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## A SOME FAILURE CASES

Although LLMs show the power of optimizing basic math problems (Section 3) and prompts (Section 4), we see some limitations across all optimizer LLMs that may impede their power of solving more challenging problems. These limitations include:

- **Hallucinating the values that need to come from math calculation:** The optimizer LLMs often output contents like “the function value at (5, 3) is 15” despite that the true value is not 15. The model will get it right if external tools that can reliably calculate the value are triggered. When and how to trigger such tool use cases remains an interesting topic (see e.g., (Schick et al., 2023; Cai et al., 2023)).
- **Generating solutions already appeared in context even if we tell it to "Give me a new (w, b) pair that is different from all pairs above":** the optimizer LLMs do not 100% reliably follow this instruction even if its own outputs often include sentences like “I will provide a new pair that is different”, making the output self-contradictory. The output is almost guaranteed to be different from in-context old solutions when the model output contains a comparison of the new pair and all old pairs, though. Thus (implicitly) triggering such behaviors may be a solution. How to implement this feature without harming the instruction following performance of other parts remains an interesting topic to study.
- **In black-box math optimization, getting stuck at a point that is neither global nor local optimal:** This often occurs in two linear regression cases: (a) The in-context exemplars all share the same  $w$  or  $b$  that is different from  $w_{\text{true}}$  or  $b_{\text{true}}$ . This case is more likely to be avoided when a larger number of past solutions are included in the meta-prompt; (b) one or several of the best previous solutions in the meta-prompt have  $w$ s and  $b$ s in quantitatively opposite directions from the global optima  $w_{\text{true}}$  and  $b_{\text{true}}$ : for example, the  $w$ s are all smaller than  $w_{\text{true}}$  while the  $b$ s are all larger than  $b_{\text{true}}$ . Since the optimizer model often proposes to only increase  $w$  or decrease  $b$  when the past solutions in meta-prompt share  $w$  or  $b$ , the optimization will get stuck if either increasing  $w$  or decreasing  $b$  would increase the objective value. This issue is mitigated by sampling multiple new solutions (thus more exploration) at each step.
- **Hard to navigate a bumpy loss landscape:** Like other optimizers, it is harder for the optimizer LLM to optimize black-box functions when the loss landscape gets more complicated. For example, when minimizing the Rosenbrock function  $f(x, y) = (a-x)^2 + b(y-x^2)^2$  with  $a = 20$  (whose global optimal point is  $x = 20, y = 400$ ) with 5 starting points in  $[10, 20] \times [10, 20]$ , the optimization often gets stuck at around (0, 0). This is because the optimizer LLM sees a decrease of objective value when it drastically decreases both  $x$  and  $y$  to 0. Then starting from (0, 0), the optimizer LLM is hard to further navigate  $x$  and  $y$  along the narrow valley in the loss landscape towards (20, 400) (Figure 13).

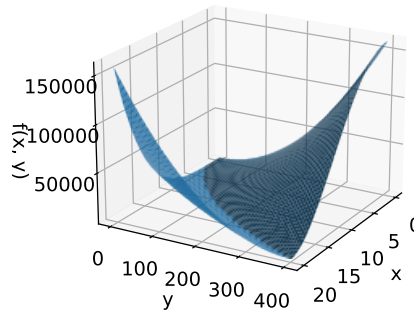


Figure 13: A visualization of the landscape of the Rosenbrock function  $f(x, y) = (a-x)^2 + b(y-x^2)^2$  with  $a = 20$  and  $b = 1$ . The global optima is at  $x = 20, y = 400$  with function value 0. The function value at  $x = 0, y = 0$  is 400. The landscape has a narrow valley between (0, 0) and (20, 400).

## B PROMPTING FORMATS FOR SCORER LLM

Figure 14, 15, and 16 show examples of the Q\_begin, Q\_end, and A\_begin prompting formats when the “QA” pattern is present. The “QA” pattern is eliminated when prompting instruction-tuned scorer models like `text-bison` with the Q\_begin and Q\_end formats (Figure 17 and 18).

Q: {instruction}

Janet’s ducks lay 16 eggs per day. She eats three for breakfast every morning and bakes muffins for her friends every day with four. She sells the remainder at the farmers’ market daily for \$2 per fresh duck egg. How much in dollars does she make every day at the farmers’ market?

A:

Figure 14: The Q\_begin prompting format on a GSM8K test exemplar with the "QA" pattern.

Q: Janet’s ducks lay 16 eggs per day. She eats three for breakfast every morning and bakes muffins for her friends every day with four. She sells the remainder at the farmers’ market daily for \$2 per fresh duck egg. How much in dollars does she make every day at the farmers’ market?

{instruction}

A:

Figure 15: The Q\_end prompting format on a GSM8K test exemplar with the "QA" pattern.

Q: Janet’s ducks lay 16 eggs per day. She eats three for breakfast every morning and bakes muffins for her friends every day with four. She sells the remainder at the farmers’ market daily for \$2 per fresh duck egg. How much in dollars does she make every day at the farmers’ market?

A: {instruction}

Figure 16: The A\_begin prompting format on a GSM8K test exemplar.

{instruction}

Janet’s ducks lay 16 eggs per day. She eats three for breakfast every morning and bakes muffins for her friends every day with four. She sells the remainder at the farmers’ market daily for \$2 per fresh duck egg. How much in dollars does she make every day at the farmers’ market?

Figure 17: The Q\_begin prompting format on a GSM8K test exemplar without the "QA" pattern.

Janet’s ducks lay 16 eggs per day. She eats three for breakfast every morning and bakes muffins for her friends every day with four. She sells the remainder at the farmers’ market daily for \$2 per fresh duck egg. How much in dollars does she make every day at the farmers’ market?

{instruction}

Figure 18: The Q\_end prompting format on a GSM8K test exemplar without the "QA" pattern.