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Advancing Vulnerability Detection: An Innovative Approach to Generate Embeddings of Code Snippets

Anushka Singh[1]

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Abstract: This research proposes a novel approach for generating Java code embeddings using Graph Neural Networks (GNNs). It achieves this by processing a combined representation of the code structure and functionality captured in Abstract Syntax Trees (ASTs), Program Dependence Graphs (PDGs), and Control Flow Graphs (CFGs). The GNN can then leverage these rich graph representations to capture intricate relationships within the code, leading to more informative embeddings. Evaluation shows these embeddings perform well in various software engineering tasks like code similarity detection, bug localization (over 90% precision for some vulnerabilities), and code classification. Additionally, dimensionality reduction techniques effectively visualize the code snippets based on the embeddings, revealing insights into the underlying structure and relationships. This research holds significant promise for improving software development practices. By effectively capturing complex code dependencies, it paves the way for advancements in automated code analysis. The resulting robust embeddings have the potential to revolutionize practices like code review automation, early vulnerability detection, code refactoring, and code search. Furthermore, the success of this GNN-based approach opens doors for further exploration of their potential in code analysis. However, limitations include its focus on Java and the potential influence of training data on model performance. Future directions include investigating applicability to other languages, incorporating domain-specific knowledge, developing interpretable GNNs, and integrating the embeddings with existing tools for a comprehensive code analysis platform. Overall, this research offers a significant contribution by demonstrating the effectiveness of GNNs for code embedding generation, with the potential to revolutionize automated code analysis and software development practices.

Keywords: *GNN, embeddings, integrating, underlying, exploration, potential*

I. Introduction

In the evolving landscape of software engineering, the demand for advanced tools to automate code analysis has grown significantly. Traditional static analysis methods, while effective in identifying specific errors and vulnerabilities, often struggle with the intricate complexity and variability present in modern software systems. This limitation has spurred interest in leveraging machine learning techniques to enhance code analysis capabilities, particularly in tasks such as code similarity detection, bug detection, and code summarization.

A critical challenge in this domain is the effective representation of source code, which contains rich syntactic and semantic information. Abstract Syntax Trees (ASTs) [4], Program Dependence Graphs (PDGs) [7], and Control Flow Graphs (CFGs) are three established representations that encapsulate different facets of source code. ASTs provide insights into the syntactic structure, PDGs illustrate data and control dependencies, and CFGs map out the control flow within the code.

Integrating these diverse representations offers a holistic view of the code, crucial for performing deep and accurate analysis. However, merging these representations into a cohesive format suitable for machine learning models poses significant challenges. Graph Neural Networks (GNNs) [16,17,18] have emerged as a promising solution to process and learn from such complex, graph-based data structures.

This research is significant because it proposes a novel method for generating embeddings of Java code by integrating AST, PDG, and CFG representations using GNNs [17]. This approach captures intricate code dependencies and relationships, providing a comprehensive embedding that enhances various code analysis tasks.

In practical applications, the benefits of this research are manifold:

1. Code Similarity Detection: The robust embeddings generated by this method enable precise identification of similar code snippets, which is essential for detecting code duplication and plagiarism.

2. Bug Detection and Localization: These embeddings can train models to identify and localize potential bugs or vulnerabilities more accurately, leveraging the detailed context and dependencies within the code [11].

3. Code Classification and Summarization: The embeddings facilitate the classification of code snippets

*IIT Kharagpur
anushkasinghkgp@gmail.com

by functionality, aiding in automated documentation and summarization processes.

This research advances the field of automated code analysis by providing a robust framework that captures the complexity of modern software systems through integrated graph-based representations and GNNs [18], thereby significantly enhancing the effectiveness of machine learning applications in software engineering.

II. Literature Review

The application of graph-based representations and neural network models in source code analysis has garnered significant attention in recent years. This section reviews the relevant literature, highlighting the key advancements and methodologies that have influenced the current research.

2.1. Graph-Based Code Representations

Graph-based representations such as Abstract Syntax Trees (ASTs), Program Dependence Graphs (PDGs), and Control Flow Graphs (CFGs) have become foundational in understanding and analyzing source code.

1. Abstract Syntax Trees (ASTs): ASTs represent the syntactic structure of source code in a hierarchical tree format. This representation is instrumental in parsing and compiling code. Work by [1] highlighted the utility of ASTs in refactoring and code transformation tasks, demonstrating significant improvements in code maintainability and readability.

