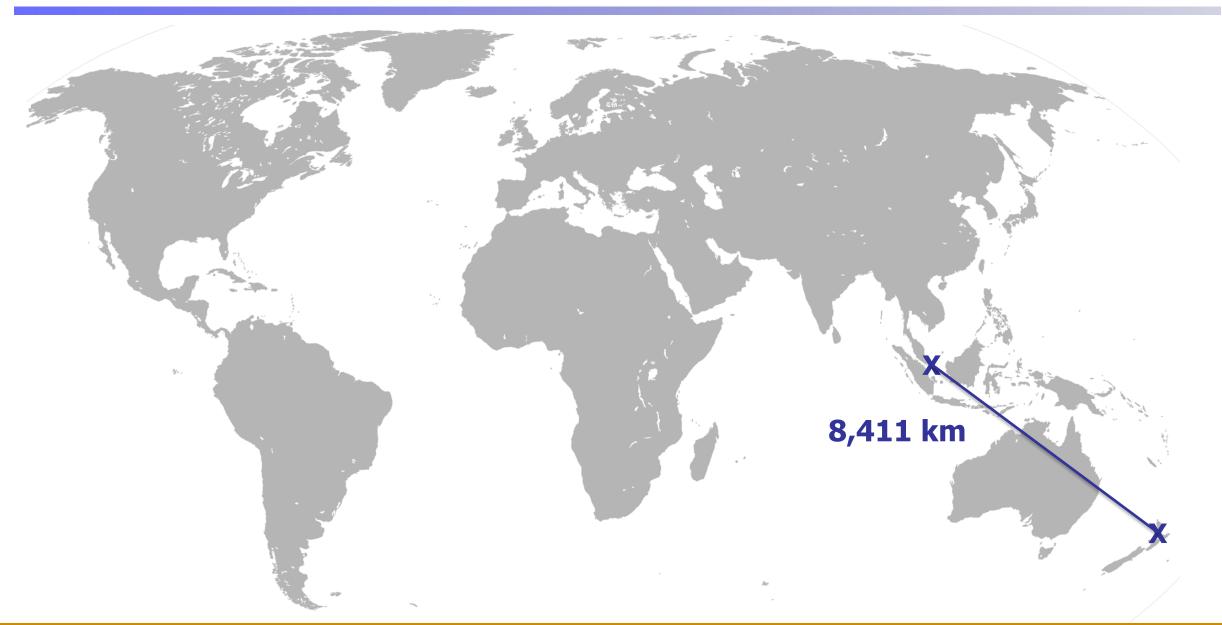


Code, Critique, Cure: Advancing LLM *Reasoning* **for AI-Augmented Software Maintenance**

David Lo, FACM, FIEEE





















Singapore Management University



- Third university in Singapore
- Number of students:
 - 8000+ (UG)
 - 1800+ (PG)
- Schools:
 - Business
 - Computing
 - Economics
 - Accountancy
 - Law
 - Social Science



School of Computing and Information Systems



Center for Research on Intelligent Software Engineering (RISE)



Elsevier JSS'21, Bibliometric Study

| Table 3 Most active institutions in software engineering | | |
|---|---------------------------------|--|
| Rank | Name | |
| 1 | University of California | |
| 2 | Carnegie Mellon University | |
| 3 | Nanjing University | |
| 4 | Microsoft Research | |
| 5 | Singapore Management University | |

CSRankings, SE, Aug 2025

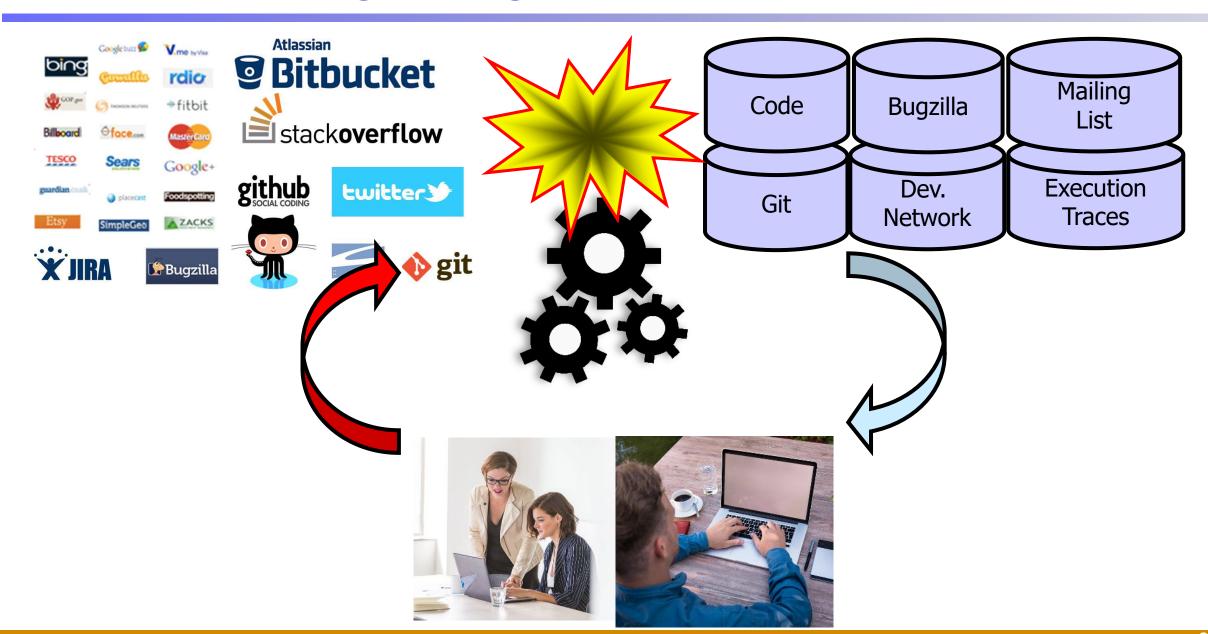
| # | Institution | Count Fa | culty |
|---|---|----------|-------|
| 1 | ▶ Nanjing University 🚾 📶 | 45.6 | 40 |
| 2 | Peking University Image: Image: Imag | 31.3 | 22 |
| 3 | ▶ Carnegie Mellon University 🔤 📊 | 31.2 | 16 |
| 4 | ▶ Singapore Management University 뜨 📊 | 25.0 | 9 |



Computing and Information Systems

Centre for Research on Intelligent Software Engineering

AI for Software Engineering



Experience with AI4SE

SMArTIC: Towards Building an Accurate, Robust and Scalable Specification Miner

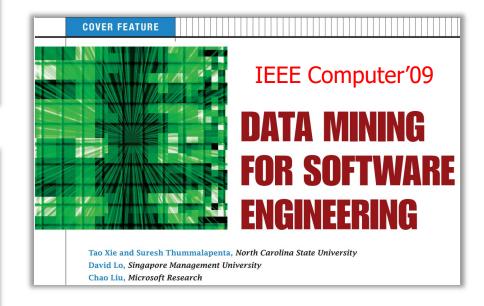
FSE'06

David Lo and Siau-Cheng Khoo Department of Computer Science, National University of Singapore {dlo,khoosc}@comp.nus.edu.sg

Efficient Mining of Iterative Patterns for Software Specification Discovery

KDD'07

David Lo and Siau-Cheng Khoo Department of Computer Science National University of Singapore {dlo,khoosc}@comp.nus.edu.sq Chao Liu
Department of Computer Science
University of Illinois-UC
chaoliu@cs.uiuc.edu







Experience with AI4SE

Classification of Software Behaviors for Failure Detection: A Discriminative Pattern Mining Approach

KDD'09

David Lo Singapore Management University davidlo@smu.edu.sq Hong Cheng *Chinese University of Hong Kong hcheng@se.cuhk.edu.hk

Jiawei Han[†]
University of Illinois at Urbana-Champaign
hanj@cs.uiuc.edu

Siau-Cheng Khoo and Chengnian Sun National University of Singapore {khoosc.suncn}@comp.nus.edu.sq

A Discriminative Model Approach for Accurate Duplicate Bug Report Retrieval

ICSE'10

Chengnian Sun¹, David Lo², Xiaoyin Wang³, Jing Jiang², Siau-Cheng Khoo¹

¹School of Computing, National University of Singapore

²School of Information Systems, Singapore Management University

³Key laboratory of High Confidence Software Technologies (Peking University), Ministry of Education suncn@comp.nus.edu.sg, davidlo@smu.edu.sg, wangxy06@sei.pku.edu.cn, jingjiang@smu.edu.sg, khoosc@comp.nus.edu.sg

Intelligent issue trackers

Test oracle generation

Tag Recommendation in Software Information Sites MSR'13

Xin Xia*[‡], David Lo[†], Xinyu Wang*, and Bo Zhou*[§]
*College of Computer Science and Technology, Zhejiang University
[†]School of Information Systems, Singapore Management University

Intelligent crowdsourced SE

History Driven Program Repair

SANER'16

Xuan-Bach D. Le, David Lo School of Information Systems Singapore Management University {dxb.le.2013,davidlo}@smu.edu.sg Claire Le Goues School of Computer Science Carnegie Mellon University clegoues@cs.cmu.edu

Intelligent program repair

"History-driven program repair influence our work, the overall pipeline is similar"

FacebookEngineers



Computing and Information Systems

Our Research Agenda in AI4SE

Trustworthy and Synergistic Artificial Intelligence for Software Engineering: Vision and Roadmaps

David Lo
School of Computing and Information Systems,
Singapore Management University,
Singapore
Email: davidlo@smu.edu.sg





<u>Trustworthy</u> and <u>Synergistic</u> AI4SE: Vision and the Road Ahead

David Lo

Computing and

ICSE'23 Future of SE Talk

AI for Software Engineering

History

Challenges

Vision













Roadmap I

Roadmap II

Call4Action

Towards Software Engineering 2.0



SMU SINGAPORE MANAGEMEN

"If you want to go far, go together" – African Proverb































University of Victoria



















































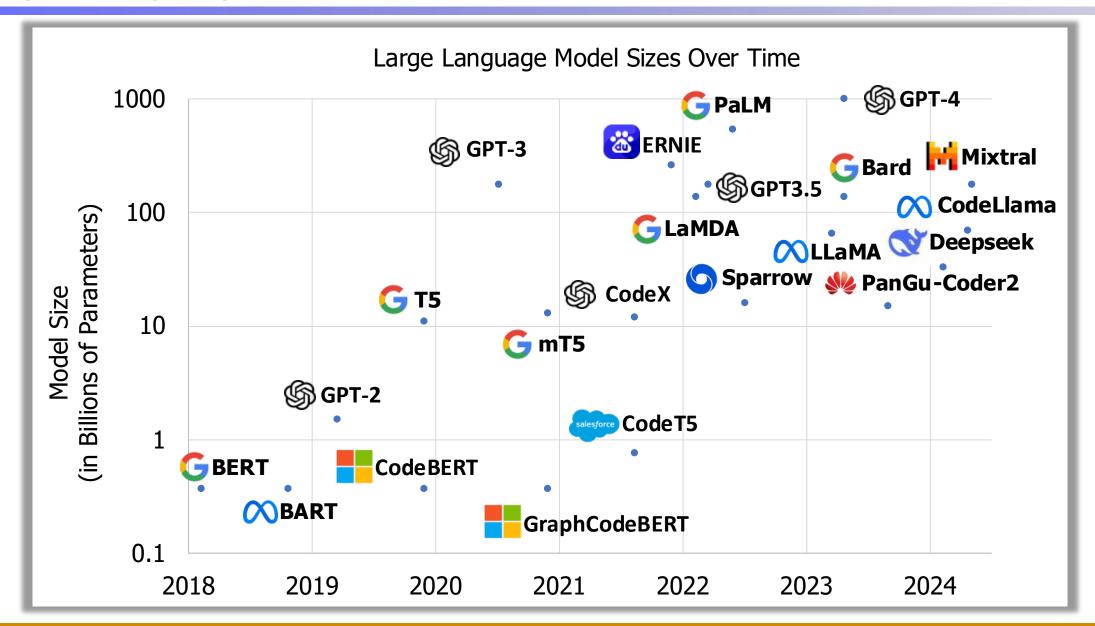




Code, Critique, Cure: Advancing LLM Reasoning for AI-Augmented Software Maintenance

Computing and Information Systems

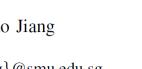
Large Language Models (LLMs)



LLM Can Greatly Help SE Tasks

2020 ICSME

Sentiment Analysis for Software Engineering: How Far Can Pre-trained Transformer Models Go?



