the Testing Dataset

Fig. 7. Effectiveness of CEREBRO *BERT*, CEREBRO *RoBERTa*, CEREBRO *T5* and AMALFI_{DT} in Different Scales of Dataset

5.4 Dataset Scale Evaluation (RQ3)

Figure 7 presents the results of our dataset scale evaluation. Overall, CEREBRO *BERT* and CEREBRO *RoBERTa* consistently outperform the state-of-the-art by a significant margin in both PyPI and NPM packages, even with limited dataset scales (i.e., 10%, 20%). In Figure 7(a), CEREBRO *BERT* and CEREBRO *RoBERTa* exhibit similar F1-Scores as the dataset scale changes. CEREBRO *RoBERTa* outperforms AMALFI_{DT} by an F1-Score of 0.045 at the 10% scale. As the dataset scale increases, CEREBRO *RoBERTa* further widens the gap, surpassing AMALFI_{DT} with an F1-Score of 0.113 at the 100% scale. In Figure 7(b), CEREBRO *BERT*, CEREBRO *RoBERTa*, and CEREBRO *T5* exhibit similar F1-Scores as the dataset scale changes. CEREBRO *RoBERTa* outperforms AMALFI_{DT} by an F1-Score of 0.09 at the 10% scale. As the dataset scale increases, CEREBRO *RoBERTa* further keeps the gap, achieving an average F1-Score difference of 0.072 across remaining dataset scales. We also observe that as the training dataset increases, the F1-score improvement for NPM packages is relatively smaller compared to PyPI packages. This is primarily due to the differing levels of package diversity between the two ecosystems. As shown in Fig. 8b, a larger proportion of NPM packages focus on information stealing. Consequently, models trained on NPM packages quickly learn and generalize malicious patterns from smaller datasets than those for PyPI, resulting in better performance at lower data percentages and smaller incremental gains as the dataset scale increases.

Summary. The effectiveness of our approach maintains an advantage over state-of-the-art across different dataset scales. CEREBRO *RoBERTa* achieves an F1-Score of 0.785 in PyPI and 0.944 in NPM even when the dataset scale is reduced by 90%, indicating the robustness of CEREBRO in situations with scarce data availability.

5.5 Ablation Study (RQ4)

We train the three ablated versions of CEREBRO in the bi-lingual scenario. As shown in Table 9, the ablated version is less effective than the original version. Specifically, the average precision and recall for CEREBRO *BERT*, CEREBRO *RoBERTa* and CEREBRO *T5* decrease 1.6% and 0.6%, increase 1.6% and decrease 3.7%, decrease 1.4% and 1.9% for CEREBRO w/o Seq in mono-lingual, cross-lingual and bi-lingual scenarios, respectively. Similarly, the

