Are Large Language Models Robust in Understanding Code Against Semantics-Preserving Mutations?

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- LLMs are widely used, and often blindly, with developers placing significant trust in their capabilities [Oh et al., 2024].

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However, this growing reliance on LLMs for coding tasks raises a fundamental question:

 \bullet To what extent do $\rm LLMs$ truly understand code and the underlying semantics of programs?

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 just reflect pattern recognition over code syntax rather than genuine semantic
 understanding [Petrov et al., 2025].
- If LLMs outputs are simply the result of statistical associations, then their reliability in critical development tasks could be overestimated [Gu et al., 2024].
- In other domains, such as mathematical competitions [Petrov et al., 2025], LLMs tend to provide accurate predictions, but based on flawed reasoning.

```
def minPossibleSum(n:int, target:int)->int:
    i = 1
    arr = {1}
    while len(arr) < n:
        i += 1
    if target - i not in arr:
        arr.add(i)
    return sum(arr)</pre>
```

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    i = 1
    arr = {1}
    while len(arr) < n:
        i += 1
    if target - i not in arr:
        arr.add(i)
    return sum(arr)</pre>
```

Given two integers n and target, function minPossibleSum finds the sum of an array arr such that:

- len(arr) == n;
- all elements in arr are distinct positive integers;
- $\sharp_0^{n-1}(i,j)$: arr[i] + arr[j] == target;

```
def minPossibleSum(n:int, target:int)->int:
    i = 1
    arr = {1}
    while len(arr) < n:
        i += 1
    if target - i not in arr:
        arr.add(i)
    return sum(arr)
    assert minPossibleSum(n=1,target=1)==????</pre>
```

LLMs for code (LLMCs)

Now imagine we ask $$\rm QWEN2.5\text{-}CODER,$$ to predict this function's output, and to explain its reasoning.

Qwen2.5-Coder's Answer

Let's walk through the execution of the code step-by-step to understand how the output is produced.

```
The function `minPossibleSum` takes
two parameters: `n` and `target`.

In this case, `n = 1` and `target = 1`.

1. The variable `i` is initialized to 1.

2. A set `arr` is initialized with the
```

3. The while loop condition checks if the length of `arr` is less than `n`. Since `n` is 1, the loop will run once.

element 1

4. Inside the loop, `i` is incremented to 2.

```
def minPossibleSum(n, target):
    i = 1
    arr = {1}
    while len(arr) < n:
        i += 1
        if target - i not in arr:
            arr.add(i)
    return sum(arr)
assert minPossibleSum(n=1,target=1)==????</pre>
```

Qwen2.5-Coder's Answer

```
5. The condition `if target - i not in
arr is checked. Here, 'target - i'
                                               def minPossibleSum(n, target):
is 1 - 2, which equals -1.
                                                   i = 1
Since `-1` is not in the set `arr`, the
                                                   arr = \{1\}
condition is true.
                                                   while len(arr) < n:
                                                       i += 1
6. The number 2 is added to the set 'arr'. 5
                                                       if target - i not in arr:
                                            6
7. The loop ends because the length of
                                                          arr.add(i)
`arr` is now `n`.
                                                   return sum(arr)
8. The function returns the sum of the
                                               assert minPossibleSum(n=1,target=1)==????
elements in `arr`. which is 1 + 2 = 3`.
Therefore, the assertion should be:
[ANSWER] assert minPossibleSum(1, 1) == 3[/ANSWER]
```

Providing some feedback to Qwen2.5-Coder

```
Your previous output prediction was INCORRECT!
Try again. Complete the initial program
assertion containing the execution output
corresponding to the given input in [ANSWER]
and [/ANSWER] tags.
For example, the answer to
'''assert sumEvenNumbers([1.2.3.4])==???'''
would be
[ANSWER]
assert sumEvenNumbers([1.2.3.4]) == 6
[/ANSWER]
Please complete the assertion and explain
your reasoning for your new prediction,
using no more than 1000 tokens.
```

Qwen2.5-Coder's Answer