Ting Zhang, Bowen Xu*, Ferdian Thung, Stefanus Agus Haryono, David Lo, Lingxiao Jiang School of Information Systems, Singapore Management University Email: {tingzhang.2019, bowenxu.2017}@phdcs.smu.edu.sg, {ferdianthung, stefanusah, davidlo, lxjiang}@smu.edu.sg



2021 **ICSME**

Assessing Generalizability of CodeBERT

Xin Zhou, DongGyun Han, and David Lo School of Computing and Information Systems, Singapore Management University xinzhou.2020@phdcs.smu.edu.sg, {dhan, davidlo}@smu.edu.sg



Early work on benchmarking code LLM, among most cited papers of ICSME 2021





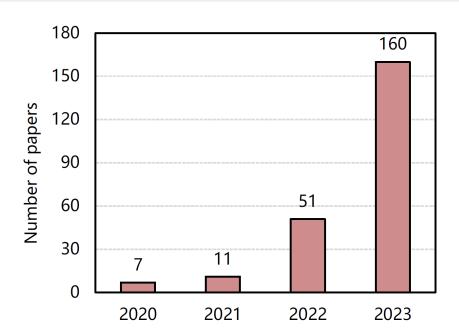
LLMs Seem to Win for Many SE Scenarios

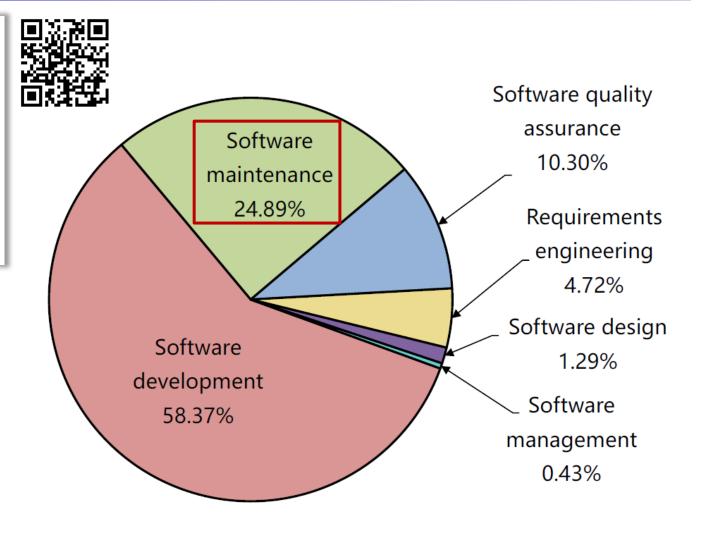
Large Language Models for Software Engineering: A Systematic Literature Review

YANJIE ZHAO*, Monash University, Australia
YUE LIU, Monash University, Australia
ZHOU YANG, Singapore Management University, Singapore
KAILONG WANG, Huazhong University of Science and Technology, China
LI LI, Beihang University, China
XIAPU LUO, The Hong Kong Polytechnic University, China
DAVID LO, Singapore Management University, Singapore
JOHN GRUNDY, Monash University, Australia

HAOYU WANG[†], Huazhong University of Science and Technology, China

XINYI HOU*, Huazhong University of Science and Technology, China





Despite Successes, Much Work Remains

Measuring the Impact of Early-2025 AI on Experienced Open-Source Developer Productivity



Joel Becker*, Nate Rush*, Beth Barnes, David Rein

Model Evaluation & Threat Research (METR)

InfoWorld

Al coding tools can slow down seasoned developers by 19%

News

Jul 11, 2025 • 6 mins

Computing and Information Systems



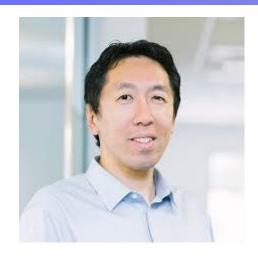
Despite Successes, Much Work Remains

| Factor | Relevant Observations |
|--|--|
| Over-optimism about AI usefulness (C.1.1) | Developers forecast AI will decrease implementation time by 24% Developers post hoc estimate AI decreased implementation time by 20% |
| High developer familiarity with repositories (C.1.2) | Developers slowed down more on issues they are more familiar with Developers report that their experience makes it difficult for AI to help them Developers average 5 years experience and 1,500 commits on repositories |
| Large and complex repositories (C.1.3) | Developers report AI performs worse in large and complex environments Repositories average 10 years old with >1,100,000 lines of code |
| Low AI reliability (C.1.4) | Developers accept <44% of AI generations Majority report making major changes to clean up AI code 9% of time spent reviewing/cleaning AI outputs |
| Implicit repository context (C.1.5) | • Developers report AI doesn't utilize important tacit knowledge or context |

LLM has **limited reasoning capabilities** for software maintenance tasks

How Can We It?

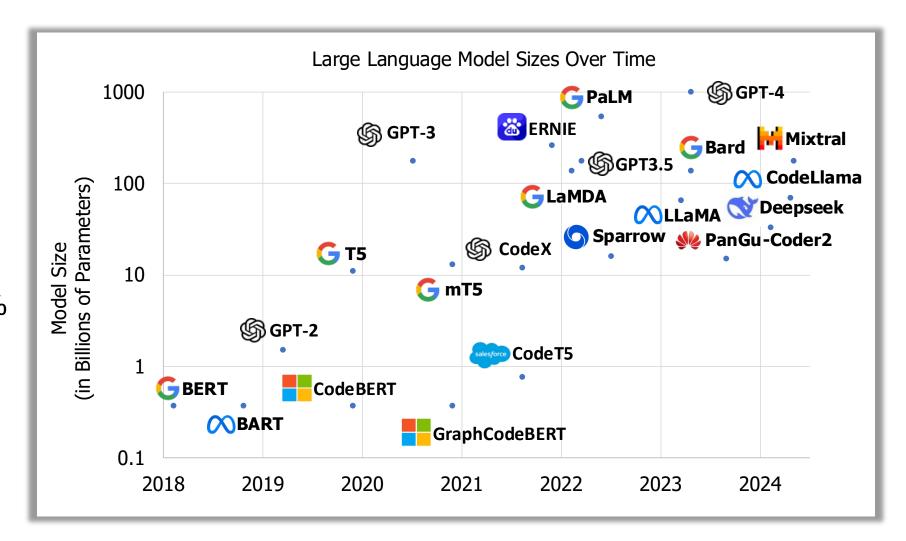
Too Much Focus on Models



"99% of the papers were model-centric with only 1% being data-centric"

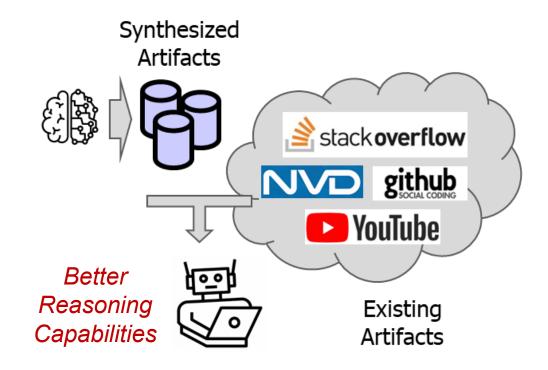
– Andrew NgGoogle Brain Co-Founder





Data-Centric LLM4SE

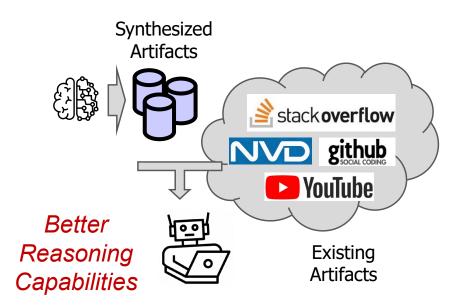
- Use SE domain knowledge for software artifact engineering
- to guide LLM reasoning
- for specific SE tasks





Data-Centric LLM4SE: Artifact Engineering

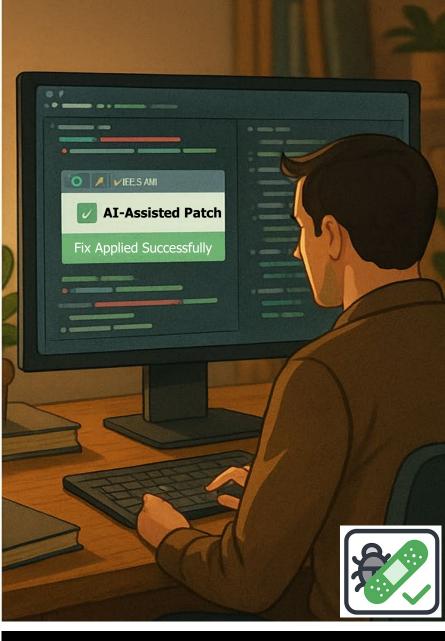
"How Can We **Systematically Engineer Software Artifacts** to Build Better LLM4SE Bots?"



- Construct LLM-reasoning friendly datasets by
 - selecting the right artefacts
 - linking related pieces of information,
 - providing examples,
 - transforming them appropriately, etc.
 leveraging domain knowledge.
- Scale up with LLM4(LLM4SE):
 LLMs themselves can assist this SE artifact engineering (crafting) step





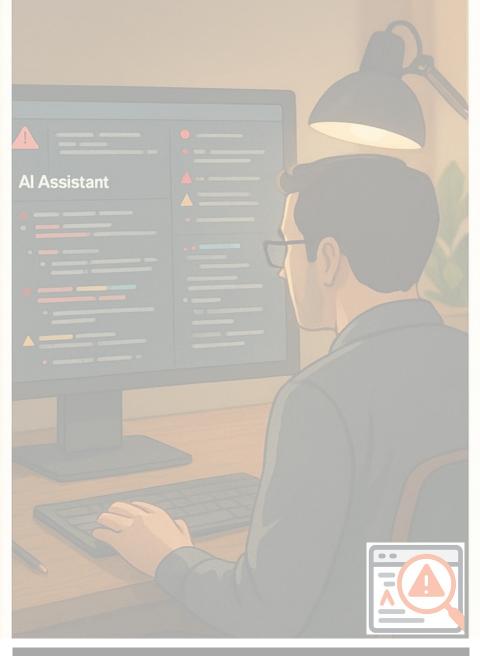


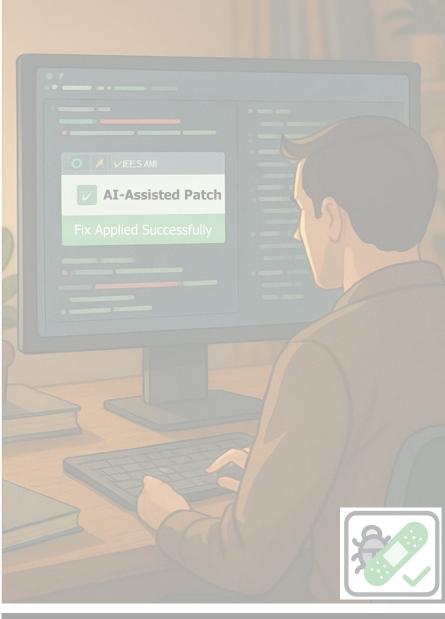
Code

Critique

Cure







Code

Critique

Cure

Structured Data Can Be Helpful for AI4SE

Deep Code Comment Generation*

Xing Hu¹, Ge Li¹, Xin Xia², David Lo³, Zhi Jin¹

¹Key Laboratory of High Confidence Software Technologies (Peking University), MoE, Beijing, China