Table 9. Evaluation Result on Ablated Versions of CEREBRO

Train	Test	CEREBRO w/o Seq						CEREBRO w/o Text						CEREBRO w/ DT	
		BERT		RoBERTA		T5		BERT		RoBERTA		T5		Pre.	Rec.
		Pre.	Rec.	Pre.	Rec.	Pre.	Rec.	Pre.	Rec.	Pre.	Rec.	Pre.	Rec.	Pre.	Rec.
PyPI	PyPI	91.3%	87.1%	92.1%	86.2%	92.1%	76.1%	92.6%	85.0%	90.6%	89.6%	94.1%	76.8%	91.4%	89.4%
		↓ 4.5%	↓ 2.3%	↓ 3.9%	↓ 5.5%	↓ 1.3%	↑ 5.2%	↓ 3.2%	↓ 4.4%	↓ 5.4%	↓ 2.1%	↑ 0.7%	↑ 5.9%	↓ 4.4%	↓ 0.0%
NPM	NPM	98.0%	92.2%	98.9%	92.1%	98.8%	90.4%	98.1%	90.4%	97.7%	90.4%	99.1%	88.3%	96.6%	92.2%
		↓ 0.2%	↑ 0.4%	↑ 0.4%	↓ 0.8%	↓ 0.1%	↓ 0.6%	↓ 0.1%	↓ 1.4%	↓ 0.8%	↓ 2.5%	↑ 0.2%	↓ 2.7%	↓ 1.6%	↑ 0.4%
NPM	PyPI	77.3%	36.0%	76.7%	42.1%	64.7%	67.6%	93.7%	18.5%	64.2%	2.0%	88.0%	8.4%	49.5%	11.0%
		↑ 5.3%	13.1%	↑ 1.6%	↓ 2.0%	↓ 0.5%	↑ 4.2%	21.7%	30.6%	10.9%	42.1%	22.8%	55.0%	22.5%	38.1%
PyPI	NPM	49.2%	92.2%	38.3%	87.2%	41.3%	86.0%	41.8%	94.0%	28.0%	98.9%	10.6%	13.6%	10.2%	8.4%
		↑ 7.3%	↓ 0.8%	↓ 8.2%	↓ 5.5%	↑ 3.8%	↓ 4.9%	↓ 0.1%	↑ 1.0%	18.5%	↑ 6.2%	26.9%	77.3%	31.7%	84.6%
Mixed	PyPI	92.3%	86.2%	93.4%	88.3%	92.6%	71.3%	95.5%	86.0%	94.7%	87.4%	92.9%	82.0%	90.5%	86.6%
		↓ 2.7%	↓ 5.8%	↓ 2.7%	↓ 2.6%	↓ 2.0%	↑ 1.7%	↑ 0.5%	↓ 6.0%	↓ 1.4%	↓ 3.5%	↓ 1.7%	12.4%	↓ 4.5%	↓ 5.4%
NPM		98.2%	91.8%	98.6%	91.7%	98.9%	90.9%	98.7%	91.1%	98.3%	91.1%	98.8%	89.5%	93.9%	92.0%
		↓ 0.5%	↓ 1.2%	↓ 0.3%	↓ 2.2%	↓ 0.0%	↓ 1.1%	↓ 0.0%	↓ 1.9%	↓ 0.6%	↓ 2.8%	↓ 0.1%	↓ 2.5%	↓ 4.8%	↓ 1.0%

Table 10. Result of Real-World Malicious Package Detection

Package Registry	Time Period	Newly Published Package Versions	Flagged by CEREBRO	False Positives	True Positives	Thankers	Lets	Removed Before Report
PyPI	March	104,512	750	521	229	173	56	
	April	101,415	661	560	101	0	101	
	May	78,528	422	324	98	30	68	
	June	102,088	768	595	173	0	173	
	July	101,600	720	670	50	10	40	
	August	56,561	298	283	15	14	1	
	September	25,193	101	88	13	4	9	
	October	29,596	16	12	4	1	3	
Total		599,493	3,746	3,053	683	232	451	
NPM	April	130,697	325	178	147	147	0	
	May	39,094	145	88	57	35	22	
	June	28,764	256	145	111	0	111	
	July	34,626	244	155	89	44	45	
	August	33,013	514	314	200	131	69	
	September	27,350	374	254	120	91	29	
	October	30,601	372	297	75	27	48	
Total		324,145	2,230	1431	799	475	324	

average precision and recall decrease 1.4% and 1.2%, decrease 2.0% and 33.0%, decrease 0.5% and 0.7% for CEREBRO w/o Text in mono-lingual, cross-lingual and bi-lingual scenarios, respectively. Further, the average precision and recall decrease 3.0% and 0.2%, 27.1% and 61.4%, 4.7% and 3.2% for CEREBRO w/ DT in mono-lingual, cross-lingual and bi-lingual scenarios, respectively.

Summary. Generating behavior sequence, transforming behavior sequence into textual description, and feeding textual description into a classifier fine-tuned from a pre-trained language model are all effective in detecting malicious packages. Averagely, the ablated versions of CEREBRO decrease 4.5% in precision and 11.8% in recall.

5.6 Real-World Usefulness Evaluation (RQ5)

To evaluate the practical usefulness of CEREBRO in analyzing newly published package versions in real-world registries, we design a monitoring system that first monitors and crawls newly published package versions from PyPI and NPM and then runs CEREBRO against the crawled package versions. Our monitoring system has lasted over 8 months for PyPI and 7 months for NPM.