```
Given n = 1 and target = 1:
There seems to be a
                                 - Initially, `arr = 1`.
misunderstanding in the
                                 - The loop runs once because `len(arr) < n`
explanation. Let's
                                 (1 < 1) is false.
re-evaluate the logic:
                                 - Therefore, the loop does not add any new
- Initially, `arr` contains {1}
- The loop runs while the length elements to `arr`. Thus, the final `arr`
                                 remains '1', and the sum is '1'.
of `arr` is less than `n`.
- In each iteration, `i` is
incremented, and if `target - i` Therefore, the correct assertion should be:
                                 [ANSWER]assert minPossibleSum(1, 1) == 1[/ANSWER]
is not in `arr`, `i` is added
to `arr`.
```

Qwen2.5-Coder's Answer

```
Given `n = 1` and `target = 1`:
There seems to be a
                                 - Initially, `arr = 1`.
misunderstanding in the
                                 - The loop runs once because `len(arr) < n`
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- Initially, `arr` contains {1}
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                                 remains '1', and the sum is '1'.
of `arr` is less than `n`.
- In each iteration, `i` is
incremented, and if `target - i` Therefore, the correct assertion should be:
                                 [ANSWER] assert minPossibleSum(1, 1) == 1[/ANSWER]
is not in `arr`. `i` is added
to `arr`.
```

Our feedback was sufficient to guide Qwen2.5-Coder toward a logically sound reasoning process and to correctly predict the output!

LLMs' Robustness

LLMs for code (LLMCs)

 When QWEN2.5-CODER and SEMCODER are presented with this semantically equivalent function, both models fail to provide the correct output;

```
def minPossibleSum(n, target):
    i = 1
    eAJMfVcq = {1}
    while len(eAJMfVcq) < n:
        i += 1
    if target - i not in eAJMfVcq:
        eAJMfVcq.add(i)
    return sum(eAJMfVcq)</pre>
```

LLMs' Robustness

LLMs for code (LLMCs)

- When QWEN2.5-CODER and SEMCODER are presented with this semantically equivalent function, both models fail to provide the correct output;
- Both models also fail to construct logically sound reasoning, even after five rounds of interactive feedback.

```
1  def minPossibleSum(n, target):
2     i = 1
3     eAJMfVcq = {1}
4     while len(eAJMfVcq) < n:
5          i += 1
6         if target - i not in eAJMfVcq:
7         eAJMfVcq.add(i)
8     return sum(eAJMfVcq)</pre>
```

In this work

 Conduct a manual expert evaluation to assess whether LLMs' code output predictions are based on logically sound reasoning, flawed reasoning, or mere guesses.

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- Conduct a manual expert evaluation to assess whether LLMs' code output predictions are based on logically sound reasoning, flawed reasoning, or mere guesses.
- Evaluate LLMs' output prediction stability across five different semantics-preserving code mutations.

Semantics-Preserving Code Mutation

Given a program P that is syntactically well-formed program, and it is semantically consistent with the test suite, i.e.,

$$\forall (t_{in}^i, t_{out}^i) \in T : P(t_{in}^i) = t_{out}^i.$$

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A semantics-preserving code mutation is a syntactic program transformation to P that generates a new program P_m by syntactically replacing a subset S_1 of P's statements $(S_1 \subseteq P)$ with another set of statements S_2 , such that

$$P_m = ((P \setminus S_1) \cup S_2)$$

and P_m is syntactically well-formed and semantically consistent with the original specification:

$$\forall (t_{in}^i, t_{out}^i) \in T : P_m(t_{in}^i) = t_{out}^i.$$

Semantics-Preserving Code Mutations

We introduce **five semantics-preserving code mutations** designed to syntactically modify Python programs without altering their semantics:

- variable renaming;
- comparison expression mirroring;
- swapping if-else statements;
- loop conversion
- partial loop unrolling.

Variable renaming

```
def f(nums):
                                      def f(nums):
                                        uoWIfiQc = 0
  sum = 0
                                        for n in nums:
  for n in nums:
    if n % 2 == 0:
                                          if n % 2 == 0:
                                           uoWIfiQc += n
      sum += n
                                          else:
    else:
                                           uoWIfiQc += 0
      sum += 0
                                        return uoWIfiQc
  return sum
```

Comparison Expression Mirroring