²Faculty of Information Technology, Monash University, Australia

³School of Information Systems, Singapore Management University, Singapore

¹{huxing0101,lige,zhijin}@pku.edu.cn, ²xin.xia@monash.edu, ³ davidlo@smu.edu.sg



First work that leverages structural information in code AST for better code comment generation; most cited paper of ICPC



Think Like Human Developers: Harnessing Community Knowledge for Structured Code Reasoning

Chengran Yang
Singapore Management University
Singapore
cryang@smu.edu.sg

Zhensu Sun
Singapore Management University
Singapore
zssun@smu.edu.sg

Hong Jin Kang University of Sydney Australia hongjin.kang@sydney.edu.au

Jieke Shi Singapore Management University Singapore jiekeshi@smu.edu.sg David Lo
Singapore Management University
Singapore
davidlo@smu.edu.sg



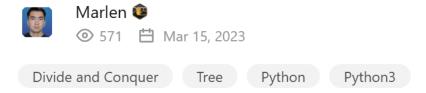
Engineers high-quality structured reasoning traces from community knowledge for better LLM-powered code generation





Community Knowledge as Code Reasoning Training Resources

558: Time 99.4%, Solution with step by step explanation



Intuition

Approach

- 1. Check if either quadTree1 or quadTree2 is a leaf node. If quadTree1 is a leaf node return quadTree1 if its value is True, else return quadTree2. If quadTree2 is a leaf node, return quadTree2 if its value is True, else return quadTree1.
- 2. Recursively check the intersection of each child node of quadTree1 and quadTree2 by calling the intersect function on each of them. Store the return values in variables tl (top-left), tr (top-right), bl (bottom-left), and br (bottom-right).

Community discussions offer peer-reviewed insights into developers' problem-solving strategies

"How Can We Leverage Community Knowledge to Help LLM Reason Better?"

RT-Distiller: From Com. Posts to Structured Reasoning Traces

 Distilling high-quality reasoning traces (RTs) for code generation from evolving community knowledge.



LeetCode Problem:

Given two binary grids as quad trees, return their logical OR result as a quad tree while maintaining minimal node representation.

User Discussion:

Intuition

Approach

- 1. Check if either quadTree1 or quadTree2 is a leaf node...
- 2. Recursively check the intersection of each child node of quadTree1 and quadTree2 by calling the intersect function...
- 3. Check if all four child nodes (tl, tr, bl, br) are leaves and have the same value...
- 4. If any of the child nodes have a different value or are not leaf nodes, create a new internal node...

Complexity

Time complexity: ...

Code

class Solution:

defintersect...

RT-Distiller: From Com. Posts to Structured Reasoning Traces

- Distilling high-quality reasoning traces (RTs) for code generation from evolving community knowledge.
 - X Mixed Quality Posts
 - Artificial
 Site-Specific
 Code Structure

LeetCode Problem:

Given two binary grids as quad trees, return their logical OR result as a quad tree while maintaining minimal node representation.

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- 1. Check if either quadTree1 or quadTree2 is a leaf node...
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RT-Distiller: From Com. Posts to Structured Reasoning Traces

- Distilling high-quality reasoning traces (RTs) for code generation from evolving community knowledge.
 - X Mixed Quality Posts
 - Artificial
 Site-Specific
 Code Structure
 - X Loosely Structured Reasoning

LeetCode Problem:

Given two binary grids as quad trees, return their logical OR result as a quad tree while maintaining minimal node representation.

User Discussion:

- # Intuition
- # Approach
- 1.Check if either quadTree1 or quadTree2 is a leaf node...
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Complexity

Time complexity: ...

Code

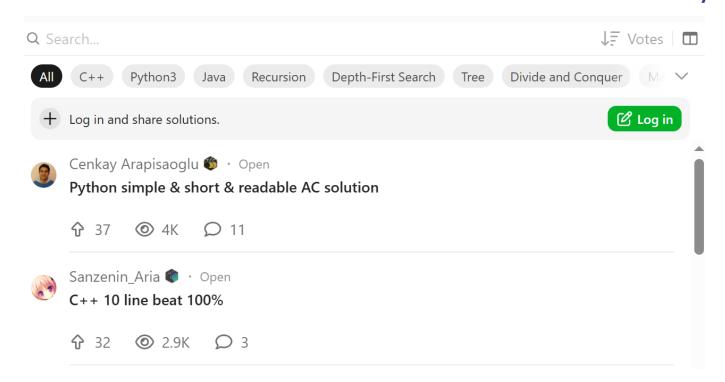
class Solution:

defintersect...

Step I: Addressing Mixed Quality Posts

- Identify High Quality Posts
- Identify rating mechanisms
- Select highly-rated posts

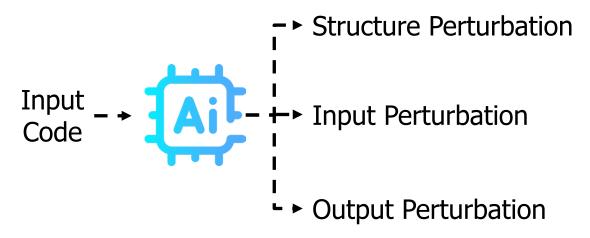
- ✓ Improve Post Quality
- Identify typical information pieces
- Detect missing pieces
- Synthesize missing pieces using LLM





Step II: Dealing with Artificial Site-Specific Code Structure



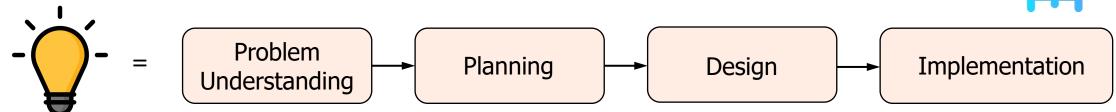


| Category | Variation Type |
|------------------------------|--|
| In most Forms of | Direct input (e.g., variables, constants) Structured input (e.g., list, tuple, dictionary) |
| Input Format | Batch input |
| | Interactive input() Boolean input |
| | Command-Line Arguments |
| | Structured input |
| | (e.g., list, tuple, dictionary) Boolean output |
| Output Format | Batch output |
| | Print statement |
| | Logging Output |
| | Class-based |
| Structural Variations | Function-based |
| | Script-based |



Rewrite a post into a structured trace inspired by SDLC





Given two binary grids as quad trees, return their logical OR result as a quad tree while maintaining minimal node representation.

User Discussion:

Intuition

Approach

- 1. Check if either quadTree1 or quadTree2 is a leaf node...
- 2. Recursively check the intersection of each child node of





First things first, I need to understand what a quad-tree is. From the description, it's a tree data structure where each internal node has exactly four children ...

Let's think about this step by step. First, I need to understand how the a leaf: quad-tree represents the matrix. If a node is a lis 1's, so the OR leaf and its `val` is true, it means ...

Let me try to outline an approach:

- 1. If `quadTree1` is
- If its `val` is true, | , quadTree2): then the entire grid with anything else is still 1's ...

Let me try to write some solutions: function intersect(quadTree1 if quadTree1.isLeaf: if quadTree1.val: return quadTree1

Problem Understanding

Planning

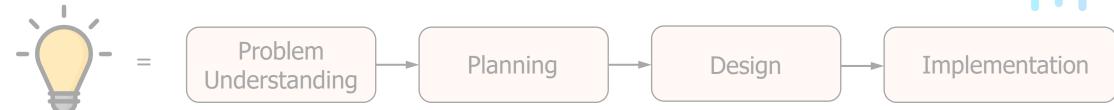
Design

Implementation



Rewrite a post into a structured trace inspired by SDLC

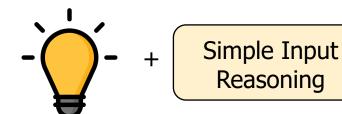






Add iterative refinement considerations





Common Mistake Reasoning

+ Edge Case Reasoning



Given two binary grids as quad trees, return their logical OR result as a quad tree while maintaining minimal node representation.

User Discussion:

- # Intuition
- # Approach
- 1. Check if either quadTree1 or quadTree2 is a leaf node...
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Let me try to write some solutions: function intersect(quadTree1 if quadTree1.isLeaf: if quadTree1.val: return quadTree1

I should think about edge cases:

- Both trees are leaf nodes.
- One tree is a leaf, the other is ...

I need to make sure that the function handles all these cases correctly. Let me consider a simple 2x2 grid...

Now, I need to think about whether there are any potential issues or edge cases that this doesn't handle...

Iterative Refinement

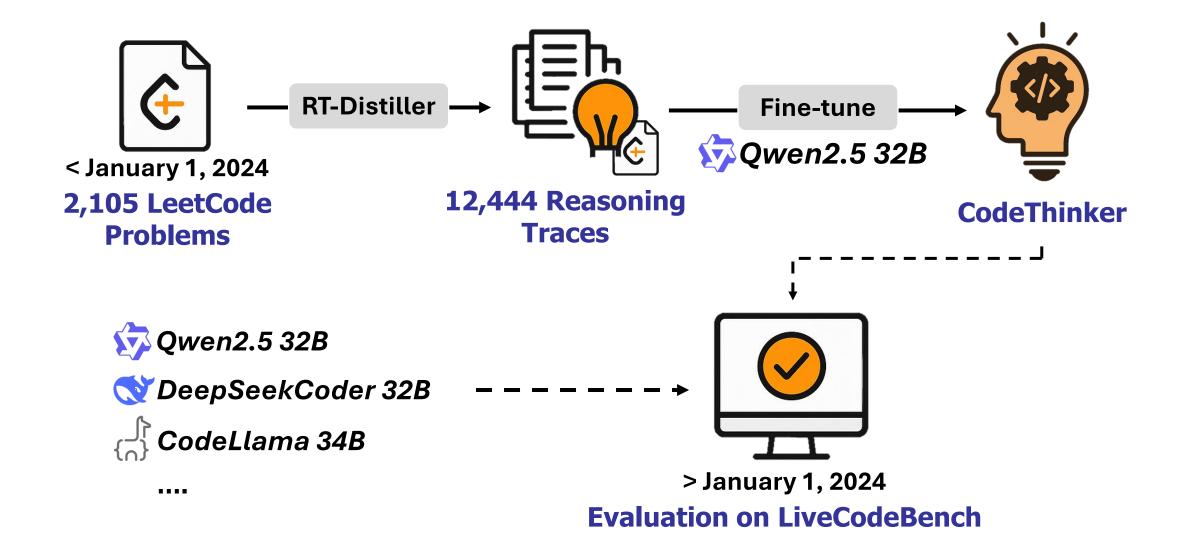
Problem Understanding

Planning

Design

Implementation

Experiment Settings



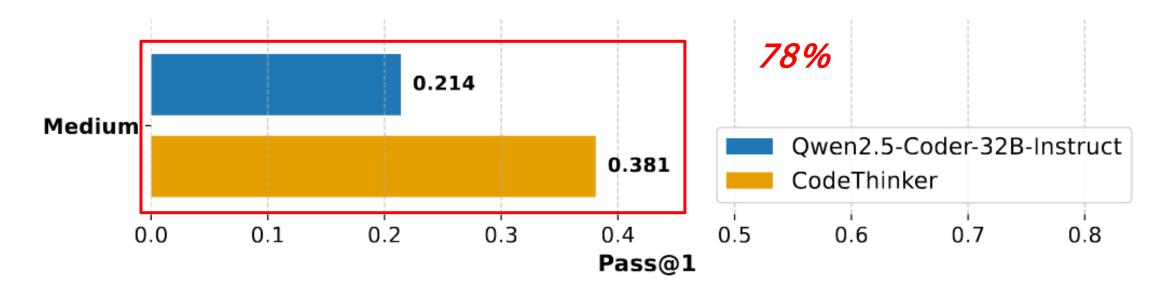
Experiment Results – Comparison with LLMs of Similar Sizes

