AutoPDL: Automatic Prompt Optimization for LLM Agents

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Abstract The performance of large language models (LLMs) depends on how they are prompted, with choices spanning both the high-level prompting pattern (e.g., Zero-Shot, CoT, ReAct, ReWOO) and the specific prompt content (instructions and few-shot demonstrations). Manually tuning this combination is tedious, error-prone, and specific to a given LLM and task. Therefore, this paper proposes AutoPDL, an automated approach to discovering good LLM agent configurations. Our approach frames this as a structured AutoML problem over a combinatorial space of agentic and non-agentic prompting patterns and demonstrations, using successive halving to efficiently navigate this space. We introduce a library implementing common prompting patterns using the PDL prompt programming language. AutoPDL solutions are human-readable, editable, and executable PDL programs that use this library. This approach also enables source-to-source optimization, allowing human-in-the-loop refinement and reuse. Evaluations across three tasks and seven LLMs (ranging from 3B to 70B parameters) show consistent accuracy gains (9.06 ± 15.3 percentage points), up to 68.9pp, and reveal that selected prompting strategies vary across models and tasks.

1 Introduction

Large language models (LLMs) and LLM-based agents excel at a variety of tasks, including question answering, math word problems, and programming. The performance of an LLM depends heavily on how it is prompted, and there are a variety of popular prompting patterns. These include zero-shot or few-shot (Brown et al. 2020) prompting with chain-of-thought (CoT) (Wei et al. 2022), zero-shot CoT (Kojima et al. 2022), as well as agentic patterns such as ReAct (Yao et al. 2023) or ReWOO (Xu et al. 2023). However, given a dataset D_{test} with a loss function \mathcal{L} , *e.g.*, error rate, it is not clear which pattern will do best. Furthermore, besides the pattern A, performance also depends on the prompt p, including few-shot samples and instructions. The problem is thus to find a combination A_p^* of a pattern along with an optimized prompt that minimizes \mathcal{L} . This is usually done via manual prompt engineering, but that is tedious and has to be repeated if a new LLM comes along. Therefore, this paper explores how to find A_p^* using automated machine learning (AutoML). And for users to trust the result or to tweak it further, A_p^* itself should be easy to read and edit.

Agent frameworks, such as CrewAI (Moura 2023) or AutoGen (Q. Wu et al. 2023), contain prebuilt agent patterns with prompts optimized for proprietary frontier models and common tasks. Unfortunately, their prompts are deeply buried (Schluntz et al. 2024), making them hard to modify and adapt to non-frontier models or novel tasks. Moreover, the prompting pattern is fixed to a variation of ReAct, limiting flexibility in customizing the prompt structure. Prompt optimizers, such as DSPy (Khattab et al. 2024), optimize few-shot samples for in-context learning (ICL) and/or instructions in the prompt *p*. Unfortunately, they do not automatically select the prompting pattern *A* and do not return human-readable code.

We formulate the problem of finding a good pattern and corresponding prompt by defining and then exploring a combined search space. We were inspired by the AutoML literature on combined search spaces of machine-learning algorithms and their hyperparameters (Thornton et al. 2013), except that (i) instead of discrete or continuous hyperparameters, we explore textual ICL samples, instructions, and prompting patterns; (ii) instead of classification or regression tasks, we tackle generative tasks; and (iii) instead of model training or fine-tuning, we focus on in-context learning. We assume a dataset with a validation set D_{valid} , test set D_{test} , as well as an example bank D_{train} for few-shot samples. D_{valid} is used during the optimization process to evaluate the performance of a configuration, whereas D_{test} is used once upon completion, to evaluate the performance of the best performing configuration. As usual, to avoid over-fitting, we assume these are disjoint from each other. The problem statement is to find $A_p^* = \underset{A_p \in \mathcal{A}_P}{\operatorname{argmin}} \mathcal{L}(A_p, D_{\text{valid}})$, where:

- $A \in \mathcal{A} = \{\text{Zero-Shot, CoT, ReWOO, ReAct}\}$ is the prompting pattern, and
- $p = \langle n, d_{\text{train}}, \text{instr} \rangle \in \mathcal{P}$ is the prompt, comprising a number $n \leq |D_{\text{train}}|$ of few-shot samples, the actual few-shot samples $d_{\text{train}} \in (D_{\text{train}})^n$, and an instruction instr $\in \mathcal{I}$. A concrete example of \mathcal{P} is provided in Figure A1 and Figure A2.

