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Debugging of AI-enabled and Quantum Software Systems

石本, 優太

https://hdl.handle.net/2324/7443462

出版情報：Kyushu University, 2025, 博士（情報科学）, 課程博士
バージョン：
権利関係：

KYUSHU UNIVERSITY

（様式 2）

氏　　名　：石本　優太

論 文 名　：Debugging of AI and Quantum Software Systems（AI および量子ソフトウェアシステムに対するデバッギング）

区　　分　：甲

論　文　内　容　の　要　旨

In recent years, software systems enhanced with the capabilities of artificial intelligence (AI) and quantum computation have attracted increasing attention. We refer to these systems as *AI-enabled software systems* and *quantum software systems*, respectively. These systems enable tasks that were difficult or even impossible to accomplish with conventional software. For example, AI-enabled software systems have realized applications such as autonomous driving and chatbots through inductive development paradigms that learn from large amounts of data. On the other hand, quantum software systems are expected to enhance applications such as optimization and cryptography by leveraging their computational power. Given their increasing deployment in critical domains, misbehavior in these systems can lead to threats to human life or substantial economic losses. This underscores the need for rigorous software engineering practices for these software systems, just as for conventional software systems.

Among software engineering practices, *debugging*, the process of isolating and correcting mistakes in computer software, is essential for ensuring software quality. To support this process, the software engineering research community has dedicated considerable effort, including automated fault localization and automated program repair. However, conventional debugging techniques may not be well suited to emerging software paradigms such as AI-enabled and quantum software systems. For AI-enabled software systems, debugging requires attention not only to the source code but also to the datasets and trained AI models, as their behavior depends on data-driven learning processes. For quantum software systems, debugging should take into account the quantum mechanical properties of quantum software, such as superposition, no-cloning theorem, and entanglement of quantum bits (qubits). These challenges motivate the development of novel debugging methodologies tailored to AI-enabled and quantum software systems.

This dissertation addresses the challenges of debugging AI-enabled and quantum software systems through four complementary studies related to fault localization and repair. The main contributions of this dissertation are as follows: the first two concern debugging for AI-enabled software systems, and the remaining two concern debugging for quantum software systems.

- *Probabilistic Automaton-based Fault Localization for Recurrent Neural Networks.*
  Deep neural networks (DNNs) play a central role in AI-enabled software systems.

Among various types of DNNs, recurrent neural networks (RNNs) present unique debugging challenges because they maintain internal states that dynamically change depending on input sequences. To address this, we propose probabilistic automaton-based fault localization (PAFL). PAFL abstracts RNNs into probabilistic finite automata (PFAs) and localizes faulty sequences of state transitions on PFAs by adapting the concept of spectrum-based fault localization (SBFL). Our evaluation demonstrates that PAFL can identify data samples leading to misbehavior more effectively and efficiently than the state-of-the-art techniques in 66.74% of the cases.

- *Repairs and Breaks Prediction for Deep Neural Networks.* DNN repair methods refer to those that target components of the model itself (e.g., neurons or weights) to reduce the specific type of misbehavior while preserving its existing correct behavior. These methods are often computationally expensive. Therefore, predicting promising repair methods in advance is crucial to reduce the number of trial-and-error iterations during the debugging process of AI-enabled software systems. To this end, we build prediction models to estimate the outcomes of DNN repair methods. Our evaluation demonstrates that these prediction models can reduce the overall time for repair application scenarios, yielding an average time savings of 16.29% compared to the naive method of applying all repair methods and checking the results.
- *Evaluating Mutation-based Fault Localization for Quantum Programs.* Quantum programs, consist of sequences of operations on qubits, known as quantum gates. While existing studies have demonstrated the effectiveness of mutation operators (e.g., deleting quantum gates) for testing quantum programs, their potential for fault localization remains unexplored. Therefore, we evaluate the effectiveness of mutation-based fault localization (MBFL) for quantum programs. While MBFL was originally proposed for classical (non-quantum) programs, we first evaluate its effectiveness in the quantum context. The experimental results demonstrate that mutation operations specific to quantum programs are more effective than classical mutation operations.
- *Leveraging Mutation Analysis for LLM-based Repair of Quantum Programs.* Although automated program repair (APR) techniques for quantum programs exits, they often show low success rates or produce patches with limited interpretability. To address these limitations, we enhance LLM-based repair for quantum programs by incorporating insights from mutation analysis. We hypothesize that mutation analysis results can provide richer dynamic context than standard execution results (e.g., simple pass/fail outcomes), thereby improving both repair success and explanation quality for repair. Our evaluation demonstrates that incorporating mutation analysis results into the prompt enabled the repair of 17 out of 18 faulty programs. Furthermore, it enhances the quality of the generated explanations.

In summary, this dissertation contributes to advancing debugging for AI-enabled and quantum software systems by proposing novel approaches and evaluating the effectiveness of existing techniques for fault localization and repair.