Table 11. Result of Incremental Learning

Added Train (#)	Time Period	New Test (#)	Pre.
None	-		7.2%
PyPI (750)	March		26.5%
Mixed (1,736)	March-April	PyPI (1,135)	36.5%
Mixed (2,303)	March-May		39.0%
Mixed (3,327)	March-June		58.2%
None	-		32.2%
PyPI (750)	March		76.3%
Mixed (1,736)	March-April	NPM (1,504)	80.3%
Mixed (2,303)	March-May		80.2%
Mixed (3,327)	March-June		80.7%

Overall Usefulness Result. In total, CEREBRO scans 923,638 newly published package versions, and flags 3,746 PyPI package versions and 2,230 NPM package versions as potentially malicious, as reported in Table 10. We first manually validate each flagged package version, and confirm 683 PyPI package versions and 799 NPM package versions as true positives. Then, following responsible disclosure process, we promptly report these package versions to administrators of the official PyPI and NPM teams. At the time of reporting, 451 PyPI package versions and 324 NPM package versions have already been removed. The PyPI and NPM teams confirm the remaining 232 PyPI package versions and 475 NPM package versions as malicious, and remove all of them. Thus, we receive 232 and 457 thank letters from PyPI and NPM.

False Positive Analysis. As shown in Table 10, the false positive rate is 81.5% for PyPI and 64.2% for NPM, which is actually high. It is worth mentioning that it takes one of our authors around one hour to manually analyze and confirm the flagged package versions every day, which is still acceptable. After analyzing all the false positives, we identify four major types of benign packages that are flagged as malicious, as their behavior sequences are similar to malicious ones.

First, some benign packages encapsulate RESTful APIs, which enable data transmission to remote servers. Their behavior sequences consist of features about *Information Reading* and *Data Transmission* (e.g., R1, D1, D2 and D3). Second, some benign packages encapsulate CLI commands into Python/JavaScript methods where their behavior sequences resemble those malicious packages in using features about *Payload Execution*. Third, some benign packages behave similarly to Trojans, but their payloads serve benign purposes. Normally, their behavior sequences resemble Trojans by starting with D1 and D3, then undertaking intermediate actions such as R1 and R4, and ending with P2 and P3. Last, some benign packages consist of a single meta utility module that incorporates features ranging from *Information Reading*, *Data Transmission*, *Encoding* to *Payload Execution*. It causes CEREBRO to recognize parts of behavior sequences as similar to those of malicious packages.

False Negative Analysis. To measure false negatives of CEREBRO, we reached out to package registries. However, PyPI replied that they did not maintain a malicious package list and NPM refused to share the list. Therefore, we try to use state-of-the-art detectors to identify true positives. Specifically, we employ AMALFI [70] to identify potentially malicious packages during the same monitoring time period. It flagged 41,434 PyPI package versions and 1,930 NPM package versions as potentially malicious. Then, we undertake a manual inspection process with a sampling rate of 95% confidence level and 5% error margin, which results in 381 PyPI packages and 164 NPM packages. After manual validation, we identify 9 malicious PyPI packages and 45 malicious NPM packages. Remarkably, only 2 PyPI packages and 5 NPM packages went undetected by CEREBRO. It indicates that the false negative rate of CEREBRO is relatively low in real-world detection.

Incremental Learning Result. As we are continuously confirming and accumulating true positives and false positives of malicious packages based on our monitoring system, one potential way to reduce false positives is to adopt incremental learning on such true positives and false positives. To this end, we add the true positives and false positives confirmed during our monitoring from March to June as two incremental datasets for retraining.