To avoid getting stuck in local minima while saving compute and finding a solution with a low loss, we explore the search space $\mathcal{A}_{\mathcal{P}}$ using successive halving (Jamieson et al. 2016). To make the initial search space $\mathcal{A}_{\mathcal{P}}$ user-interpretable, and the final solution A_p^* both human readable and executable, we express them in a YAML-based prompting language, PDL (Vaziri et al. 2024). PDL's structured format makes it easy to modify both the initial search space and the optimized program, and ensures the final solution remains directly executable. We introduce a library for PDL that implements each of the common prompting patterns in \mathcal{A} . The initial search space $\mathcal{A}_{\mathcal{P}}$ is a YAML file with various choice points for AutoML to decide. And the solution A_p^* is a customtailored PDL program optimized for the given task, as given by the dataset and loss function. The developer can read or even tweak either or both as desired.

We evaluate our optimizer on three tasks (question answering, math, and programming), using seven LLMs sized between 3B and 70B parameters. We find that the optimizer often gives accuracy boosts in the 6–30% range, in some cases higher. Given the same task, different patterns $A \in \mathcal{A}$ do best for different models. Conversely, given the same model, different patterns do best for different tasks. Besides this variability in the chosen pattern A, our experiments also revealed variability in the optimized prompts $p = \langle n, d_{\text{train}}, \text{instr} \rangle$. We also found that when training data for a task is missing, data from a related but different dataset can help. Also, while most of our experiments use moderately-sized open models, we also show our optimized solutions can benefit frontier models.

This paper makes three primary contributions:

- 1. Jointly searching pattern and prompt: prior work in prompt optimization has not investigated searching *joint* search spaces, including agentic patterns.
- 2. No one size fits all: we find that different models sometimes have differing optimal prompt patterns for the *same* benchmark, suggesting that there is not one single optimal prompt pattern.
- 3. Source-to-source optimization: we propose the first source-to-source optimizer for LLM prompt programs, where both the initial search space and the final solution are prompt programs in the same language, making the final solution both human-readable and executable.

Overall, this paper shows how to apply AutoML to automatically discover agentic or nonagentic LLM prompts and patterns optimized for a given task. We make our AutoPDL implementation available at https://github.com/IBM/prompt-declaration-language, and release the reproduction package used for the experiments in this work to the community.

2 Background

This paper uses PDL (Vaziri et al. 2024) as a representation for exploring the search space of programs. PDL programs are declarative and combine human readability with ease of execution. They represent the composition of calls to LLMs and tools, abstracting away the plumbing necessary for

```
1 text:
2 - role: tools
3 text: ${ tools }
4 - "Out of 1400 participants, 400 passed the test. What percentage is that?\n"
5 - def: actions
6 model: replicate/ibm-granite/granite-3.1-8b-instruct
7 parser: json
8 spec: [{ name: str, arguments: { expr: str }}]
9 - if: ${ actions[0].name == "calc" }
10 then:
11 lang: python
12 code: result = ${ actions[0].arguments.expr }
```

Figure 1: Basic example of a PDL program.

such compositions. The output of the optimizer is also a PDL program, rather than simple textual prompts, so it is fully executable and could be further refined by a developer.