```
def f(nums):
                                      def f(nums):
  sum = 0
                                         sum = 0
  for n in nums:
                                         for n in nums:
    if n % 2 == 0:
                                           if 0 == n % 2:
      sum += n
                                             sum += n
                                    5
    else:
                                           else:
      sum += 0
                                             sum += 0
  return sum
                                         return sum
```

Swap If-Else Statements

```
def f(nums):
                                     def f(nums):
  sum = 0
                                       sum = 0
  for n in nums:
                                       for n in nums:
    if n % 2 == 0:
                                         if not n % 2 == 0:
                                           sum += 0
    sum += n
    else:
                                         else:
    sum += 0
                                           sum += n
  return sum
                                       return sum
```

For-to-While Loop Conversion

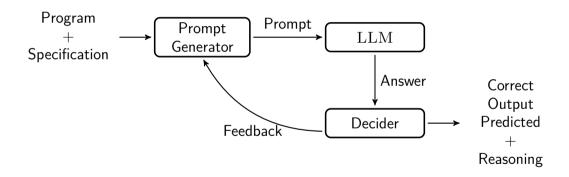
```
def f(nums):
    sum = 0
    for n in nums:
    if n % 2 == 0:
        sum += n
    else:
        sum += 0
    return sum
```

```
def f(nums):
     sum = 0
2
     i = 0
     while i < len(nums):
       n = nums[i]
       if n \% 2 == 0:
          sum += n
7
       else:
         sum += 0
       i += 1
10
     return sum
11
```

Partial Loop Unrolling

```
def f(nums):
                                                sum, i = 0, 0
                                           2
   def f(nums):
                                                while i < (len(nums)-1):
                                                  n = nums[i]
      sum = 0
                                                  if n % 2 == 0:
      i = 0
                                                  sum += n
      while i < len(nums):
                                                else:
        n = nums[i]
                                                 sum += 0
        if n % 2 == 0:
                                                  i += 1
                                                if len(nums) > i:
                                          10
          sum += n
                                                  n = nums[i]
                                          11
        else:
                                                  if n % 2 == 0:
                                          12
          sum += 0
                                                 sum += n
                                          13
        i += 1
10
                                          14
                                                  else:
                                                  sum += 0
                                          15
     return sum
11
                                                  i += 1
                                          16
                                          17
                                                return sum
```

LLM-Based Program Output Prediction



Prompt Example

Simulate the Execution: You are given a Python function and an assertion containing a function input. Complete the assertion containing the execution output corresponding to the given input in [ANSWER] and [/ANSWER] tags.

```
For example, the answer to
'''assert sumEvenNumbers([1,2,3,4])==???'''
would be
[ANSWER]
assert sumEvenNumbers([1,2,3,4]) == 6
[/ANSWER]
```

Please complete the assertion and explain your reasoning for your prediction, using no more than 1000 tokens.

```
python
def f(nums):
    # python function
assert f([1, 2, 3, 4, 5]) == ???
```

Prompt Example for Feedback