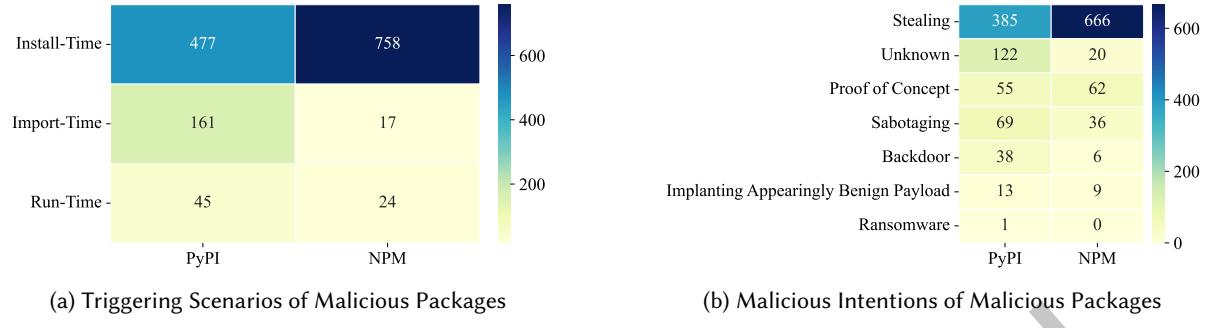


Fig. 8. Triggering Scenarios and Malicious Intentions of New Malicious Packages

In particular, we add 750 packages from March, 1,736 packages from March to April, 2,303 packages from March to May and 3,327 packages from March to June, as reported in the third to sixth row, and eight to eleven row under the column of *Added Train* in Table 11. Note that the added training dataset for March contains only PyPI packages because monitoring NPM packages starts from April. Then, we retrain four models of CEREBRO by augmenting the original mixed training dataset with the new mixed PyPI and NPM packages. Finally, we select true positives and false positives confirmed during our monitoring from July to October as the new testing dataset. In particular, there are 1,135 PyPI packages and 1,504 NPM packages as reported in the third column in Table 11.

Overall, by incorporating new malicious and benign packages into the training dataset, the precision of CEREBRO improves significantly. Specifically, when CEREBRO is retrained with new mixed packages, the precision of detecting malicious PyPI packages reaches 58.2%, while the precision of detecting malicious NPM packages reaches 80.7%, achieving a precision increase of 51.0% for PyPI packages and 48.5% for NPM packages in total.

Malicious Package Characteristics. For each of the 683 PyPI and 799 NPM malicious package versions which are previously unknown, we manually look into their malicious behavior to understand their characteristics. On the one hand, we determine their triggering scenarios, and report the result in Figure 8a. We can observe that 477 (69.8%) of the malicious PyPI package versions and 758 (94.9%) of the malicious NPM package versions trigger their malicious behavior at install-time. This is reasonable because install-time execution can achieve the highest probability of successfully carrying out attacks. Moreover, a small number of malicious PyPI package versions opt to trigger malicious behavior other than install-time, accounting for 161 (23.6%) at import-time and 45 (6.6%) at run-time. Noticeably, there are only 17 (2.1%) of the malicious NPM package versions that adopt import-time triggering, and 24 (3.0%) malicious NPM package versions adopt run-time triggering.

On the other hand, we explore the intentions of malicious package versions by executing them in a sandbox, and present the result in Figure 8b. Generally, the malicious intentions include stealing (e.g., personal data or credentials), sabotaging (e.g., shutting down firewalls), proof of concept (which is harmless but to demonstrate something malicious can be done), backdoor (i.e., enabling remote-controlled operations for an attack to exploit an infected machine), implanting apparently benign payload (e.g., the benign payload might change to be malicious via morphing Trojan), and ransomware. Besides, we fail to execute the payload for 142 of the malicious package versions due to non-existent URLs or run-time exceptions, and thus we label their malicious intentions as unknown.

Summary. CEREBRO detects 683 and 799 previously unknown malicious PyPI and NPM package versions. All of them have been removed by the official PyPI and NPM teams, and we also receive 707 thank letters from them. Further, by incorporating new malicious and benign packages, CEREBRO learns new knowledge to improve its precision. Besides, most (83.3%) of these new malicious package versions execute the malicious behavior at install-time; and most (70.9%) of them attempt to steal sensitive information.

5.7 Threats and Limitations

Threats. First, as the campaign against malware continues, new strains of malicious packages emerge daily. This implies that the original dataset of malicious packages used in our evaluation may not encompass the full spectrum of new malicious packages, hindering CEREBRO’s effectiveness. However, we have demonstrated the effectiveness of CEREBRO in learning from newly published packages and adapting to detect emerging threats. Second, while we thoroughly examine the potentially malicious package versions identified by CEREBRO, we acknowledge that the vast workload makes it impractical to validate every potentially benign package version. Therefore, we only systematically report the result of precision but not the result of recall. Third, CEREBRO can generate false positives. To address this, we conduct manual validation on identified package versions before reporting them to PyPI and NPM teams. While this process can also introduce false positives, the fact that the reported packages are subsequently removed indicates the validity of our validation. Fourth, as pre-trained language models continue to advance rapidly, we expect to see new and more powerful models. Nevertheless, the choice of language models is orthogonal to our approach. We plan to test the effectiveness of additional language models on this task. Fifth, the varying behavior sequences between malicious and benign packages may reduce the accuracy of CEREBRO in cross-lingual scenarios. Nevertheless, the cross-lingual setting represents an extreme case in real-world where there are no malicious samples within the same ecosystem.

