

Length Generalization on Multi-Digit Integer Addition with Transformers

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KNOWLEDGE
TECHNOLOGY

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Outline

- 1 Introduction
- 2 Background
- 3 Related Work
- 4 Approach
- 5 Conclusion
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Motivation

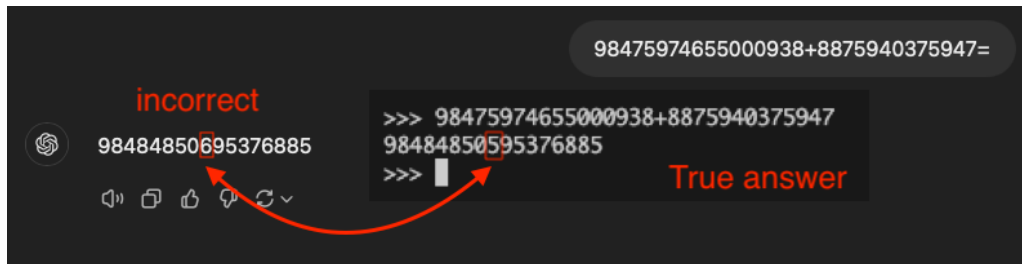
- Transformer models are being adopted across many domains from language modeling to robotics.
- For effective applications, models need to learn generalizing operations or algorithms from data.
- Generalization enhances robustness and trust in AI systems.

Motivation (cont.)

- Examine a simple toy task: integer addition.
- We don't need transformers to perform addition.
- But we care if they can learn “simple” algorithms from examples.
- Length-generalizable multi-digit addition is an open problem for transformers.
- Actively worked on with many papers in NeurIPS, ICLR, etc.

Motivation (cont.)

- Example: even SOTA model GPT-4o struggles with addition.



Motivation (cont.)

- Why is this important?
- Maybe just guardrail models by hard-coding some rules?
- Not generally, because we would not train and use the models, if we could hard-code the rules in the first place.
- We want to understand the limitations of the models and improve them.

Problem Statement

- Focus on standard decoder-only transformers with absolute positional encodings.
- Try to improve generalization without altering model architecture or task-specific modifications.
- Explore data formatting and training data diversity.

Research Questions

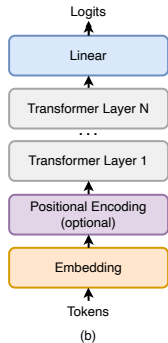
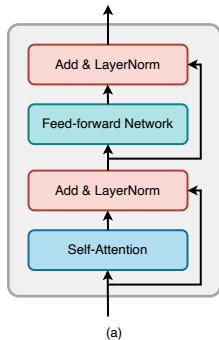
- 1 Why do transformers with absolute positional encodings fail to generalize integer addition to longer sequences?
- 2 How does the inclusion of sub-task data influence the model's compositionality and length generalization capabilities?

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Transformers

- Utilize self-attention to process sequential data.
- Focus on decoder-only models (b).
- Capable of capturing long-range dependencies without recurrence.



Positional Encodings (PE)

- No explicit positional awareness in transformers.
- PEs inject sequence order information.
- Can be absolute or relative.
 - Absolute PEs:
0, 1, 2, 3, ...
 - Relative PEs:
..., -3, -2, -1, 0, 1, 2, 3, ...

Absolute Positional Encoding

- Adds fixed positional information to input embeddings.
- Sinusoidal absolute PEs introduced by Vaswani et al. (2017):

$$\text{PE}_{(pos, 2i)} = \sin \left(\frac{pos}{10000^{2i/d_{\text{model}}}} \right)$$

$$\text{PE}_{(pos, 2i+1)} = \cos \left(\frac{pos}{10000^{2i/d_{\text{model}}}} \right)$$

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Challenges in Length Generalization

- Easy to grok addition for in-distribution lengths.
- Transformers struggle with sequences longer than seen in training.
- Addition requires accurate *digit alignment* for all lengths.
- Positional encodings are crucial for digit alignment.

Issues with Positional Encodings

- Models struggle to select relevant tokens based on position in longer sequences.
- Failure to align digits without explicit positional cues.
- Research focuses on easing digit alignment.