```
Your previous output prediction was INCORRECT!
Try again. Complete the initial program
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For example, the answer to
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```
compatible content of the conte
```

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- For each program mutation, we generate a separate transformed version of the benchmark, producing up to two mutated variants per program, each containing at most one mutation;
- We also check that the semantics of the original program is preserved in the mutated versions.

• Large Language Models (LLMs): We evaluated six different LLMs.

Experimental Setup

- Large Language Models (LLMs): We evaluated six different LLMs.
 - Five of these models are LLMCs, i.e., LLMs fine-tuned for coding tasks:
 - IBM's GraniteCode;
 - Google's CodeGemma;
 - Alibaba's QWEN2.5-CODER;
 - Mistral's MISTRAL;
 - SemCoder;

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 - SemCoder:
 - The other model is a general-purpose LLM: Meta's LLAMA3.2;
- Experiments were conducted using a timeout of **90s**.

Analysis of LLMs' Reasoning About Code

Large Language Models (LL	Ms) CodeGemma	GraniteCode	Qwen2.5-Coder	Mistral	SemCoder	Llama3.2
% Failed Predictions	61.38	65.97	38.00	68.06	51.98	58.87
% Correct Predictions	38.62	34.03	62.00	31.95	48.01	41.13

Expert Analysis of LLMs' Reasoning About Code

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% Correct Predictions	38.62	34.03	62.00	31.95	48.01	41.13
% Correct Guesses based on flawed reasoning	51.35	42.34	12.79	49.67	16.08	60.90
% Correct Predictions based on sound reasoning (> 1 it.)	3.78	14.72	8.76	_	_	14.22
% Correct Predictions based on sound reasoning $(= 1 \text{ it.})$	44.87	42.93	78.45	50.33	83.92	24.87

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% Correct Predictions based on sound reasoning (= 1 it.)	44.87	42.93	78.45	50.33	83.92	24.87

RQ1. Are Large Language Models (LLMs) truly reasoning about code semantics, or merely guessing likely answers?

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RQ2. Does the interactive querying process help LLMs arrive at correct predictions supported by logically sound reasoning?

LIVECODEBENCH

Large Language Models (LLMs)	F2W	MCE	Original Benchmark	RV	SIE	UL
CODEGEMMA	34.0 (-5)	33.0 (-6)	38.6	34.0 (-5)	34.0 (-5)	32.0 (-7)
GraniteCode	34.0 (+0)	34.0 (+0)	34.0	34.0 (+0)	33.0 (-1)	27.0 (-7)
Llama3.2	40.0 (-1)	38.0 (-3)	41.1	35.0 (-6)	34.0 (-7)	33.0 (-8)
Mistral	30.0 (-2)	33.0 (+1)	32.0	32.0 (+0)	33.0 (+1)	33.0 (+1)
QWEN2.5-CODER	57.0 (-5)	60.0 (-2)	62.0	62.0 (+0)	55.0 (-7)	60.0 (-2)
SemCoder	44.0 (-4)	48.0 (+0)	48.0	49.0 (+1)	42.0 (-6)	48.0 (+0)

Table 1: Output prediction correction rate of each LLM on LIVECODEBENCH when applying different code mutations: converting for to while loops (F2W), mirroring comparison expressions (MCE), renaming variables (RV), swap if-else statements (SIE), and unroll loops (UL).

CRUXEVAL

Large Language Models (LLMs) F2W	MCE	Original Benchmark	RV	SIE	UL
CodeGemma	33.0 (-2)	34.0 (-1)	35	32.0 (-3)	34.0 (-1)	32.0 (-3)
GraniteCode	29.0 (-3)	30.0 (-2)	32	32.0 (+0)	30.0 (-2)	31.0 (-1)
Llama3.2	29.0 (+1)	29.0 (+1)	28	31.0 (+3)	29.0 (+1)	23.0 (-5)
Mistral	23.0 (-1)	24.0 (+0)	24	23.0 (-1)	22.0 (-2)	25.0 (+1)
QWEN2.5-CODER	56.0 (-4)	62.0 (+2)	60	61.0 (+1)	52.0 (-8)	62.0 (+2)
SemCoder	51.0 (+0)	51.0 (+0)	51	50.0 (-1)	46.0 (-5)	47.0 (-4)

Table 2: Output prediction correction rate of each LLM on CRUXEVAL when applying different code mutations: converting for to while loops (F2W), mirroring comparison expressions (MCE), renaming variables (RV), swap if-else statements (SIE), and unroll loops (UL).

RQ3. Do different code mutations lead LLMs to produce different predictions for the same program?