Limitations. First, our method is designed for PyPI and NPM packages. However, our method can be easily generalized into other ecosystems by implementing the feature extractor and behavior sequence generator for a new ecosystem. The feature set is language-agnostic. By leveraging the existing AST parser and call graph generator of the new ecosystem, we believe that the integration can be straightforward. Second, large packages may have a large size of the behavior sequence which can exceed the 512 token limit of BERT. However, based on our analysis of packages in Table 10, we identify a relatively modest proportion (13.6%) of packages that exceed the limit. We plan to split the behavior sequence into multiple segments to circumvent the limit while maintaining their sequential integrity. Third, the proposed approach encounters higher false positives in real-world setting. We foresee several challenges and opportunities that could help reduce false positive rates. On the one hand, we can leverage ensemble methods. Utilizing a combination of different detection tools could be advantageous. An ensemble approach, where decisions are based on the consensus among multiple tools, might improve accuracy and reduce false positive rates. On the other hand, we can utilize dynamic analysis during our detection. Incorporating dynamic analysis into the detection process could provide deeper insights into the behavior of packages by capturing detailed runtime behaviors, potentially reducing false positives by confirming suspicious activities through actual execution rather than static analysis. Nonetheless, with a large number of new packages being released daily, it remains an open question how to leverage the benefits of dynamic analysis while mitigating its computational and time costs.

6 RELATED WORK

Malicious Package Detection. Recently, there has been an increasing number of OSS supply chain attacks that inject malicious code into packages, with package registries such as NPM and PyPI being the largest targets [44, 54]. Ohm et al. [59] were the first to systematically investigate malicious packages. They collected 174 real-world malicious packages from NPM, PyPI and RubyGems. Using this dataset, they manually analyzed how malicious behavior was injected (e.g., via typosquatting) and triggered (e.g., on installation), what the objective (e.g., data exfiltration) of malicious behavior was, and whether obfuscation was employed. Similarly, Guo et al. [89] conducted an empirical study to understand the characteristics of the malicious code lifecycle in the PyPI ecosystem. Various approaches have also been proposed to detect malicious packages, mostly in NPM and PyPI.

In the NPM ecosystem, Zahan et al. [94] identified six signals of security weakness in NPM supply chain, and proposed a rule-based malicious package detector that searches for keywords in install scripts. Garrett

et al. [21] selected features about whether libraries that access the network, file system and operating system processes are used, whether code is evaluated at runtime, and whether new files, new dependencies and new hookup script entries are present, and adopted clustering to build a benign behavior model which is used to detect malicious NPM packages. Differently, Ohm et al. [58] adopted AST (abstract syntax tree)-level clustering to establish a malicious behavior model. Instead of using unsupervised methods, Fass et al. [15, 16] built a random forest classifier based on the frequency of specific patterns extracted from AST, CFG (control flow graph) and PDG (program dependency graph) of benign and malicious JavaScript samples. This approach is specifically designed for obfuscated JavaScript programs, and thus could be ineffective for non-obfuscated ones. Ohm et al. [57] extended the feature set of Garrett et al.’s work [21] by including features about package metadata and obfuscation. Similarly, Sejfia et al. [70] proposed AMALFI, which uses an extended feature set from Garrett et al.’s work [21] to train classifiers. These approaches capture malicious behavior as discrete features, hindering their accuracy in detecting malicious packages. Differently, we model malicious behavior in a sequential manner, which can model the maliciousness more precisely. Notice that Ferreira et al. [18] proposed a lightweight permission system to protect applications from malicious package updates at runtime. Recently, Huang et al. [33] proposes SpiderScan to identify malicious NPM packages based on graph-based behavior modeling and matching.