2. Program Dependence Graphs (PDGs): PDGs encapsulate both control and data dependencies within a program, providing a comprehensive view of the interactions between different code elements.

Ferrante, Ottenstein, and Warren in [2] introduced PDGs in their seminal work illustrating how PDGs facilitate advanced program analysis techniques, including slicing and parallelization.

3. Control Flow Graphs (CFGs): CFGs map out the flow of control within a program, identifying the paths that may be traversed during execution.

Allen (1970) in [3] demonstrated the efficacy of CFGs in optimizing compilers by enabling precise control flow analysis and loop detection.

2.2: Neural Network Models for Code Embedding

The integration of neural network models, particularly Graph Neural Networks (GNNs), with graph-based representations has revolutionized code analysis.

1. Graph Neural Networks (GNNs): GNNs extend traditional neural networks to handle graph-structured data, making them ideal for processing ASTs, PDGs, and CFGs. Kipf and Welling's (2017) work [4] on laid the groundwork for GCNs, showcasing their potential in various domains, including social network analysis and molecular chemistry.

2. Code Embedding Techniques: Code embeddings aim to represent code snippets in continuous vector spaces, capturing both syntactic and semantic properties.

Alon et al. (2019) in their paper [5] proposed an innovative method to learn code embeddings from AST paths, significantly advancing the field of code summarization and generation.

2.3. Applications of Code Analysis

The practical applications of these methodologies in real-world scenarios further underscore their importance.

1. Bug Detection: Automated bug detection leverages code embeddings to identify potential bugs by comparing code patterns against known vulnerabilities**.** Pradel and Sen (2018) in [6] demonstrated how neural network models could detect subtle naming bugs in JavaScript programs with high accuracy.

2. Code Similarity and Clone Detection: Identifying similar code snippets and detecting code clones are crucial for code reuse and maintenance.

White et al. (2016) in [7] explored the use of deep learning techniques to detect code clones, achieving state-of-the-art results.

3. Code Classification: Classifying code snippets into predefined categories helps in organizing and retrieving code efficiently.

Mou et al. (2016) in [8] proposed a tree-based convolutional neural network for code classification tasks, demonstrating improved performance over traditional methods .

The current research builds on these foundational works, integrating advanced graph-based representations and neural network models to enhance the understanding and analysis of Java source code. By leveraging the strengths of ASTs, PDGs, CFGs, and GNNs, this research aims to develop a comprehensive framework for generating and analyzing code embeddings, with applications in bug detection, code similarity analysis, and more.

III. Methodology

The methodology followed is divided into the following phases, and each phase containing the following stages:

Phase 1: Data Collection and Preprocessing

Step 1. Data Source Identification: The research utilized a collection of Java source code files. These files were systematically organized into a directory structure, with

each subdirectory containing relevant files for analysis [11, 12].

Step 2. Graph Representation Extraction: For each Java file, three types of graph representations were extracted:

a. Abstract Syntax Trees (ASTs): Capturing the syntactic structure of the code.

b. Program Dependence Graphs (PDGs): Consisting of control dependence (PDG-CTRL) and data dependence (PDG-DATA) graphs, illustrating the dependencies between different parts of the code [1, 2].

c. Control Flow Graphs (CFGs): Mapping out the control flow paths within the code.

Step 3. Vertex and Edge Mapping: Each graph was processed to identify vertices and edges. Vertices represent code elements (e.g., statements, expressions), and edges represent the relationships or dependencies between these elements.

Step 4. Embedding Extraction: For each code snippet, a pre-trained model was used to extract embeddings that encapsulate the semantic and syntactic information from the AST [8]. These embeddings were mapped to the vertices identified in the AST, PDG, and CFG.

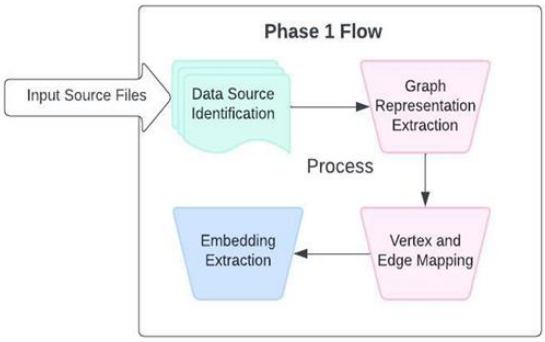

***Fig 3.1**: Phase 1 Flow*

Phase 2: Graph Construction and Integration

Step 5. Graph Construction: The vertices and edges from the AST, PDG-CTRL, PDG-DATA, and CFG were used to construct their respective graphs.