| Model | Prompting | Size | Easy pass@1 | Medium pass@1 | Hard pass@1 | Overall pass@1 | |
|--------------------|-------------------|------|----------------|------------------------|----------------|------------------------|--|
| Open-source LLMs | | | | | | | |
| CodeLlama-Instruct | Standard | 34B | 0.290 | 0.028 | 0 | 0.078 | |
| CodeLlama-Instruct | CoT | 34B | 0.298 | 0.028 | 0 | 0.106 | |
| s1-32B | Standard | 32B | 0.306 | 0.098 | 0 | 0.134 | |
| s1-32B | CoT | 32B | 0.315 | 0.112 | 0 | 0.142 | |
| DeepSeekCoder | Standard | 32B | 0.589 | 0.126 | 0 | 0.235 | |
| DeepSeekCoder | CoT | 32B | 0.565 | 0.133 | 0 | 0.233 | |
| Qwen2.5-Instruct | Standard | 32B | 0.847 | 0.343 | 0 | 0.398 | |
| Owen2.5-Instruct | СоТ | 32B | 0.823 | 0.371 | 0 | 0.401 | |
| CodeThinker | CodeThinker Style | 32B | 0.831 (\1.89%) | 0.490 (†42.86%) | 0 | 0.447 (†12.31%) | |

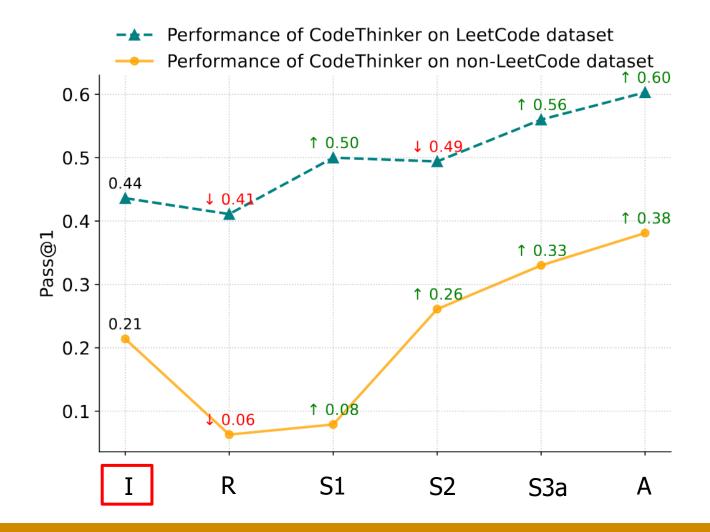


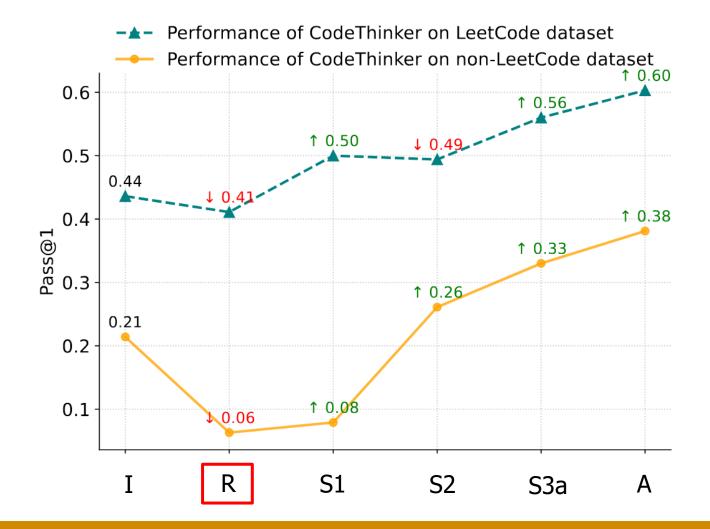
Experiment Results – Generalizability Beyond LeetCode

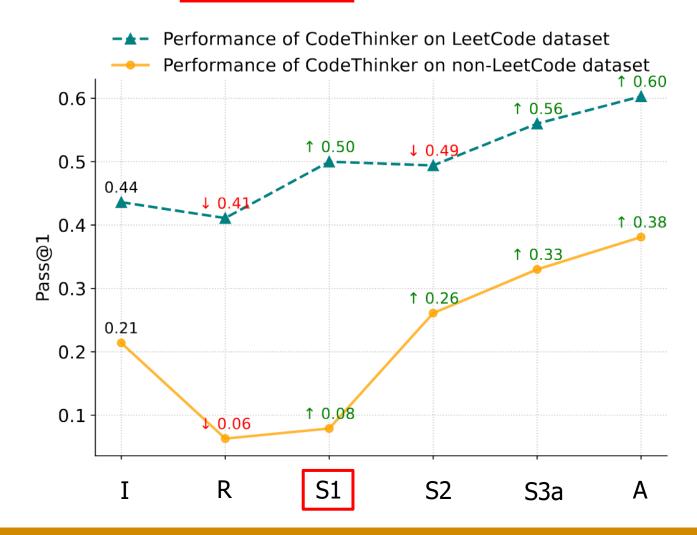
Figure 3: Comparison of CodeThinker and its base model on non-LeetCode coding problems (AtCoder and Codeforces), highlighting improved reasoning performance on medium-difficulty tasks.

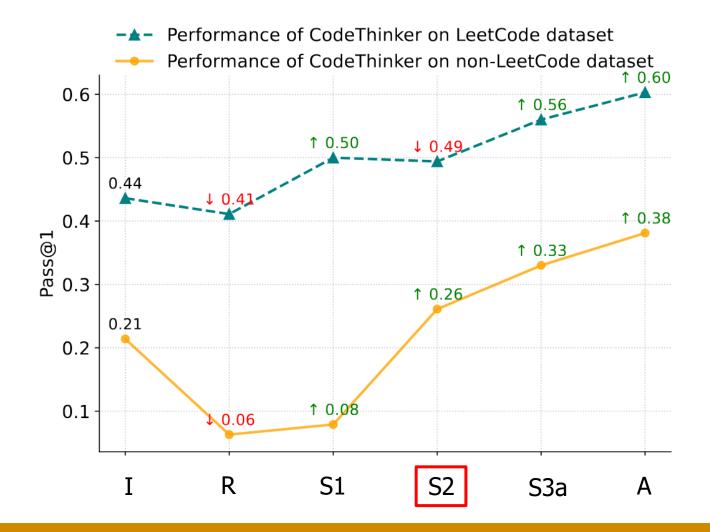


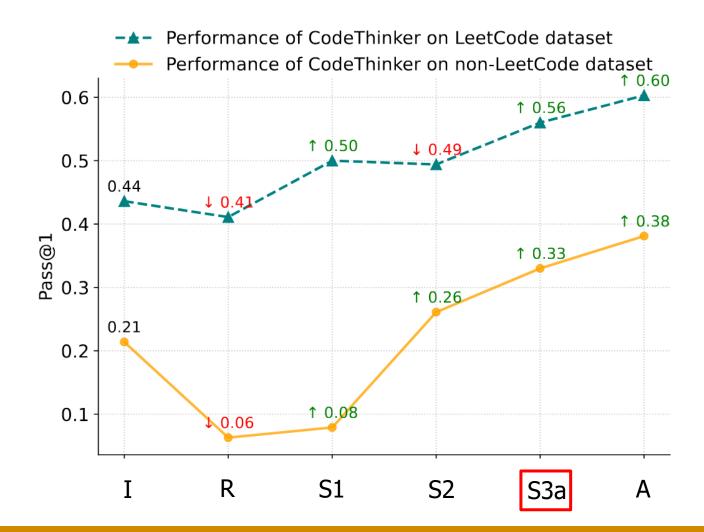
CodeThinker shows **strong generalization ability** to problems from **non-LeetCode platforms**, achieving significant improvements

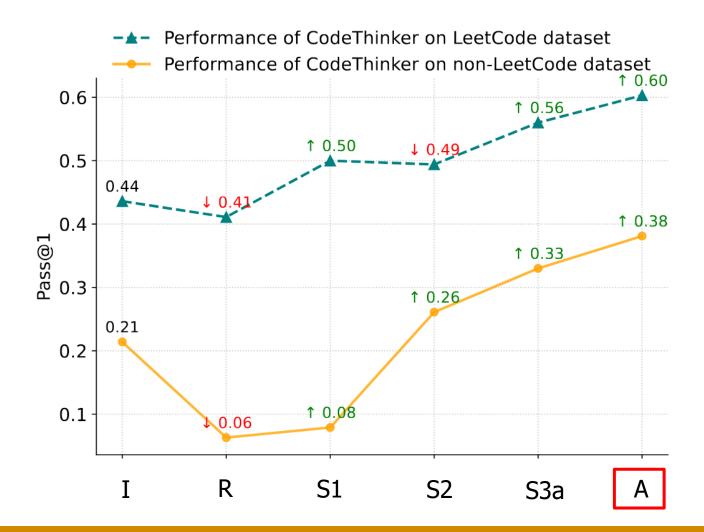




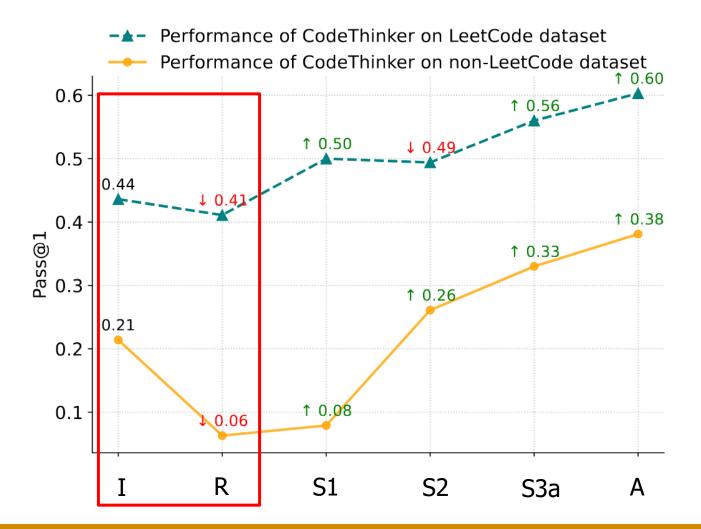






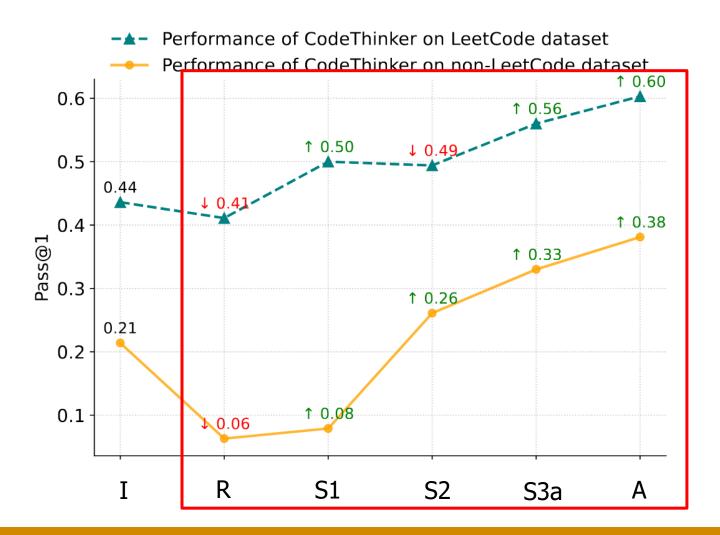


*I: Initial checkpoint; R: Fine tune using raw LeetCode discussion posts; S1: Step 1 only; S2: Step 1+2 only; S3a: Step 1+2+3a only; A: All steps of RT-Distiller