In the PyPI ecosystem, Vu et al. [87] proposed a rule-based approach to detect malicious PyPI packages that are spread by typosquatting and combosquatting attacks. The rule checks whether the package has the name similar to a Python standard library or a package with known source code repository. Besides, there are several other rule-based detectors, e.g., Bandit4Mal [83] and Malware Checks [88]. Vu et al. [85] conducted a comprehensive evaluation of these detectors. Instead of relying on rules, Vu et al. [84, 86] identified malicious packages based on discrepancies between the source code repository and distributed artifact of a Python package. Liang et al. [47] used both package metadata features and code features to learn an isolated forest model for detecting malicious packages. Recently, Liang et al. [90] utilized clustering techniques to group the PyPI installation scripts so that outliers can be identified. Sun et al. [76] proposes to integrate deep code behavior features with metadata features to detect malicious PyPI packages. These approaches share the same limitation with those detectors in NPM because they also model malicious behavior as discrete features.

Moreover, some approaches support different ecosystems. OSS Detect Backdoor [51] is a rule-based detector that support 15 ecosystems. Taylor et al. [80] leveraged package name similarity and package popularity to detect malicious packages caused by typosquatting in NPM, PyPI and RubyGems. Ladisa et al. [43] utilized language-independent feature (e.g. number of URLs, entropy of strings in code files, etc.) to detect malicious packages in NPM and PyPI. However, these approaches are not based on high-level semantics of source code, which can produce high false positives. Different from the simple rule in Taylor et al. and Ladisa et al., Duan et al. [12] derived five metadata analysis rules, four static analysis rules and four dynamic analysis rules to detect malicious packages in NPM, PyPI and RubyGems. However, it is heavyweight as it relies on program analysis.

Squatting attacks are also common in other domains, e.g., domain name system [1, 38, 40, 78, 79], container registry [49] and mobile app [31]. Malware detection has been widely studied [89, 93]. OSS opens up new opportunities for malware detection due to the availability of source code.

Security Threats in OSS Supply Chain. Apart from malicious packages, there exist various security threats in OSS supply chain. Several studies [3, 7, 29, 36, 94] have been conducted to investigate security threats in package registries such as NPM and PyPI. Ladisa et al. [42] reported a taxonomy of attacks on all OSS supply chain stages from code contributions to package distribution. They also assessed the safeguards against OSS supply chain attacks. Koishybayev et al. [41] and Gu et al. [28] characterized security threats in continuous integration workflows that produce OSS.

Enck and Williams [13] summarized five challenges in OSS supply chain security, with the top one being updating vulnerable dependencies. Specifically, the vulnerability impact analysis along the supply chain has been widely explored in various ecosystems, e.g., NPM [48, 95, 96], Maven [25, 32, 63], PyPI[2, 63, 68] and

RubyGems [63, 95]. To cope with vulnerable dependencies, various software composition analysis tools have been proposed [32, 48, 62, 92]. Besides, several advances have been made on detect maliciousness in different stages of software development. Goyal et al. [27] and Gonzalez et al. [26] proposed to detect malicious commits on GitHub. Cao and Dolan-Gavitt [6] tried to identify malware in GitHub forks. Lamb and Zaccarioli [46] and Wheeler [91] attempted to avoid the injection of maliciousness in compilation by ensuring reproducible builds.

7 CONCLUSION AND FUTURE WORK

We have proposed and implemented CEREBRO to detect malicious packages in NPM and PyPI. CEREBRO leverages a comprehensive feature set that models high-level abstraction of malicious behavior sequence, enabling bi-lingual knowledge fusing. Our extensive evaluation results have demonstrated the effectiveness, efficiency and practical usefulness of CEREBRO in detecting malicious packages. In the future, we plan to enhance the multi-lingual capability of CEREBRO by incorporating support for both interpreted and compiled languages. The challenge is to design feature extractors for new languages, and improve the generalizability of our feature set. We also plan to equip CEREBRO with the capability to pinpoint the specific malicious sequence from the whole behavior sequence, further aiding administrators to go through the manual confirmation promptly.

8 DATA AVAILABILITY

The data of our evaluation is available at <https://doi.org/10.5281/zenodo.8277447>.

ACKNOWLEDGMENT

This work was supported by the National Natural Science Foundation of China (Grant No. 62332005, 62372114 and 62402342).

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just Accepted