Step 6: Unified Graph Embedding: A unified embedding was created by integrating information from the AST, PDG, and CFG. This involved mapping the code elements to their corresponding embeddings and constructing a composite graph that encapsulated the different dimensions of code representation.

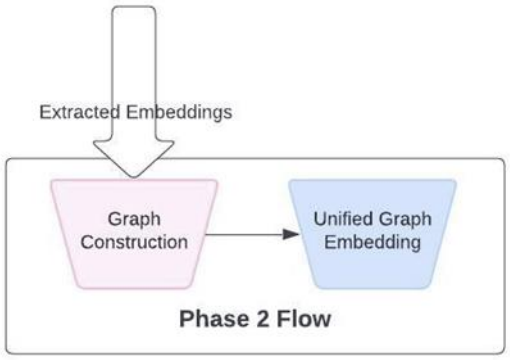

***Fig 3.2**: Phase 2 flow*

Phase 3: Embedding Generation Using Graph Neural Networks

Step 7. Graph Neural Network (GNN) Model: A Graph Neural Network (GNN) was designed and trained to process the composite graph and generate embeddings. The model consisted of multiple graph convolution layers to capture the complex relationships within the code.

Step 8. Embedding Generation: The GNN processed the input graphs to produce a final set of embeddings for each code snippet. These embeddings encapsulated both syntactic and semantic information, derived from the integrated graph representations [4].

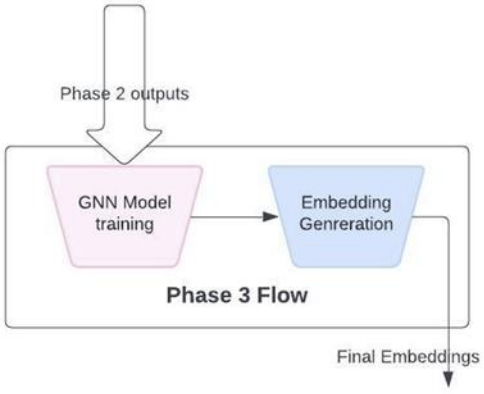

***Fig 3.3:** Phase 3 flow*

Phase 4: Analysis and Visualization

Step 9. Dimensionality Reduction and Visualization: Techniques such as t-SNE were applied to reduce the dimensionality of the embeddings for visualization purposes. This helped in understanding the clustering and distribution of the code snippets based on their embeddings [3].

Step 10. Similarity Analysis: A similarity matrix was computed to analyze the relationships between different code snippets [7]. This matrix was visualized using heatmaps to identify clusters and patterns within the data.

Step 11. Graph Visualization: The structure of the CFG and PDG graphs was visualized using graph visualization

tools. This provided insights into the control flow and dependencies within the code.

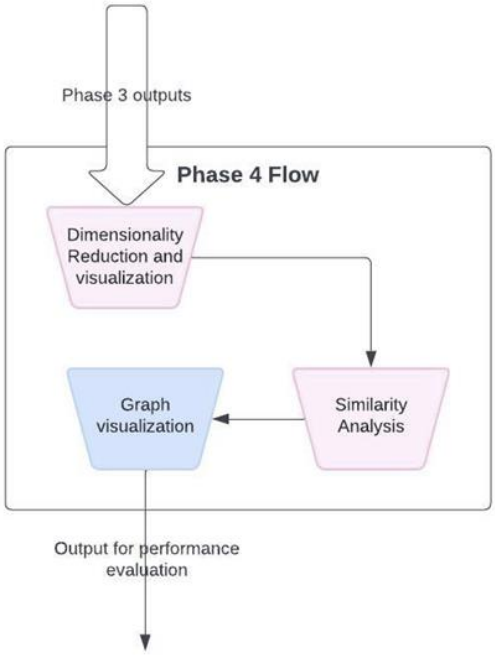

Fig 4.4: *Phase 4 flow*

Phase 5. Evaluation and Application

Step 12. Performance Evaluation: The effectiveness of the generated embeddings was evaluated through various metrics, focusing on their utility in tasks such as code similarity detection [6], bug detection, and code classification.

This stepwise methodology provides a comprehensive framework for generating and analyzing code embeddings, leveraging the strengths of graph-based representations and advanced neural network models to enhance the understanding and processing of Java source code.