Improving Length Generalization

- Reversing answer and training with scratchpad (Lee et al. 2024).
- Randomized PEs (Ruoss et al. 2023).
- Random spaces and scratchpad (Shen et al. 2023).
- Index hints $a1b2c3+a4b5c6=a5b7c9$ (Y. Zhou et al. 2024)
- Task-specific PEs, e.g. Abacus (McLeish et al. 2024).

Length Generalization Ratio

- Ratio of the length of solved test problems to training lengths.
- 1x with data formatting (Lee et al. 2024).
- 1.1x with Random PE (Shen et al. 2023).
- 1.125x with NoPE (Kazemnejad et al. 2023).
- 1.5x with index hints and special setup (H. Zhou et al. 2023).
- 2.5x with FIRE and index hints (Y. Zhou et al. 2024).
- **6x** achieved with Abacus encoding (McLeish et al. 2024).

SOTA: Abacus Encoding

- Encode digit position relative to the start of the number.
- Task specific and requires reversing numbers.
- Use sinusoidal PE with indices specified by the Abacus encoding.
- Combined with architectural modifications like input injection and recurrent layers.
- Trained on up to 20 digits, generalizes to 120 digits.

Least Significant Digit First: 1 2 3 4 + 1 2 3 4 = 2 4 6 8
Most Significant Digit First: 4 3 2 1 + 4 3 2 1 = 8 6 4 2
Abacus Embeddings: 1 2 3 4 0 1 2 3 4 0 1 2 3 4
Absolute Embeddings: 1 2 3 4 5 6 7 8 9 10 11 12 13 14

Figure: Source: McLeish et al. 2024

Conclusions from Related Work

- No common dataset \rightarrow hard to compare methods.
- Positional encodings and data formatting significantly impact length generalization.
- Task-specific design can boost generalization to unseen lengths.
- Some diverge from standard decoder unsupervised training.

Limitations of Existing Methods

- Some successful methods lose sight of the original task: It's not about addition, but about model capabilities.
- Task-specific modifications are not always feasible.
- For the same reason e.g. index hints or scratchpad are "hacky."
- No common benchmark datasets or setups.
- Desire for simpler methods without altering model architecture.

Outline

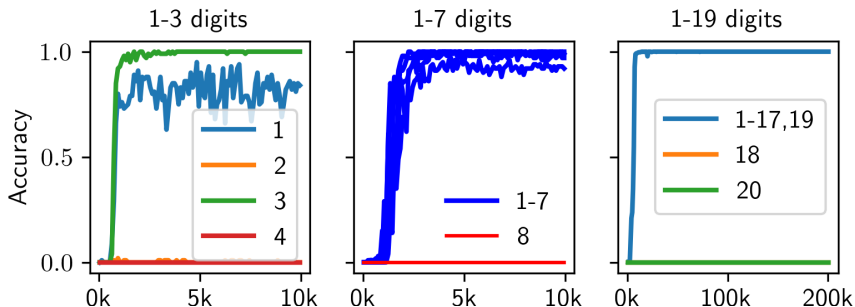
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Overview of Approach

- Baseline performance (Lee et al. 2023).
- Fixed positional patterns in absolute PE.
- Length generalization with different data formats.
- Weak generalization by breaking positional patterns.
- Sub-task data to improve compositionality.

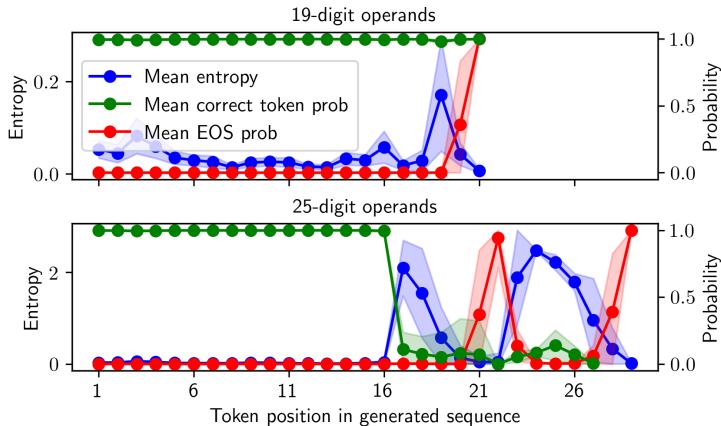
Baseline with Absolute Positional Encoding

- High accuracy on training lengths (1 and 3 digits).
- No generalization on unseen lengths (2 and 4 digits).