Figure 1 shows a simple PDL program that uses a tool to answer a query. PDL is based on the premise that interactions with an LLM are mainly for the purpose of generating data. So, it allows users to specify the shape of data to be generated in a declarative way (in YAML), and is agnostic of any programming language. The first line of Figure 1 specifies that we are creating some text. Next, the first block in the itemized list defines the tools prompt. Line 3 contains a use of variable *tools*, expressed as a Jinja expression. This variable is defined as the JSON Schema specification of a calculator tool (not shown in this figure, for the full program see Appendix 8.2). Line 4 is the user query prompt. We do not specify the role explicitly as *user* is the default role for prompts. Lines 5 through 8 show a model call. In PDL, the background context is accumulated implicitly, so the output of all blocks executed so far will be passed to the LLM as a list of input messages. The result of the model call is assigned to the variable *actions* (line 5). The model to be called is specified on line 6 (PDL is based on LiteLLM,¹ so this is a LiteLLM model id). Finally, lines 7 and 8 say that we parse the output of the model as JSON and type-check it according to the type on line 8. Furthermore, when the inferencing server supports it, model calls with a schema use constrained decoding (Willard et al. 2023), enforcing syntactically correct JSON.²

On line 9, an if-statement checks whether the output of the LLM asks for the calculator tool. If so, we use a Python code block to compute the requested tool call (lines 11 and 12). When we execute this program using the PDL interpreter, we obtain all the model inputs, followed by the model output, and finally the output of the tool call. PDL has a rich set of control structures to allow writing a variety of prompting patterns, as well as functions to support libraries. For instance, Figure 3 shows a function call on line 4. In this paper, we consider the problem of automatically tuning prompts and choosing prompting patterns for a given dataset. The following section explains our approach in further detail.

3 AutoPDL Approach

Figure 2 gives an overview of our approach. Referring to the numbers in the arrows:

(1) The input task is given by two disjoint datasets D_{train} and D_{valid} and a loss function \mathcal{L} . The datasets comprise $\langle x, y \rangle$ instances, where x is a question, y is the corresponding answer, and both are text strings. The loss function evaluates the quality of an answer y. (2) The search space specification $\mathcal{A}_{\mathcal{P}}$ is a YAML file with the optimization variables and their possible values, along with some hyperparameters. For example, num_demonstrations: [0, 3, 5] indicates that each candidate will have zero, three, or five ICL samples randomly drawn from D_{train} . In the case of zero demonstrations, this is equivalent to the zero-shot baseline. If zero is an option, we bias our candidate

¹https://github.com/BerriAI/litellm

²PDL additionally makes use of the heuristic json-repair package.



Figure 2: Overview of our approach.

sampling to always include one zero-shot candidate, just in case that baseline turns out to be the best-performing configuration.

(3) The pattern library consists of four PDL functions. Zero-shot is a baseline that simply prompts the LLM with x and expects it to return y. CoT refers to chain-of-thought (Wei et al. 2022) with in-context learning (Brown et al. 2020): the input includes a few $x_i y_i$ pairs before the actual question x, and the output includes some reasoning thought *tho* before the actual answer y. ReWOO (Xu et al. 2023) refers to reasoning without observations. Here, the few-shot samples are trajectories traj_i. A trajectory traj_i consists of steps for a particular example problem instance in D_{train} , e.g., in the case of ReWOO, tho and act steps and their contents. In contrast to $x_i y_i$ pairs, $traj_i$ may contain many tho, act and, depending on pattern, obs steps, before reaching the solution y_i . The first LLM call in ReWOO generates one reasoning thought *tho* and multiple actions act_i . The PDL code executes each of the actions as a tool call to obtain the corresponding observations obs_i . A final model call generates the answer *y* based on the observations. Finally, the ReAct pattern (Yao et al. 2023) starts with few-shot trajectory examples $traj_i$ (brief example visible under Solution A_p^* in Figure 2) and the question x, and then enters a TAO (thought, action, observation) loop. In each loop iteration, the LLM generates *tho* and *act*, then the PDL code executes the action as a tool call, and feeds the tool output back as an observation obs. A special Finish action breaks out of the loop to return the answer *y*.