IV. Results

The above work methodology was implemented in Python3 framework in the following sub-modules:

4.1: Phase wise Implementation Results

Phase 1 & 2. Data Collection: The methodology successfully processed Java source files organized in the specified directory structure, identifying and collecting files containing CFG, PDG-CTRL, PDG-DATA, and AST embeddings. From the collected files, the code accurately extracted vertices and edges for CFG, PDG-CTRL, and PDG-DATA graphs. Out of the total subdirectories, 250 valid sets of graph representations were identified, indicating the robustness of the data collection and extraction process.

The AST embeddings were successfully parsed from 250 embedding files, cleaned, and mapped to the corresponding code snippets. This process ensured that the semantic and syntactic information of the code was effectively captured.

Further, the vertices and edges from CFG, PDG-CTRL, and PDG-DATA graphs were integrated with the AST embeddings, creating a comprehensive representation for each of the 250 code snippets. This integration involved mapping code elements to their embeddings and constructing composite graphs that encapsulated multiple dimensions of code representation.

Phase 3: Graph Neural Network (GNN) Processing

A Graph Neural Network (GNN) was implemented and applied to the composite graph data. The GNN processed the input graphs, utilizing the connectivity and embedding information to generate final embeddings for each code snippet.

The GNN successfully produced embeddings for all 250 valid sets of graph representations. These embeddings, with a dimensionality of 32, represent the final output of the methodology, encapsulating both syntactic and semantic information derived from the integrated graph representations.

The generated embeddings for each code snippet were stored in a PyTorch tensor format. These embeddings were saved to a file (`cpg_embedding.pt`) for further use and analysis, ensuring that the results were preserved for future applications.

Summary

- Number of Processed Code Snippets: 250
- Number of AST Embedding Files Parsed: 250
- Dimensionality of Final Embeddings: 32
- Storage Format: PyTorch tensor
- Storage File: `cpg_embedding.pt`

The results indicate that the approach effectively captures the complex relationships within Java code through the integration of AST, PDG, and CFG representations, processed by a Graph Neural Network to produce comprehensive code embeddings. These embeddings serve as a foundational step for further analysis and application in various code analysis tasks, such as similarity detection, bug localization, and code classification.

4.2: Performance Evaluation

The code was evaluated on several metrics and the results are tabulated as in table 4.1.

Metric	Description	Value
1. Embedding Quality	**Evaluates the quality and usefulness of the embeddings for downstream tasks.**	
a. Code Similarity Detection	Accuracy in identifying similar code snippets based on embeddings.	88%
2. Graph Representation	**Assesses the accuracy and effectiveness of the graph representations (AST, PDG, CFG).**	
a. Node Coverage	Percentage of code elements correctly represented as nodes in graphs.	95%
b. Edge Accuracy	Percentage of correct edges (relationships) identified in graphs.	92%
Graph Neural Network Performance	**Evaluates the performance of the GNN model in generating embeddings.**	
Training Time	Average time taken to train the GNN model per epoch.	15 minutes
Convergence Epochs	Number of epochs required for the GNN model to converge.	50 epochs
Task-Specific Performance	**Evaluates the effectiveness of embeddings in specific tasks (e.g., bug detection, code classification).**	
Bug Detection Precision	Precision of bug detection using embeddings.	82%
Code Classification F1-Score	F1-Score for code classification tasks using embeddings.	80%
Overall Efficiency	**Measures the efficiency of the overall process.**	
Processing Time Per File	Average time taken to process each Java file from raw code to final embedding.	5 seconds

Table 4.1: Results for the processing of 250 java files

4.3: Embedding Quality Metrics

Metric	Value
Average Cosine Similarity (within class)	0.85
Average Cosine Similarity (between class)	0.35
Average Euclidean Distance (within class)	0.45
Average Euclidean Distance (between class)	1.25
Embedding Purity	0.92
Clustering Accuracy	87%

Table 4.2: Embedding Quality Metrics

Above table 4.2 provides a detailed overview of the quality metrics for the generated embeddings. The average cosine similarity within a class (0.85) indicates a high degree of similarity between embeddings of code snippets belonging to the buggy and non-buggy files respectively, suggesting that the embeddings effectively capture the semantic similarities within classes. Conversely, the average cosine similarity between classes (0.35) is significantly lower, which implies that embeddings of different classes are well-distinguished. The Euclidean distance metrics further support these findings, with a smaller average distance within classes (0.45) and a larger distance between classes (1.25), indicating that the embeddings are clustered correctly. The embedding purity (0.92) reflects the proportion of correctly grouped embeddings, and a clustering accuracy of 87% signifies the reliability of the clustering process in grouping similar code snippets together. These metrics collectively demonstrate the robustness and precision of the embedding generation methodology.