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• It is crucial to analyse the set of distinct output predictions generated under different mutations to assess the stability of each ${\rm LLM}$.

 $\mathbf{RQ3}$. Do different code mutations lead LLMs to produce different predictions for the same program?

- It is crucial to analyse the set of distinct output predictions generated under different mutations to assess the stability of each LLM.
- This allows us to determine whether the models maintain consistent reasoning and predictions across semantically equivalent program variants.

LIVECODEBENCH

LLMs	Original Benchmark	Original + F2W	Original + MCE	Original + RV	Original + SIE	Original + UL	Original + All Mutations
CodeGemma	38.6%	47.2 (+8.6)	52.2 (+13.6)	51.8 (+13.2)	52.6 (+14.0)	42.0 (+3.3)	66.8 (+28.2)
GraniteCode	34.0%	37.6 (+3.5)	39.5 (+5.4)	43.2 (+9.2)	38.4 (+4.4)	34.7 (+0.6)	46.8 (+12.7)
Llama3.2	41.1%	50.7 (+9.6)	50.9 (+9.8)	56.6 (+15.4)	49.3 (+8.1)	43.4 (+2.3)	64.9 (+23.8)
Mistral	31.9%	35.3 (+3.3)	35.7 (+3.8)	40.1 (+8.1)	36.1 (+4.2)	33.4 (+1.5)	44.7 (+12.7)
Qwen2.5-Coder	62.0%	75.6 (+13.6)	80.2 (+18.2)	82.9 (+20.9)	78.1 (+16.1)	67.6 (+5.6)	93.1 (+31.1)
SemCoder	48.0%	63.0 (+15.0)	66.6 (+18.6)	71.6 (+23.6)	62.8 (+14.8)	52.0 (+4.0)	84.6 (+36.5)

Table 3: Output prediction stability of LLMs on LIVECODEBENCH when running a portfolio approach, applying different code mutations: converting for to while loops (F2W), mirroring comparison expressions (MCE), renaming variables (RV), swap if-else statements (SIE), and unroll loops (UL).

CRUXEVAL

LLMs	Original Benchmark	Original + F2W	Original + MCE	Original + RV	Original + SIE	Original + UL	Original + All Mutations
CodeGemma	34.6%	38.6 (+4.0)	39.8 (+5.1)	44.1 (+9.5)	40.9 (+6.2)	35.9 (+1.2)	49.2 (+14.6)
GraniteCode	32.4%	34.2 (+1.9)	34.8 (+2.4)	38.6 (+6.2)	34.5 (+2.1)	33.1 (+0.8)	40.9 (+8.5)
Llama3.2	28.0%	33.5 (+5.5)	32.6 (+4.6)	43.5 (+15.5)	33.2 (+5.2)	30.1 (+2.1)	48.1 (+20.1)
Mistral	24.1%	24.9 (+0.8)	25.6 (+1.5)	28.2 (+4.1)	26.0 (+1.9)	24.5 (+0.4)	30.4 (+6.3)
Qwen2.5-Coder	59.8%	63.2 (+3.5)	64.8 (+5.0)	70.4 (+10.6)	64.1 (+4.4)	61.9 (+2.1)	73.4 (+13.6)
SemCoder	50.6%	55.2 (+4.6)	55.8 (+5.1)	61.8 (+11.1)	56.6 (+6.0)	52.2 (+1.6)	65.5 (+14.9)

Table 4: Output prediction stability of LLMs on CRUXEVAL when running a portfolio approach, applying different code mutations: converting for to while loops (F2W), mirroring comparison expressions (MCE), renaming variables (RV), swap if-else statements (SIE), and unroll loops (UL).

RQ4. Are LLMs robust in understanding code against semantics-preserving mutations?

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LLMs	LiveCodeBench + Mutations	CruxEval + Mutations
CodeGemma	66.8 (+28.2)	49.2 (+14.6)
GraniteCode	46.8 (+12.7)	40.9 (+8.5)
Llama3.2	64.9 (+23.8)	48.1 (+20.1)
Mistral	44.7 (+12.7)	30.4 (+6.3)
QWEN2.5-CODER	93.1 (+31.1)	73.4 (+13.6)
SemCoder	84.6 (+36.5)	65.5 (+14.9)

 We investigate the reasoning capabilities and semantic robustness of Large Language Models (LLMs) in the context of program output prediction;

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- We examine whether the correct outputs are grounded in sound reasoning and whether $\rm LLMs$ are robust to semantics-preserving code mutations;

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- We examine whether the correct outputs are grounded in sound reasoning and whether LLMs are robust to semantics-preserving code mutations;
- ullet Our evaluation using six LLMs, reveals two key findings:

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- We examine whether the correct outputs are grounded in sound reasoning and whether LLMs are robust to semantics-preserving code mutations;
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 - LLMs often change predictions in response to our code mutations, indicating **limited** robustness in their semantic understanding.

Thank you!

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