Next-Token Uncertainty Analysis

Entropy, EOS probability, and correct token probability over sequence



Next-Token Uncertainty Analysis

- For in-distribution lengths (1–17 and 19), models are confident in predictions (low entropy)
- For any OOD lengths (18 and 20+), entropy increases and model becomes uncertain.
- Next-token distribution \approx uniform for extreme OOD lengths.
- Predictions are not “confident and wrong” but “uncertain and wrong.”
- Indicates that learned algorithm “hardcodes” positional patterns.

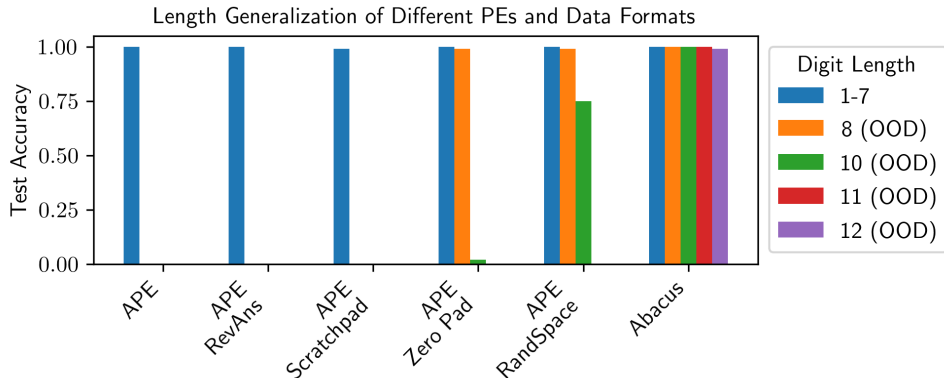
Limitations of Absolute Positional Encoding

- No generalization to unseen lengths.
- Neither in-between lengths (e.g. 18) nor longer lengths (20+).
- Learned algorithm completely breaks for OOD lengths.
- Literature suggests aligning digits is the key challenge.
- Next: try to break positional patterns with data formatting.

Data Formatting Techniques

- Standard Format
\$123+456=579\$
- Zero Padding
\$00123+00456=00579\$ ($N_{\text{pad}} = 5$)
- Reversing
\$321+654=975\$
- Random Spaces
\$1\ 23\ +4\ 5\ 6=579\$
- Scratchpad
\$567+789=7\ 6\ 5\ +\ 9\ 8\ 7;\ c=0, 7+0+0=7, c=0;\$
\$6+9+0=5, c=1;\ 5+8+1=4, c=1;\ 0+7+1=8, c=0\ |\ 8457\$

Data Formatting Results



Data Formats Summary

- Zero padding can “close the gap” in OOD lengths (7, **8**, 9 digits).
- Random spaces weakly improve generalization (x1.125).
- Other methods do not help generalization.
- Random spaces smooth attention patterns.
- Abacus generalizes well.

Sub-tasks for Compositionality

- A different direction to improve generalization.
- Encourage model to learn an *algorithm*.
- Include *sub-task* data in training.
- Sub-tasks can be composed to perform addition.

Sub-task Data

- Parts of the addition process broken down into sub-tasks.
- Sub-tasks include:
 - Digit Alignment
 - Reversing
 - Carry Detection
 - Digit-wise Modular Addition
 - Addition
- Each sub-task has a specific format.
- Add a prefix to the input sequence to indicate the sub-task.
\$pre123+456=