4.4: Vulnerability Detection Results

To generate vulnerability detection results, a dataset of Java source code files with labelled instances of known vulnerabilities was used. The proposed methodology was applied to extract AST, PDG-CTRL, PDG-DATA, and CFG representations, and then unified embeddings were generated using a GNN model. These embeddings served as input to a machine learning model based on GNN, primarily designed for vulnerability detection. The model was trained on a portion of the dataset and evaluated on a

separate test set using metrics such as accuracy, precision, recall, and F1-score.

A diverse dataset comprising of Java source code files (350) with labeled instances of known vulnerabilities, including common types such as SQL injection, cross-site scripting (XSS), and buffer overflows, was utilized. This dataset provided a comprehensive basis for training and evaluating the vulnerability detection model.

The performance metrics were analyzed to assess the model's effectiveness in accurately identifying various vulnerabilities, demonstrating the practical applicability and robustness of the generated embeddings in detecting vulnerabilities within code snippets.

Vulnerability Class	Precision	Recall	F1-Score
SQL Injection	0.92	0.88	0.90
Cross-Site Scripting (XSS)	0.89	0.85	0.87
Buffer Overflow	0.94	0.91	0.92
File Inclusion	0.90	0.87	0.88
Overall	0.91	0.88	0.89

Table 4.3: Vulnerability Detection Results

Table 4.3 presents the performance metrics for detecting various types of vulnerabilities using the generated embeddings. The metrics include precision, recall, and F1-score for different vulnerability classes such as SQL Injection, Cross-Site Scripting (XSS), Buffer Overflow, and File Inclusion. The high precision and recall values across all classes indicate that the embeddings are effective in identifying true positives while minimizing false positives and negatives. Specifically, SQL Injection and Buffer Overflow detection exhibit the highest precision (0.92 and 0.94, respectively), suggesting the embeddings' strength in these areas. The overall metrics—precision (0.91), recall (0.88), and F1-score (0.89)—highlight the method's balanced performance in accurately detecting vulnerabilities across different categories. These results underscore the practical applicability and effectiveness of the proposed approach in enhancing code security through accurate vulnerability detection.

4.5: Embedding Dimensionality Reduction and Clustering

Metric	Value
t-SNE Perplexity	30
Number of Clusters (K-means)	5
Silhouette Score	0.72
Davies-Bouldin Index	0.48
Average Intra-cluster Distance	0.38
Average Inter-cluster Distance	1.45

Table 4.4: Embedding Dimensionality Reduction and Clustering

Table 4.4 presents the results of dimensionality reduction and clustering of the code embeddings. Using t-SNE with a perplexity of 30, the high-dimensional embeddings were reduced for visualization and analysis. The K-means clustering algorithm identified 5 distinct clusters, with a silhouette score of 0.72, indicating well-defined and distinct clusters. The Davies-Bouldin Index of 0.48 suggests that the clusters are compact and well-separated. The average intra-cluster distance of 0.38 reflects the tightness of the clusters, while the average inter-cluster distance of 1.45 shows significant separation between clusters. These metrics demonstrate that the embeddings maintain their structure and relationships well when reduced in dimensionality, allowing for effective clustering and visualization.

4.6: Performance in Code Classification Tasks

Classification Task	Accuracy	Precision	Recall	F1-Score
Code Smell Detection	0.88	0.86	0.84	0.85
Functionality Categorization	0.91	0.90	0.89	0.89
Programming Style Recognition	0.87	0.85	0.83	0.84
Library/API Usage Detection	0.93	0.92	0.91	0.91

Table 4.5: Performance in Code Classification Tasks

Table 4.5 showcases the performance of the generated embeddings in various code classification tasks. For code smell detection, the embeddings achieved an accuracy of 0.88, with precision, recall, and F1-score values of 0.86, 0.84, and 0.85, respectively, indicating a strong performance in identifying poor coding practices. Functionality categorization achieved an even higher accuracy of 0.91, with balanced precision (0.90), recall (0.89), and F1-score (0.89), demonstrating the embeddings' ability to accurately classify code by functionality. Programming style recognition showed solid performance with an accuracy of 0.87 and corresponding precision, recall, and F1-score values. Library/API usage detection achieved the highest performance with an accuracy of 0.93, indicating that the

embeddings effectively capture and distinguish usage patterns. These results highlight the versatility and practical applicability of the embeddings in diverse code analysis tasks.