I vs. R: Training with raw LeetCode discussion posts results in performance drop

*I: Initial checkpoint; R: Fine tune using raw LeetCode discussion posts; S1: Step 1 only; S2: Step 1+2 only; S3a: Step 1+2+3a only; A: All steps of RT-Distiller



I vs. R: Training with raw LeetCode discussion posts results in performance drop

R vs. S1: Synthesizing missing information in LeetCode discussion posts helps

S1 vs. S2: Applying code perturbation improves generalization to non-LeetCode

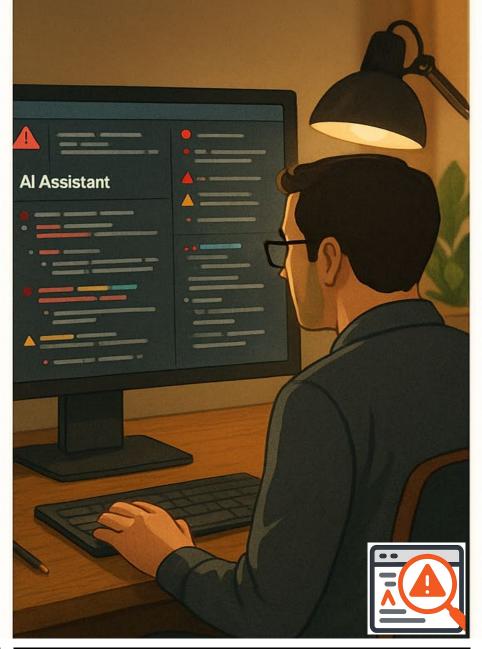
S2 vs. S3a: Introducing SDLC-inspired structure to reasoning traces helps

S3a vs. A: Adding iterative refinement considerations helps

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Engineering structured reasoning traces help LLM reasoning for code generation







Code

Critique

Cure

Contrastive Patterns Can Help AI Reasoning

Classification of Software Behaviors for Failure Detection: A Discriminative Pattern Mining Approach

David Lo Singapore Management University davidlo@smu.edu.sg

Jiawei Han University of Illinois at Urbana-Champaign hanj@cs.uiuc.edu Hong Cheng
Chinese University of Hong Kong
hcheng@se.cuhk.edu.hk

Siau-Cheng Khoo and Chengnian Sun National University of Singapore {khoosc,suncn}@comp.nus.edu.sg



Distills rich discriminative (contrastive) patterns for AI-powered failure detection (aka. test oracle generation); early SE paper in a top AI venue

Distilling **Contrastive** Reasoning Trace Pairs

R2VUL: Learning to Reason about Software Vulnerabilities with Reinforcement Learning and Structured Reasoning Distillation

Martin Weyssow^{1*}, Chengran Yang¹, Junkai Chen¹, Ratnadira Widyasari¹, Ting Zhang¹, Huihui Huang¹, Huu Hung Nguyen¹, Yan Naing Tun¹, Tan Bui¹, Yikun Li¹, Ang Han Wei², Frank Liauw², Eng Lieh Ouh¹, Lwin Khin Shar¹, David Lo¹

¹Singapore Management University ²GovTech Singapore



Engineers contrastive reasoning trace pairs to help LLM reason about vulnerabilities

TOSEM 2025

Vulnerability Detection with LLMs

- Vulnerability detection demands a binary judgement:
 - Is the input code safe or vulnerable?

Large Language Model for Vulnerability Detection and Repair: Literature Review and the Road Ahead

XIN ZHOU, School of Computing and Information Systems, Singapore Management University, Singapore, Singapore

SICONG CAO and XIAOBING SUN, Yangzhou University, Yangzhou, China DAVID LO, School of Computing and Information Systems, Singapore Management University, Singapore, Singapore





Vulnerability Detection with LLMs

Limited efficacy

ICSE 2024

Large Language Model for Vulnerability Detection: Emerging Results and Future Directions

Xin Zhou, Ting Zhang, and David Lo School of Computing and Information Systems, Singapore Management University, Singapore {xinzhou.2020,tingzhang.2019}@phdcs.smu.edu.sg,davidlo@smu.edu.sg



From a developer viewpoint, a binary judgement is also not sufficient:

Why is this input code vulnerable or safe?
What is the mechanism of a vulnerability and its impact?





R2Vul: Beyond Binary Judgement

Fine-tune an LLM to **better detect vulnerabilities** and generate **structured reasoning**.

 The LLM outputs a structured reasoning covering key aspects of code safety and vulnerability.

Vulnerable Code

- 1. Discuss specific code constructs responsible for the vulnerability
- 2. Explain the mechanism of the vulnerability
- 3. Discuss its potential impact
- 4. Relate the vulnerability to a relevant CWE

Safe Code

- 1. Discuss key aspects contributing to code safety
- 2. Discuss the absence of key vulnerabilities
- 3. Provide evidence-based justification why a code is safe

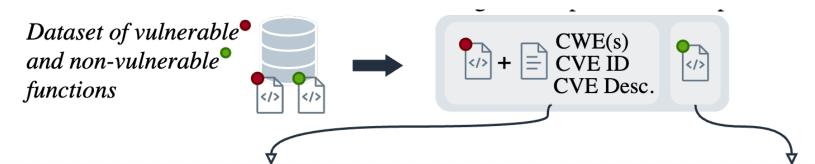


Step 1: Generate Contrastive Reasoning Trace Pairs

- Given a labeled dataset $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N$
 - (x_i : function, $y_i \in \{Vuln, Safe\}$)
- Prompt a base LLM to generate:
 - A **valid** reasoning r_i^+ conditioned on the *true* sample label y_i
 - A **flawed** reasoning r_i^- conditioned on the *flipped* sample label $-y_i$
 - $\rightarrow \mathcal{D} = \{(x_i, y_i, r_i^+, r_i^-)\}_{i=1}^N = \text{preference dataset}$



Step 1: Generate Contrastive Reasoning Trace Pairs



```
The following function has been flagged as vulnerable.

[ `{ lang }

[ function }

[ This function contains a nulnerability associated with the
```

This function contains a vulnerability associated with the following CWE(s):

```
{ cwe_list }.
```

Specifically, it is linked to { cve_id }, which is described as follows: { cve_description }

Given this information, generate a detailed and coherent thought process ...

- 1. Specific Code Constructs: Identify parts [...]
- 2. Mechanism of the Vulnerability: Explain how [...]
- 3. **Potential Impact**: Describe the consequences [,,,]
- 4. Contextual Relevance: Relate to CWE(s) and CVE [...]

The following function has been flagged as **non-vulnerable**.

```
`{ lang }
{ function }
```

This function has been reviewed and determined to not contain any known vulnerabilities.

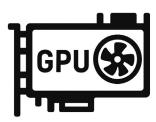
Given this information, generate a detailed and coherent thought process ...

- 1. Analysis of Code Safety: [...]
- 2. Absence of Common Vulnerabilities: [...]
- 3. Validation of the Non-Vulnerable Label: [...]

Step 2: Use Contrastive Reasoning Trace Pairs

- Combines supervised fine-tuning (SFT) and odds-ratio (OR) losses
 - → SFT: trains the model to generate high-quality structured reasoning
 - → OR: distinguish valid vs. flawed reasoning
- Additional feature: Distill smaller models
 - → constraints from deployment environment









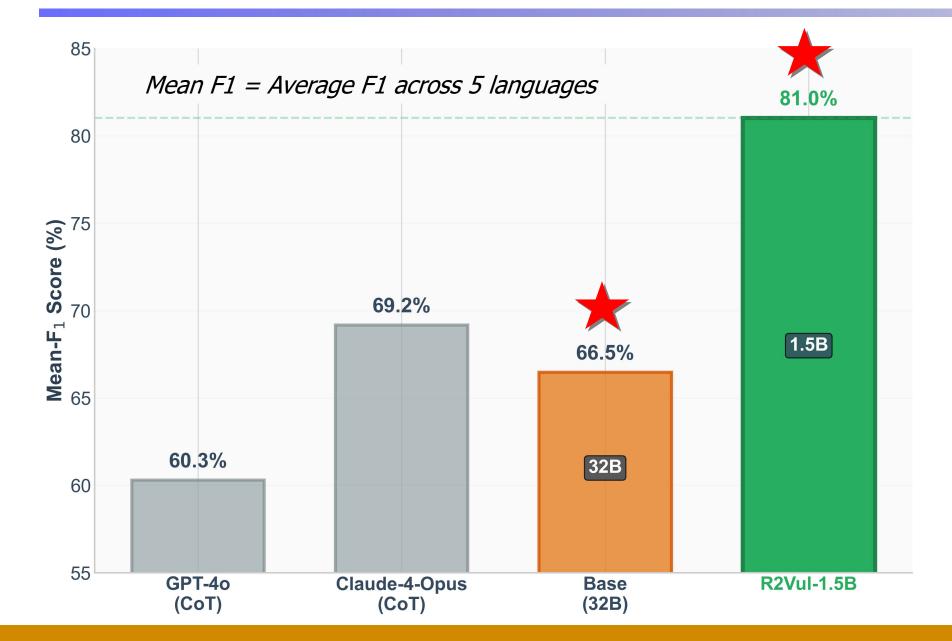
Experiment Details

- Step 1:
 - Base LLM: Qwen2.5-Coder-Instruct with 32B parameters
 - About **18,000 pairs** of contrastive traces
 - **Five** programming languages: C#, JavaScript, Java, Python, and C

- Step 2:
 - Target LLMs: Qwen2.5-Coder-Instruct with 0.5B, 1.5B, and 7B parameters

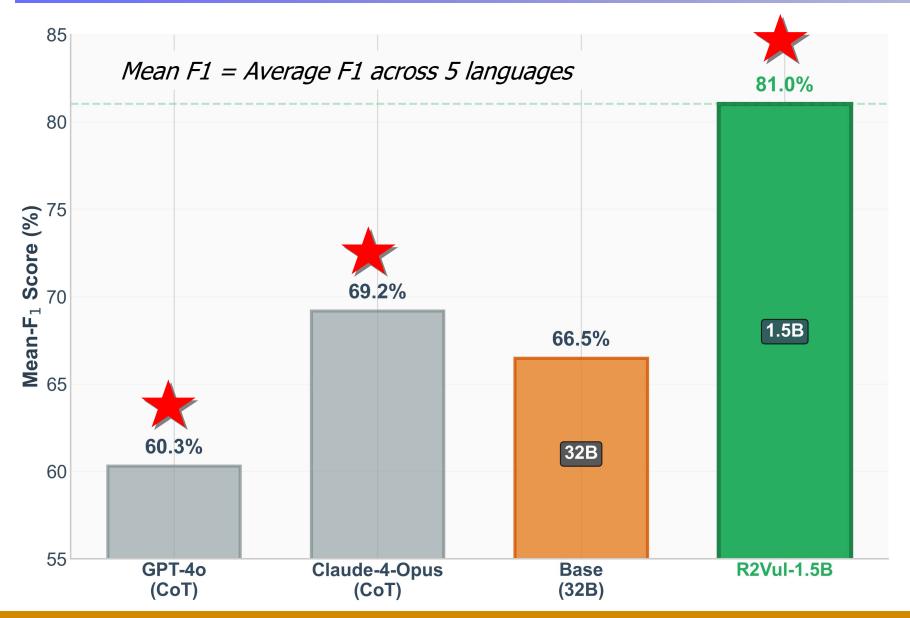


Main Results: Detection Performance



R2Vul-1.5B wins over Base (32B)