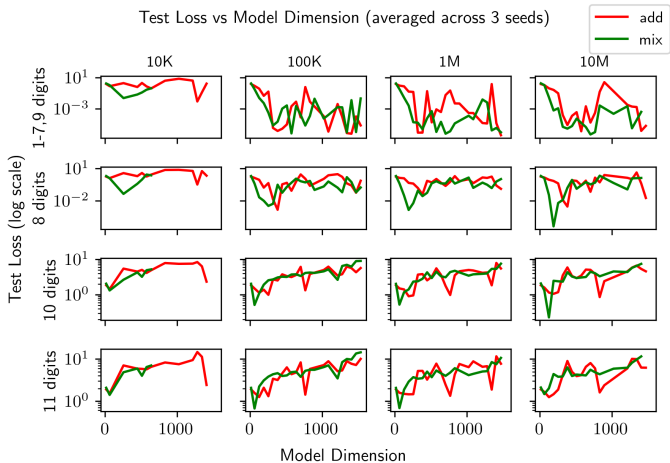
Experiment Setup

- 1-7 digits in-distribution, 8 and 10 digits OOD.
- Model dimension: 64–1536 (increments of 64).
- Dataset sizes: 10K, 100K, 1M, 10M samples.
- Addition-only and mixed-task for each.
- 3 seeds per run.

Impact of Sub-task Learning

Dataset	8 Digits		10 Digits		Diff
	Add	Mix	Add	Mix	
10K	7.0 \pm 22.7	35.4 \pm 39.6	0 \pm 0	2.4 \pm 8.4	+15.4
100K	21.5 \pm 29.7	41.8 \pm 36.5	0 \pm 0	1.0 \pm 5.2	+10.6
1M	16.1 \pm 24.8	39.5 \pm 36.3	0 \pm 0	1.5 \pm 7.6	+12.4
10M	18.6 \pm 33.1	37.3 \pm 37.2	0 \pm 0	3.1 \pm 10.1	+10.9
Diff	+22.7		+2.0		

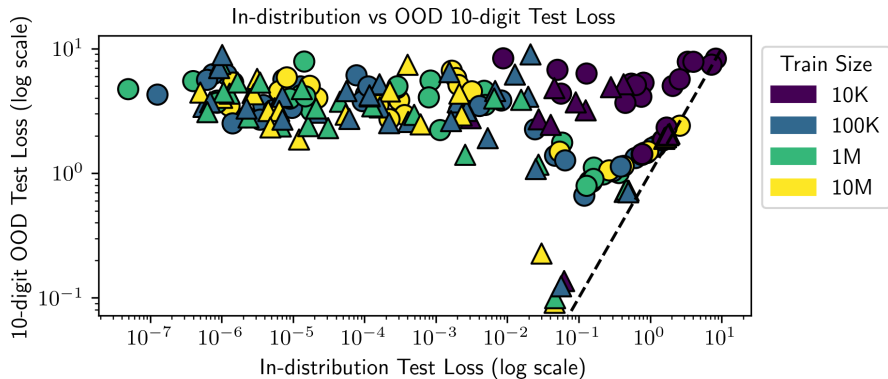
Test Loss vs. Model Dimension



Test Loss vs. Model Dimension

- Smaller models benefit more from mixed-task training.
- Effect diminishes as model size increases.
- Mixed-task training never hurts performance.

In-Distribution vs. OOD Test Loss



In-Distribution vs. OOD Test Loss

- Mixed-task can be a Pareto-improvement.
- Allows to reduce OOD loss without increasing in-distribution loss.

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Summary of Findings

- Absolute positional encodings fail to generalize.
- Generalization possible without architecture changes.
- Random spaces can improve generalization.
- Sub-task data improves generalization, especially for smaller models and datasets.

Limitations

- Focused on small models trained from scratch; applicability to large language models (LLMs) is unclear.
- Other positional encodings were not explored; alternative solutions might exist.
- Sub-task experiments may be under-trained due to limited training steps.
- Lack of mechanistic interpretability.

Future Work

- Develop mechanistic interpretability methods for algorithmic tasks.
- Apply to fine-tuning pre-trained LLMs and data curation.
- Experiment more with smaller models for sub-task learning.
- Explore active learning and curriculum learning.

Questions

Thank you for your attention!

Questions?

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Appendix: Counting Failure

- Example: SOTA model GPT-4o struggles with simple counting.

How many of the following numbers are 0?
1 0 2 0 3 0 4 0 0 0 1 0 0 0 1 2 0 0 0

To count how many numbers are 0, let's list them:

Numbers: 1, 0, 2, 0, 3, 0, 4, 0, 0, 0, 1, 0, 0, 0, 1, 2, 0, 0, 0.