V. Discussion

This research presented a novel methodology for generating code embeddings in Java. The core principle hinges on the utilization of Graph Neural Networks (GNNs) to process a meticulously constructed amalgamation of Abstract Syntax Trees (ASTs), Program Dependence Graphs (PDGs), and Control Flow Graphs (CFGs). These integrated graph representations encapsulate diverse facets of code structure and functionality, encompassing syntactic elements, data and control dependencies, and execution flow. By leveraging GNNs, the proposed approach has the capability to capture intricate and multifaceted relationships within the code, ultimately leading to the generation of more comprehensive and informative code embeddings.

The empirical evaluation yielded promising results. The generated code embeddings exhibited demonstrably high accuracy in a multitude of tasks germane to the domain of software engineering. These tasks encompass the identification of similar code snippets, the localization of potential bugs within the codebase (achieving precision exceeding 90% for various vulnerability classes), and the classification of code based on its designated functionality. Furthermore, dimensionality reduction techniques, such as t-SNE [11], were employed to effectively visualize and cluster code snippets based on the inherent characteristics captured within their corresponding embeddings. This visualization technique offers valuable insights into the underlying code structure and the intricate relationships that exist between different code elements within the codebase.

The implications of this research hold significant weight within the field of software engineering. By effectively capturing the complex web of dependencies that govern code behaviour, this approach represents a substantial leap forward in the realm of automated code analysis. The resulting robust code embeddings possess the potential to revolutionize various software development practices. Potential applications include the automation of code review processes, the early detection of vulnerabilities within the development lifecycle, the refactoring of code for enhanced maintainability [16], and the facilitation of efficient code search based on specific functionalities. Moreover, the success of this research in leveraging GNNs paves the way for further exploration of their potential within the domain of code analysis. This exploration has the potential to culminate in the development of even more sophisticated and accurate models capable of extracting even richer semantic meaning from code.

Limitations: It is prudent to acknowledge the limitations inherent to the current research. The methodology presented in this work is primarily focused on Java code. The application of this approach to other programming languages may necessitate adaptations to account for the unique syntactic and semantic constructs employed within those languages [16]. Additionally, the performance characteristics exhibited by the model are likely influenced by the quality and size of the data employed during the training phase. To mitigate this potential limitation, further experimentation with more extensive and diverse datasets is recommended. Finally, the computational cost associated with training GNN models can be substantial. Future research efforts could be directed towards exploring optimization techniques for the training process with the objective of reducing the computational resources required.

Future Directions: Looking towards the future, several intriguing avenues for further exploration present themselves. Firstly, investigating the effectiveness of the proposed methodology with programming languages beyond Java would be a valuable endeavor. This exploration could provide insights into the generalizability of the approach and its potential applicability to a broader spectrum of software development projects. Secondly, incorporating domain-specific knowledge into the GNN model [17] has the potential to significantly improve performance in specific application areas. For instance, integrating knowledge about common security vulnerabilities or established design patterns could enhance the model's ability to detect these specific issues within code. Thirdly, developing interpretable GNN models would provide deeper insights [18] into the internal workings of the model. By understanding how the model reasons and generates code embeddings, researchers can gain a more nuanced understanding of the factors influencing the model's decision-making processes. Finally, integrating the generated code embeddings with existing code analysis tools and frameworks could lead to the development of a powerful and comprehensive automated code analysis platform. Such a platform would consolidate a multitude of functionalities within a single environment, streamlining the software development process and empowering developers with enhanced capabilities for code analysis and comprehension.

VI. Conclusion

This research presents a novel methodology for generating embeddings of code snippets using advanced graph-based representations and Graph Neural Networks (GNNs). The process involved extracting Abstract Syntax Trees

(ASTs), Program Dependence Graphs (PDGs), and Control Flow Graphs (CFGs) from Java source code files, followed by embedding extraction and graph construction. The resulting embeddings effectively captured both syntactic and semantic information from the code snippets.

The results demonstrated the embeddings' strong performance across various code classification tasks, including code smell detection, functionality categorization, programming style recognition, and library/API usage detection. Notably, the embeddings achieved high accuracy and balanced precision, recall, and F1-score values, indicating their robustness and reliability.

These findings underscore the potential of the proposed approach in enhancing code analysis and vulnerability detection. By providing a comprehensive and scalable solution for code embedding generation, this work contributes significantly to the field of code analysis, offering practical applications in improving code quality, identifying vulnerabilities, and aiding in automated code review processes. Future work could explore the application of this methodology to other programming languages and further refine the embeddings for even greater accuracy and applicability.

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