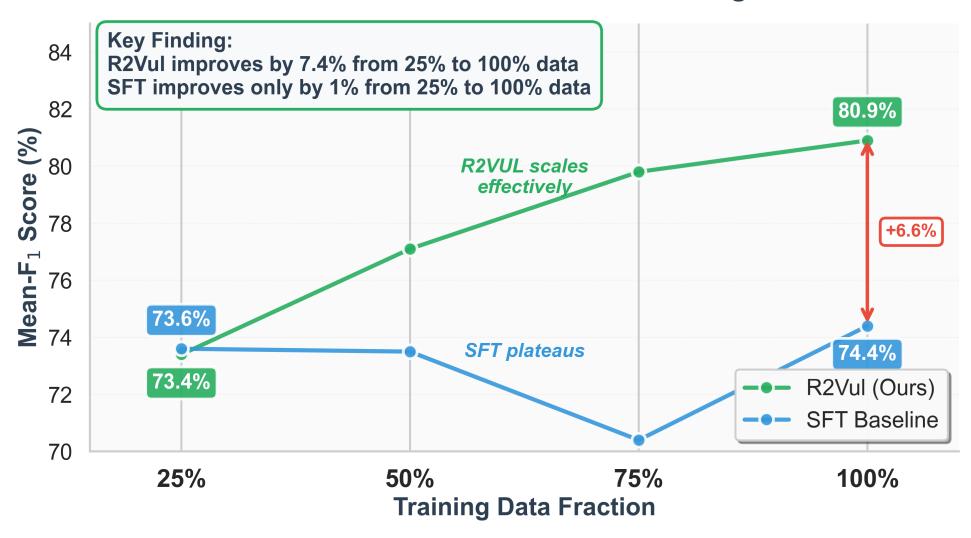
Main Results: Detection Performance



R2Vul-1.5B wins over commercial LLMs

R2Vul vs. SFT: Impact of Contrastive Reasoning Trace Pairs

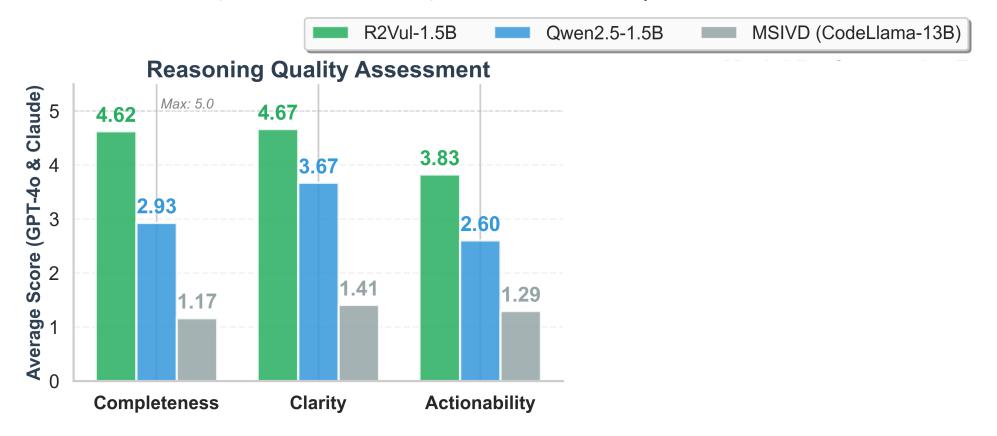
R2Vul Scales Better with More Training Data



Reasoning Quality Assessment

Baselines: Qwen2.5-1.5B-Coder-Instruct and MSIVD (CodeLlama-13B): reasoning-based LLM [1]

Evaluators: GPT-4o, Claude-3.5-Sonnet, and two human experts





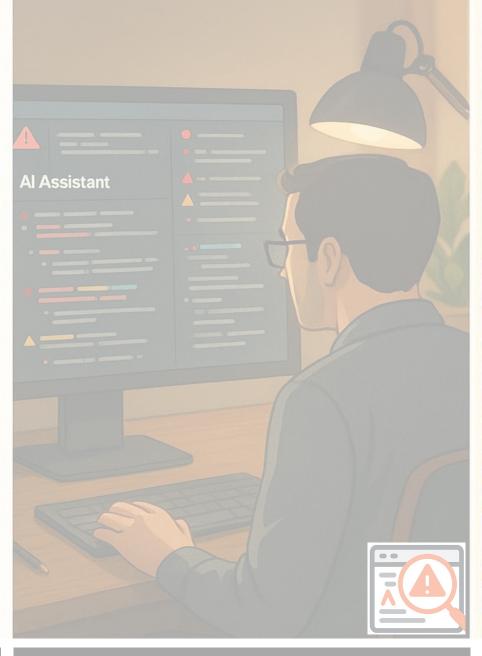




Engineering contrastive reasoning trace pairs help LLM reasoning for vulnerability detection

Critique







Code

Critique

Cure

Integrating Diverse Inputs from Diverse Sources Can Help AI

SANER 2016

History Driven Program Repair

Xuan-Bach D. Le, David Lo School of Information Systems Singapore Management University {dxb.le.2013,davidlo}@smu.edu.sg Claire Le Goues School of Computer Science Carnegie Mellon University clegoues@cs.cmu.edu



First MSR-powered APR work: mines hundreds of GitHub repositories for repair patterns serving as augmented inputs to test cases for search-based automated program repair (APR); most-cited SANER 2016 paper that inspired Facebook



Integrating Diverse Inputs for LLM-Powered Vulnerability Repair

Out of Sight, Out of Mind: Better Automatic Vulnerability Repair by Broadening Input Ranges and Sources

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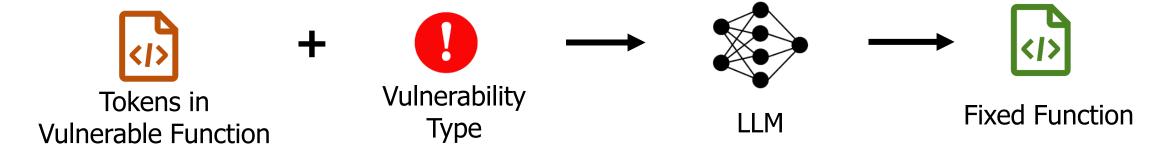
First LLM-powered automated program repair work that (i) links vulnerable code to LLM-enriched CWE knowledge and (ii) leverages AST contents to double the efficacy of prior work

Computing and Information Systems



Integrating Diverse Inputs for LLM-Powered Vulnerability Repair

Previous solutions:



Many **other inputs** have not been leveraged:

Abstract Syntax Tree AST Parser LLM

CWE Knowledge

Vulnerability Type





→ CWE Description

Simple VulnerableCode Examples

→ Detailed Analyses

VulMaster's Design

Data-Centric Innovations



Multi-LLM Collaboration

Incorporate AST

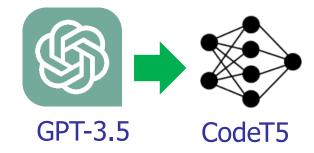


Incorporate CWE knowledge



Address lengthy inputs





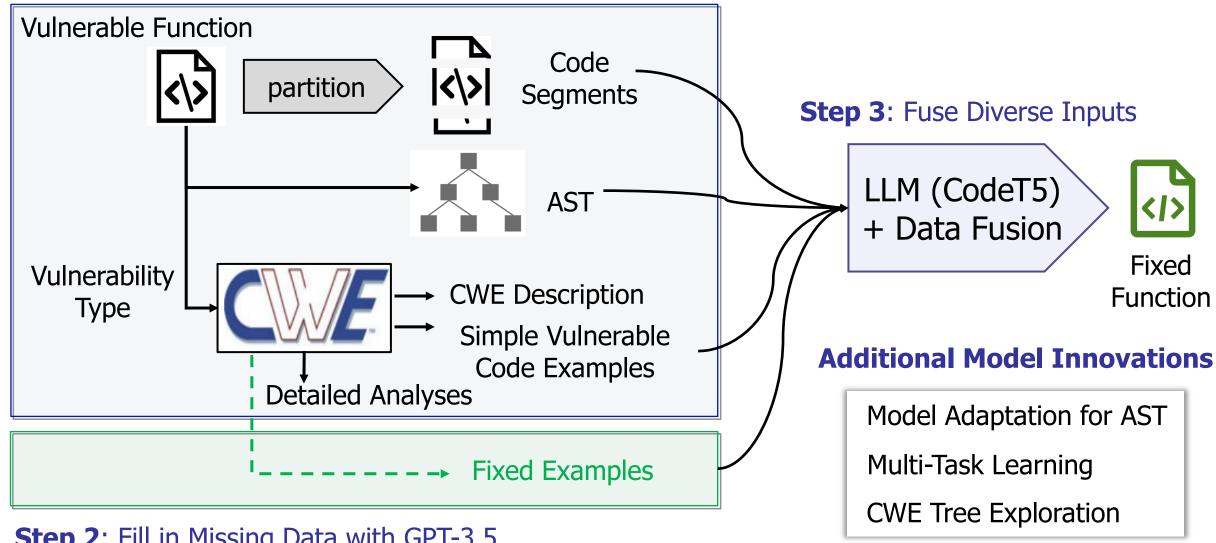
2x Fixed Vulnerabilities

Computing and Information Systems



Overall Framework

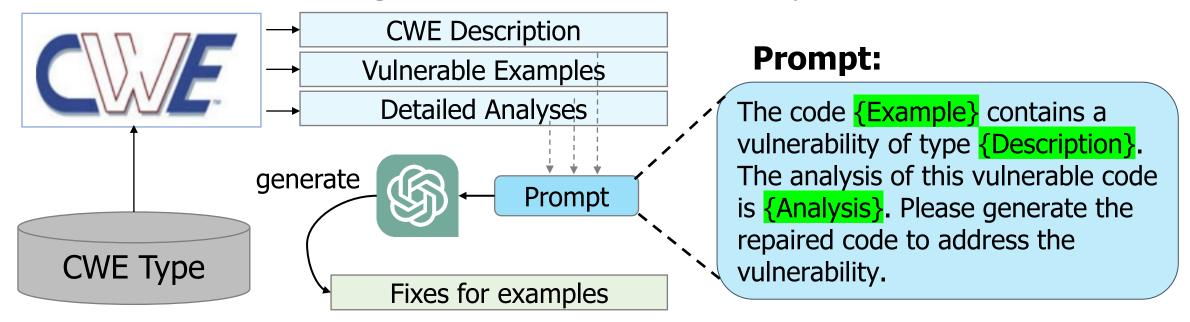
Step 1: Collect Diverse Inputs



Step 2: Fill in Missing Data with GPT-3.5

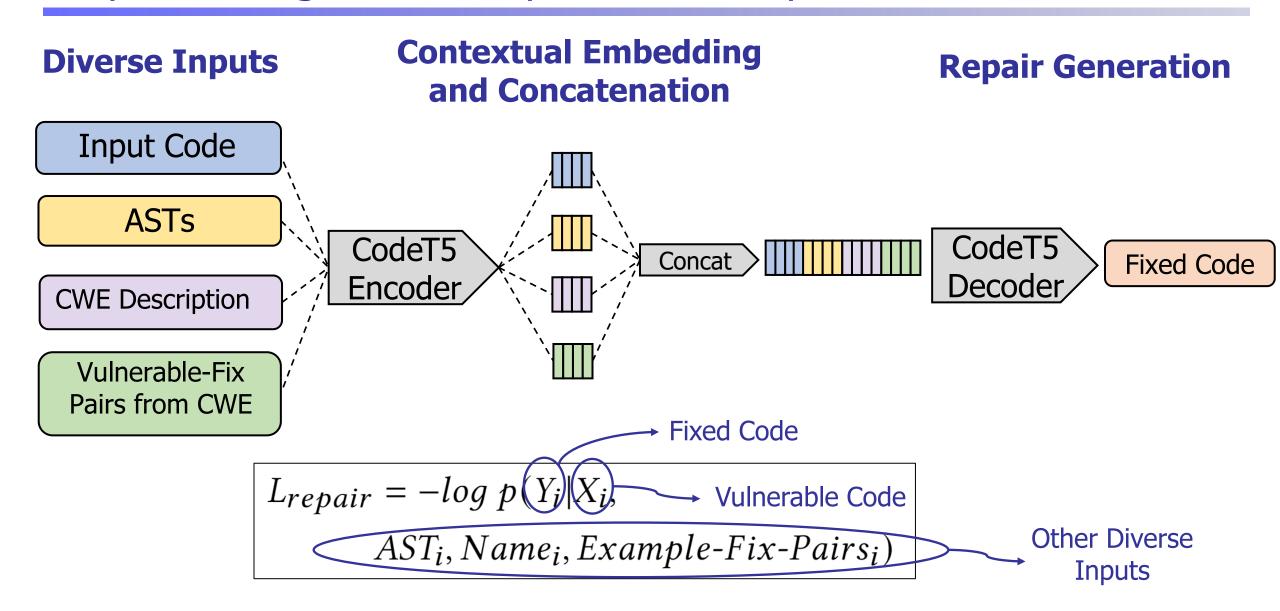
Step 2: Fill In Missing Data with GPT-3.5

- General-purpose LLMs are effective for
 - Fixing simple (toy) vulnerable examples when *detailed analysis* is given.
- Thus, we use GPT-3.5 to generate the fixed CWE examples:



Note: Real vulnerability fixes are not simple or come with detailed analysis

Step 3: Fusing Diverse Input Data Components

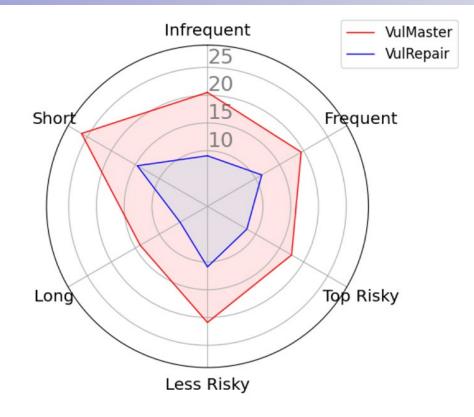


Results: Comparisons with SOTA

Main Results

| Type | Approach | EM | BLEU |
|---------------|-----------------------|------|------|
| LLM | GPT-3.5 [55] | 3.6 | 8.8 |
| | GPT-4 [56] | 5.3 | 9.7 |
| task-specific | VRepair [9] | 8.9 | 11.3 |
| | VulRepair [19] (SOTA) | 10.2 | 21.3 |
| Ours | VulMaster | 20.0 | 29.3 |

- VulMaster doubles the Exact Match (EM) score
- VulMaster consistently outperforms for vulnerabilities of different characteristics



- *long/short*: the length of the code
- *frequent/infrequent*: the vulnerability type frequencies
- *top/less risky*: top 10 most dangerous CWEs or not



Latest Extension

More Diverse Data

+

Reinforcement Learning

Incorporate AST



Incorporate CWE knowledge



Incorporate Data Flow



Reasoning steps for repair





Qwen-2.5 7B Instruct

+34.96%
Performance Gain

Please stay tuned: Paper will be released on arXiv soon







Engineering holistic representation from diverse inputs and sources help LLM reasoning for repair

Cure





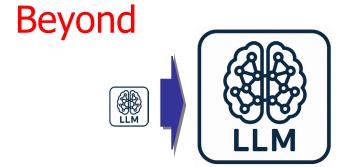


Code

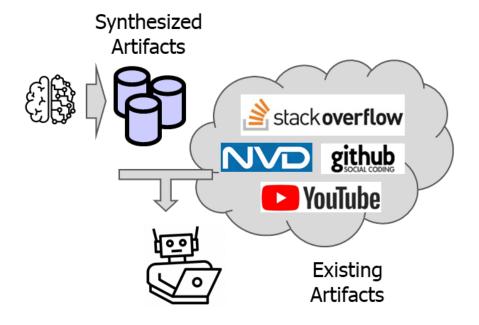
Critique

Cure

"How Can We **Systematically Engineer Software Artifacts** to Build Better LLM4SE Bots?"



Prompt Engineering



- We want to elevate the data:
 - enriching it, restructuring it, contrasting it, and linking it in ways that promote deeper reasoning
- And utilizing them effectively to train LLMs to reason and do better for specific SE tasks



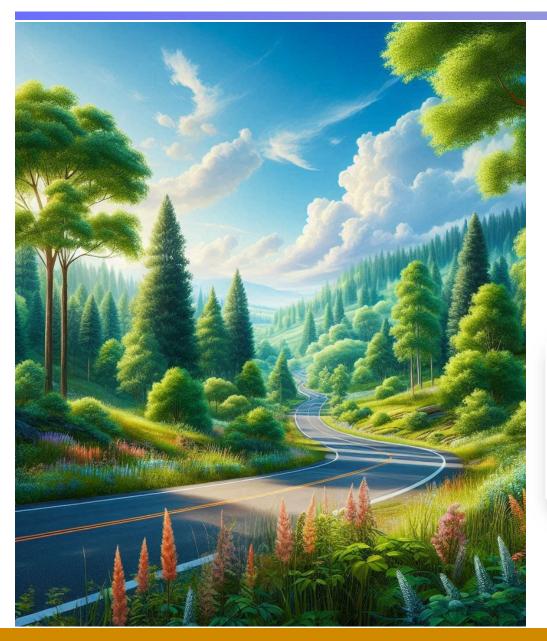
"Because in software engineering, how we craft the data is how we shape the intelligence"







Road Ahead



Multi-Agent LLM4SE

Real-world problems demand "synergistic collaboration". Multi-agent LLM4SE transforms isolated agents into a coordinated group of experts.

LLM-Based Multi-Agent Systems for Software Engineering: Literature Review, Vision and the Road Ahead

JUNDA HE, Singapore Management University, Singapore CHRISTOPH TREUDE, Singapore Management University, Singapore DAVID LO, Singapore Management University, Singapore

TOSEM 2025

Multi-Agent LLM4SE: Vulnerability Detection

Let the Trial Begin: A Mock-Court Approach to Vulnerability Detection using LLM-Based Agents

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Eng Lieh Ouh elouh@smu.edu.sg Singapore Management University Singapore

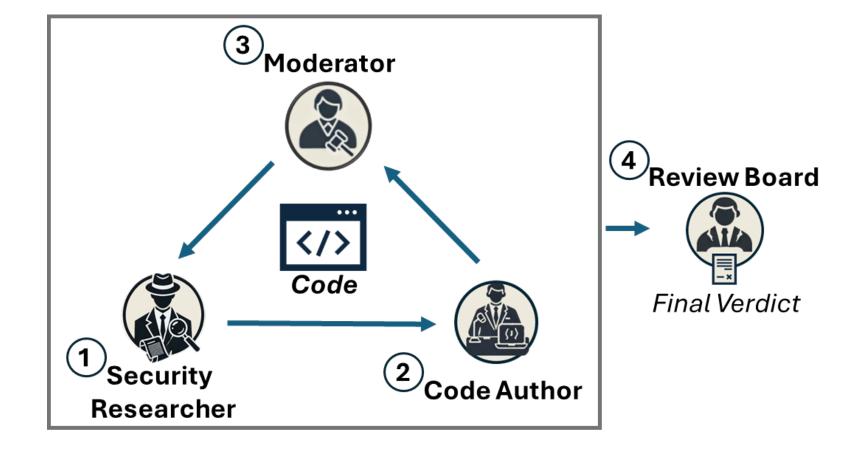
David Lo davidlo@smu.edu.sg Singapore Management University Singapore







Multi-Agent LLM4SE: VulTrial





VulTrial's Design

```
TfLiteStatus EvalGatherNd(TfLiteContext* context,
                          const TfLiteTensor* params,
                          const TfLiteTensor*comment indices,
                          TfLiteTensor* output) {
  // Vulnerability: There's no check to ensure that 'indices' are
  // within valid bounds for 'params'. Negative or out-of-range
  // indices lead to out-of-bounds reads.
  switch (params->type) {
    case kTfLiteFloat32:
      return GatherNd<float, IndicesT>(params, indices, output);
 // ... other types ...
    default:
      context->ReportError(
          context, "Params type '%s' not supported by gather_nd.",
          TfLiteTypeGetName(params->type));
      return kTfLiteError;
```

Example of Vulnerable Code CWE-125 (Out-of-bounds Read)

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Security Researcher vulnerability: Out-of-Bounds Read reason: The function `EvalGatherNd` does not perform any bounds checking on the `indices` tensor. [...]. impact: Exploiting this vulnerability could lead to information disclosure, [...] could be leveraged for further attacks such as Denial of Service (DoS). vulnerability: Type Handling reason: [...] if the new type is not properly validated [...], it could lead to unexpected behavior or crashes. impact: [...] could be exploited by an attacker to cause a DoS

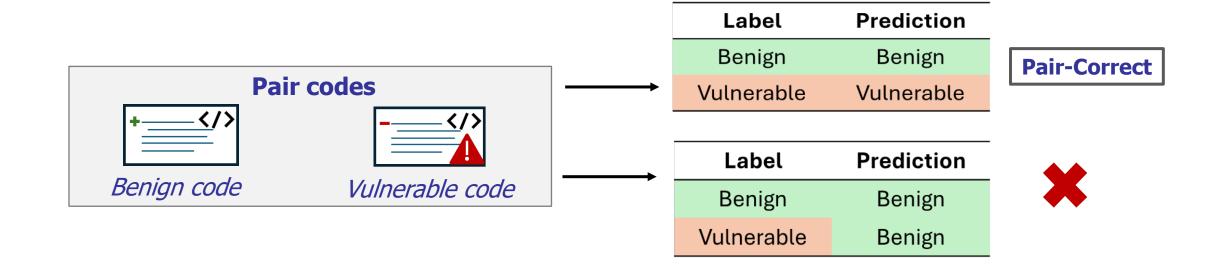
| Code A | luthor | | | | |
|---------------|--|--|--|--|--|
| vulnerability | :Out-of-Bounds Read | response : mitigation | | | |
| reason | :The concern regarding out-of-bounds reads is valid. [] I propose implementing a bounds checking []. | | | | |
| vulnerability | : Type Handling | response : refutation | | | |
| reason | : [] any unsupported type will reports an error. This is a stand | be caught in the default case, which dard practice []. | | | |

Moderator researcher summary: [...] could result in information disclosure [...] author summary : The author acknowledges the concern [...].

| | | | Review Board | |
|---------------|---|---------------|-----------------|----|
| vulnerability | : Out-of-Bounds Read | decision: | valid | -x |
| severity | : high | action : | fix immediately | |
| reason | : [] function does not perform bounds checking [] | | | |
| vulnerability | : Type Handling | decision : | partially valid | |
| severity | : medium | action : | monitor | |
| reason | : [] potential for new tensor t | ypes w/o prop | er handling[] | |
| | | | | |