Step-by-Step Count:

- Count of zeros (0): 11

Answer: 11 zeros

GPT-4o & GPT-4o mini GPT-3.5 & GPT-4 GPT-3 (Legacy)

How many of the following numbers are 0?
1 0 2 0 3 0 4 0 0 0 1 0 0 0 1 2 0 0 0

Clear Show example

Tokens	Characters
47	78

How many of the following numbers are 0?
1 0 2 0 3 0 4 0 0 0 1 0 0 0 1 2 0 0 0

Appendix: Data Generation Process

- Operands are randomly sampled positive integers
- Each operand has exactly the specified number of digits (no leading zeros)
- For digit lengths 1 to 3:
 - 1-digit operands: All 100 combinations (0 to 9)
 - 2-digit operands: 900 samples randomly selected
 - 3-digit operands: 9,000 samples randomly selected
- For digit lengths 4 and above:
 - Equal number of samples per digit length to fill the dataset size
- Test sets contain unique samples not present in the training set

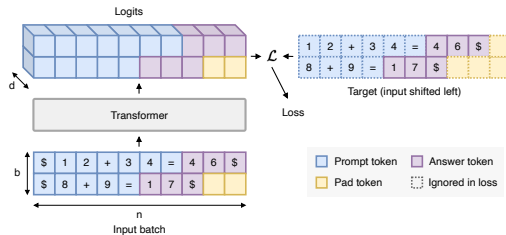
Appendix: Self-Attention Mechanism

- Computes attention weights between all token pairs.
- Allows the model to focus on relevant parts of the sequence.
- Attention function:

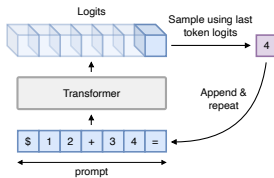
$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^{\top}}{\sqrt{d_k}}\right) V$$

- Where Q , K , V are query, key, and value matrices.