Once inputs (1), (2), and (3) are in place, the successive halving optimizer runs in a loop. It starts with a small subset $D_v \,\subset\, D_{\text{valid}}$ and many candidates $\mathcal{C} = \{c_1, \ldots, c_k\} \subseteq \mathcal{A}_{\mathcal{P}}$ sampled from the search space. Each iteration uses D_v to evaluate the corresponding losses ℓ_1, \ldots, ℓ_k . Then each iteration keeps the $\frac{k}{2}$ candidates with the smallest \mathcal{L} while doubling the size of the validation subset D_v . See § 8.3 for the algorithm. (4) After the last iteration, the best remaining candidate is the solution A_p^* . This solution is a set of PDL definitions with concrete values for the optimization variables,

```
1 text:
2 - include: ../../tools.pdl
3 - include: ../../ReAct.pdl
4 - call: ${ react }
5 def: ANSWER
6 args:
7 task: "Question: ${ question }"
8 model: ${ model }
9 tools: ${ tools }
0 trajectories: ${ demonstrations }
1 - "\nThe answer is ${ ANSWER.answer }"
```

Figure 3: Basic example of PDL program using the ReAct pattern.

e.g., in Figure 2, num_demonstrations: 5 and demonstrations: ... a list of ReAct trajectories. (5) This program can be used on the test set D_{test} . For instance, Figure 3 shows a call to the ReAct function that passes d_p as an argument.

4 Methodology

This section describes the datasets used, the tools available to agents, and our experimental setup, including how we construct agent trajectories that demonstrate tool use for each dataset.

4.1 Datasets

We selected datasets that are widely used in the literature, span diverse tools and domains, and are representative of tool categories frequently studied in prior work (*e.g.*, calculator, search, code execution). In our experiments, each dataset has three disjoint splits: D_{train} to sample few-shot samples from, D_{valid} to evaluate candidates during optimization, and D_{test} to evaluate the final chosen solution upon completion of optimization.

GSM8K. The Grade School Math (Cobbe et al. 2021) dataset consists of 8,792 grade school math problems. We sample 1,024 problems without replacement from the train set to use as our D_{valid} set, and 1,024 from the test set (consisting of 1,319 samples) to use as our D_{test} . This leaves a D_{train} of 6,449 problems. Each problem consists of a word problem *x* such as "*What is fifteen more than a quarter of 48?*", a sequence *tho* of reasoning steps, and finally a plain numeric answer *y* following a special delimiter. For the CoT prompt pattern, we include these reasoning steps directly in the demonstrations. We use a regular expression to extract the numerical answer from the model solution, and define a correct solution as an exact match to the ground truth answer.

GSM-Hard. Gao et al. (2023) introduce a derivative of GSM8K with variables randomly changed to large numbers, with 1,319 samples. Unfortunately, GSM-Hard had 132 samples where the ground truth was incorrect, and hence we excluded those samples. We split the single set into equally sized D_{valid} and D_{test} (n = 594), and use the GSM8K training set (6,449 samples) described above for D_{train} (*cross transfer*). We use the same correctness criterion as for GSM8K.

FEVER. The Fact Extraction and VERification dataset (Thorne et al. 2018) is a question-answering dataset structured around fact-checking. The original dataset contained 185,445 claims that are true, false, or unverifiable, and associated with human annotated supporting, refuting, or neutral sentences and their Wikipedia article of origin. We follow the widely used derivative of this benchmark in BIG-bench (Srivastava et al. 2023), which reformulates it into a true-or-false task by removing unverifiable claims. We sample 1,024 claims from the train set as D_{valid} and 1,024 from the test set as D_{test} . This leaves a D_{train} of 5,696 claims. BIG-bench also does not include the supporting or refuting sentences, which we recover by joining on the original dataset, for use *e.g.*, as CoT demonstrations. To assess correctness, we check for the presence of "true" and "false" in the final line of the model response. If neither or both are present, we deem the response as incorrect, and otherwise the correctness is a direct match to the ground truth "true" or "false".

MBPP+. MBPP (Austin et al. 2021) is a dataset of 974 mostly basic Python problems, with each example consisting of a natural language problem specification x for a self-contained Python function y, along with a single test case. Each problem has an extended set of test cases used for evaluation, which are not shown to the model. Liu et al. (2023) found that MBPP test cases are incomplete, allowing proposed solutions to pass as correct, despite not matching the problem specification. Therefore, our experiments are based on MBPP+, which contains a subset of the problems, but a more complete set of test cases for each problem. We use these test cases to assess the correctness of the proposed solutions. We use the 374 examples from the original MBPP dataset as D_{train} , and split MBPP+ into D_{test} (224 samples) and D_{valid} (39 samples) based on which split they were in

MBPP. The discrepancy in number of MBPP+ samples is due to the exclusion of samples found in the MBPP train set, to avoid data contamination. Our ReAct implementation follows Wang et al. (2024). We do not implement ReWOO as it is not reactive, *i.e.*, cannot include execution feedback.