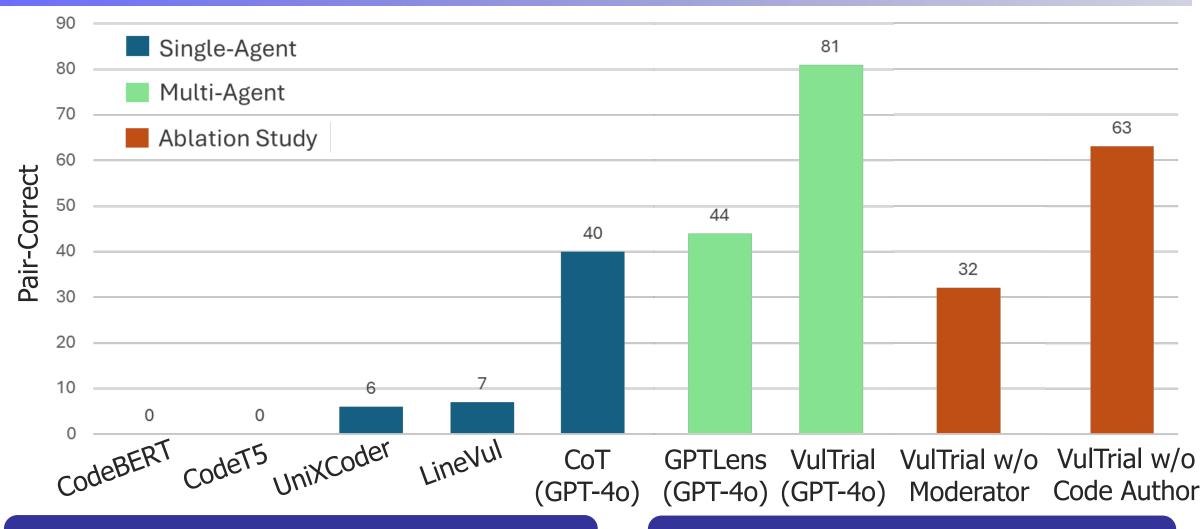
Evaluation Settings

Evaluation on PrimeVul Pair [1] data.



[1] Yangruibo Ding, Yanjun Fu, Omniyyah Ibrahim, Chawin Sitawarin, Xinyun Chen, Basel Alomair, David A. Wagner, Baishakhi Ray, Yizheng Chen: Vulnerability Detection with Code Language Models: How Far are We? ICSE 2025: 1729-1741

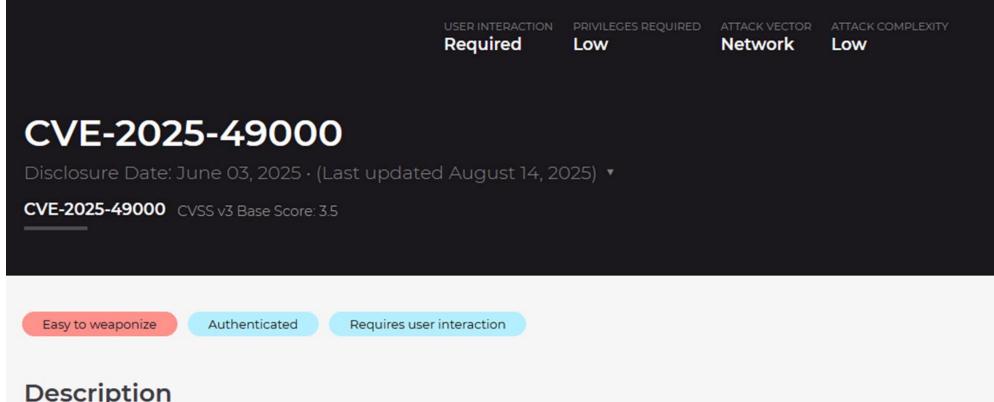
Evaluation Results



Multi-agent methods **outperform** the single-agent methods

Each agent in VulTrial is **necessary** to achieve the best performance

VulTrial in the Wild



Description

InvenTree is an Open Source Inventory Management System. Prior to version 0.17.13, the skip field in the built-in label-sheet plugin lacks an upper bound, so a large value forces the server to allocate an enormous Python list. This lets any authenticated label-printing user trigger a denial-of-service via memory exhaustion, the issue is fixed in versions 0.17.13 and higher. No workaround is available aside from upgrading to the patched version.





Related Paper @ ICSME 2025

SAEL: Leveraging Large Language Models with Adaptive Mixture-of-Experts for Smart Contract Vulnerability Detection

Lei Yu^{†‡1}, Shiqi Cheng^{†1}, Zhirong Huang^{†‡}, Jingyuan Zhang^{†‡}, Chenjie Shen^{†‡},

Junyi Lu^{†‡}, Li Yang^{†*}, Fengjun Zhang^{†§*}, Jiajia Ma[†]

[†]Institute of Software, Chinese Academy of Sciences, Beijing, China

[‡]University of Chinese Academy of Sciences, Beijing, China

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shenchenjie22@mails.ucas.ac.cn, {yangli2017, fengjun, majiajia}@iscas.ac.cn



Session 12 - Security 1

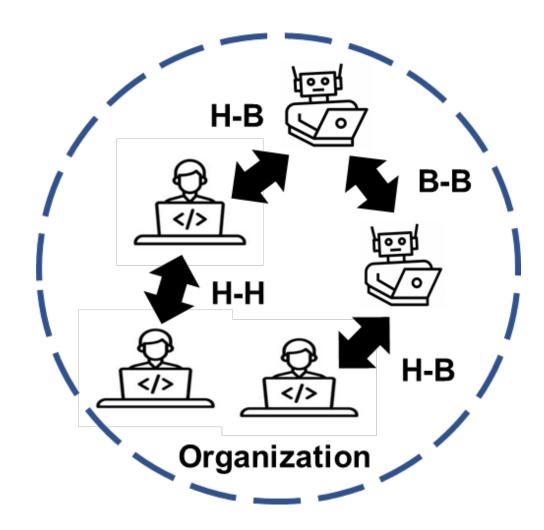
Thu 11 Sep 2025 15:45 - 16:00 Case Room 260-057

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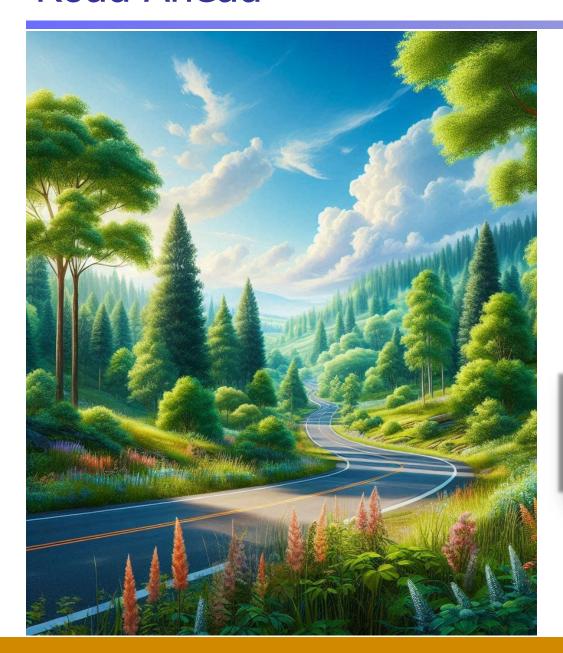
Towards Full Multi-Agent Solution: Humans (H) and Bots (B)







Road Ahead



Greening LLM4SE

LLM4SE solutions are large, slow, and not green, introducing much cost, latency, and carbon footprint

TOSEM 2025

Efficient and Green Large Language Models for Software Engineering: Vision and the Road Ahead

JIEKE SHI, ZHOU YANG, and DAVID LO, Singapore Management University, Singapore



Greening LLM4SE: Three **S**trategies



Stop

Simplify

Shrink

Greening LLM4SE

ISSTA 2024



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Stop



Improve code generation speed by up to 4.5x by **terminating inference early**





Greening LLM4SE



Simplify



Al Coders Are Among Us: Rethinking Programming Language **Grammar Towards Efficient Code Generation**

Zhensu Sun Singapore Management University Singapore zssun@smu.edu.sg

Xiaoning Du* Monash University Australia xiaoning.du@monash.edu

Zhou Yang Singapore Management University Singapore zyang@smu.edu.sg

Li Li **Beihang University** China lilicoding@ieee.org

David Lo Singapore Management University Singapore davidlo@smu.edu.sg



Won ACM SIGSOFT Distinguished Paper Award

First work to propose a programming language grammar for AI agents





Greening LLM4SE



Shrink

ESEC/FSE 2023

Towards Greener Yet Powerful Code Generation via Quantization: An Empirical Study

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Reduce size by 3x and latency by 50% by **quantizing parameter** into int8

School of Computing and Information Systems



Related Paper @ ICSME 2025

Is Quantization a Deal-breaker? Empirical Insights from Large Code Models

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Session 2 - Quality Assurance 1

Wed 10 Sep 2025 10:45 - 11:00 Case Room 260-057

Computing and Information Systems



Many Open Problems wrt. Non-Functional Properties



Robustness, Security, Privacy, Explainability, Efficiency, and Usability of Large Language Models for Code

ZHOU YANG, Singapore Management University, Singapore

ZHENSU SUN, Singapore Management University, Singapore

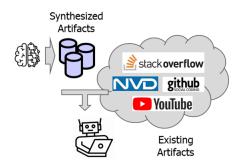
TERRY ZHUO YUE, Singapore Management University, Singapore

PREMKUMAR DEVANBU, Department of Computer Science, UC Davis, USA

DAVID LO, Singapore Management University, Singapore



"How Can We **Systematically Engineer Software Artifacts** to Build Better LLM4SE Bots?"



Beyond



Prompt Engineering

- We want to **elevate the data**:
 - enriching it, restructuring it, contrasting it, and linking it in ways that promote deeper reasoning
- And utilizing them effectively to train LLMs to do better for SE tasks



Engineering **structured reasoning traces** help LLM reasoning
for code generation

Code





Engineering contrastive reasoning trace pairs help LLM reasoning for vulnerability detection



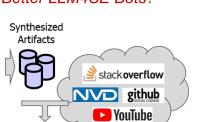
Engineering **holistic** representation from **diverse inputs and sources** help LLM reasoning for repair

Cure

SINGAPORE MANAGEMENT UNIVERSITY

Critique

"How Can We Systematically Engineer Software Artifacts to Build Better LLM4SE Bots?"



Existing Artifacts Beyond



Prompt Engineering

We w



Road Ahead



Real-world problems demand "synergistic

collaboration" and multi-agent AI transforms isolated AI into coordinated

Multi-Agent LLM4SE

experts.

LLM-Based Multi-Agent Systems for Software Engineering: Literature Review, Vision and the Road Ahead

JUNDA HE, Singapore Management University, Singapore CHRISTOPH TREUDE, Singapore Management University, Singapore DAVID LO, Singapore Management University, Singapore

TOSEM 2025



Engine

And I

LLMs

trace pairs help LLM reasoning for vulnerability detection

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Critique

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Acknowledgements





OUB Chair Professorship Fund





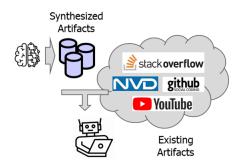




Computing and Information Systems



"How Can We **Systematically Engineer Software Artifacts** to Build Better LLM4SE Bots?"



Beyond



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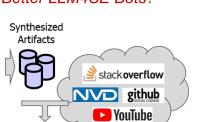
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"How Can We Systematically Engineer Software Artifacts to Build Better LLM4SE Bots?"



Existing Artifacts Beyond



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Road Ahead



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