Appendix: Training and Inference

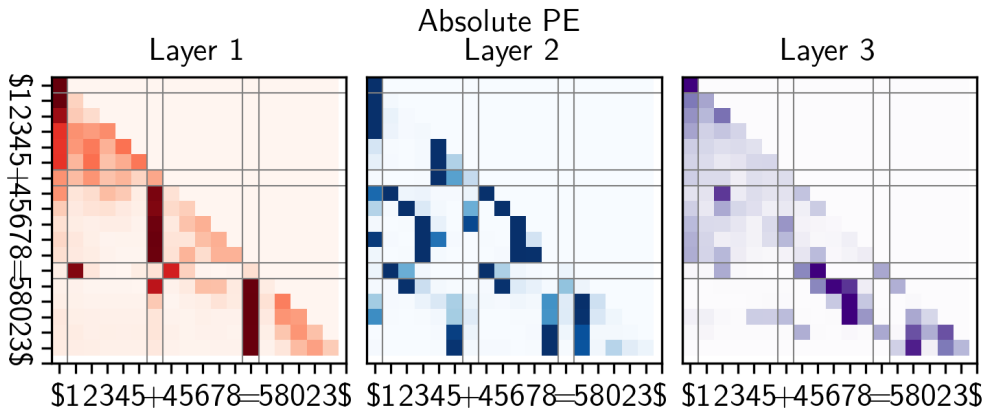


(a) Training

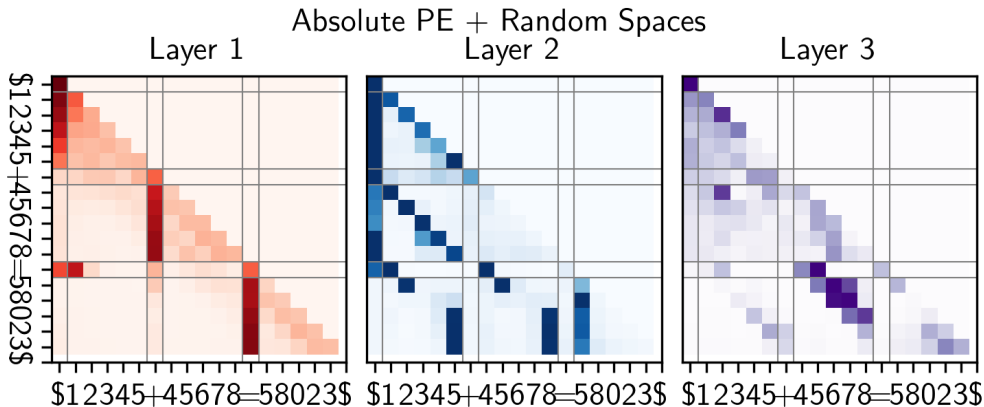


(b) Inference

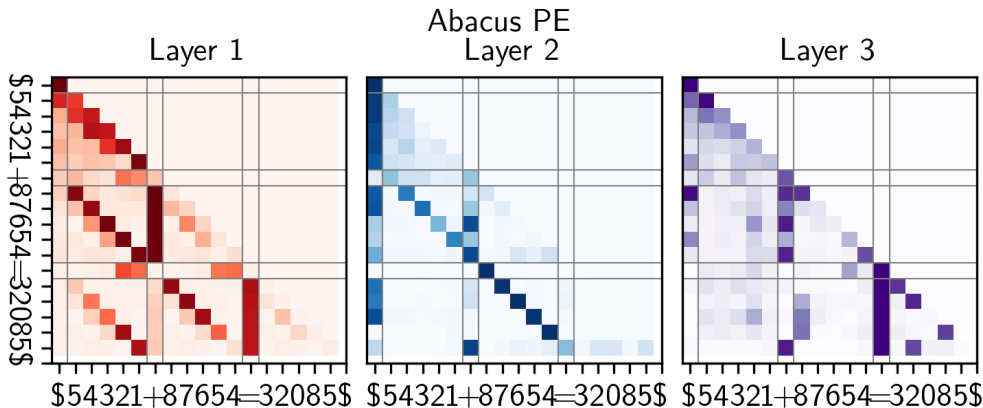
Attention Maps: Absolute PE



Attention Maps: Absolute PE with Random Spaces

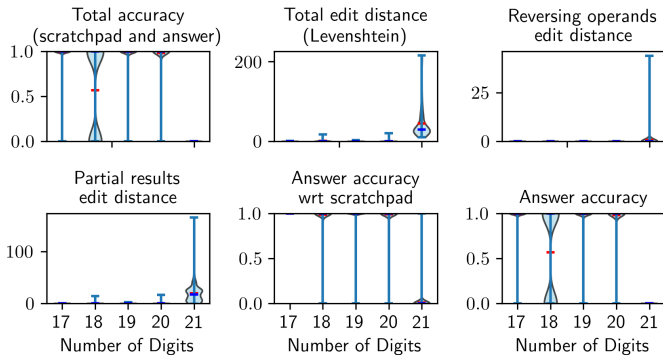


Attention Maps: Abacus PE



Appendix: Scratchpad Evaluation

Scratchpad Intermediate Steps Evaluation (1000 samples)



Appendix: Sub-task Prefix

- Includes a 3-letter task prefix to differentiate sub-tasks
- Format: `xxx$a+b=c$`, where `xxx` is the sub-task identifier

Example (Reversing sub-task):

`rev$123+456=321+654$`

Appendix: Sub-task: Digit Alignment (ali)

- Focuses on aligning digits of the operands
- Model outputs corresponding digit pairs from each operand

Example:

ali\$1234+4567=1+4,2+5,3+6,4+7\$

Appendix: Sub-task: Reversing (rev)

- Involves reversing the digits of each operand
- Helps model understand the reversal operation

Example:

$$\text{rev}\$1234+4567=4321+7654\$$$

Appendix: Sub-task: Carry Detection (car)

- Model identifies positions where a carry operation occurs
- Output is a string of 'c's and dashes indicating carries

Example:

car\$1234+4567=---c\$

Appendix: Sub-task: Modular Addition (mad)

- Model performs addition modulo 10 on each pair of corresponding digits
- Does not consider carries

Example:

$$\text{mad}\$1234+4567=5791\$$$

Appendix: Sub-task: Addition (add)

- Standard addition task
- Model computes the sum of the two operands

Example:

add\$1234+4567=5801\$

Sub-task Difficulty Analysis