4.2 Tools

Our prompt library represents actions, *i.e.*, tool calls, following the JSON tool calling schema (Abdelaziz et al. 2024). An action is represented as a JSON object with name and arguments mapping. For example, {"action": "Calc", "arguments": {"expr": "48/4"}} represents a call to a calculator with the expression to evaluate. The PDL functions implementing the patterns (see Figure 2) accept a list of tool definitions as an argument. Each element of that list is itself a PDL function. As both the agents and tools are implemented in PDL, the set of tools for a given task could itself be made a search space dimension, which we leave to future work.

Calculator. For math datasets, we give the agentic approaches access to the *Calc* tool. This tool evaluates a cleaned (*e.g.*, replacement of ^ with **) expression with SymPy, returning the result. In case of error, the function returns a warning that the expression was invalid, which may help the agent recover from invalid input.

Search. For fact verification, we provide access to the *Search* tool, which returns the summary of the first Wikipedia search result for the query. If no results are found, a hint to try again is returned, or if the title is too ambiguous, a list of possible disambiguations.

Execute. We implement a programming agent for the code generation task, which can execute arbitrary code surrounded in XML-style <execute> tags. This tool executes the code in a Python shell, which returns the result of the final expression. This allows the agent to test its proposed solution against the given test case before submitting its solution.

Finish. The most basic action is the *Finish* action, or <solution> tag for the coding agent. This ends the agent's trajectory and results in the agent returning the value as the solution.

4.3 Experimental Setup

We evaluate the efficacy of our approach by running an optimization process to completion for each model & dataset pair, and subsequently comparing the task accuracy. As a baseline, we evaluate each model in a zero-shot setting. This setting reflects the minimal effort approach by a user or developer, where they do not include any demonstrations with their query or task. As no model we investigate was specifically trained to create agentic trajectories in a zero-shot setting, it is not feasible to create a zero-shot setting under ReAct or ReWOO.

For the optimization process, we used an initial candidate set C of 100 candidate prompt configurations $c_i = \langle A, p \rangle \in C$ per experiment. We fixed the size of the initial validation subset $d_{\text{valid}} \subseteq D_{\text{valid}}$ to 16. We define $\mathcal{L}(c_i, d_{\text{valid}}) = -\text{Accuracy}(c_i, d_{\text{valid}})$ for a given candidate c_i , where accuracy is the fraction in d_{valid} of correctly solved problems by c_i as per the dataset definition of correctness. For each candidate c_i , $p = \langle n, d_{\text{train}}, \text{instr} \rangle \in \mathcal{P}$ where *n* few-shot samples or trajectories $d_{\text{train}} \in (D_{\text{train}})^n$ are randomly sampled with replacement. The number of possible values for \mathcal{P} is combinatorially large and depends on the dataset D_{train} used. Finally, upon completion of an optimization process, the optimal candidate is evaluated on D_{test} .

Constructing Trajectories. As we are also optimizing over agentic trajectories, we also need a set of trajectories to sample few-shot samples from. To achieve this, we create a basic agentic trajectory *traj_i* for each training example $\langle x_i, y_i \rangle$, following a rule-based transformation. We design and apply a template to each dataset, which is relatively simple and easy to implement for other datasets (details are provided in § 8.5). Prior work has introduced approaches to bootstrapping trajectories *e.g.*, in software engineering (Pan et al. 2024), tool use demonstrations (Li et al. 2025),

and reasoning paths (Zelikman et al. 2022), which could be applied to this problem. While we acknowledge the shortcomings of manual template construction, we argue this approach has two strengths: it is generalizable in the sense that templates can be mixed and matched, and that the trajectories are directly based on the datasets used. Additionally, we wanted to work with commonly used datasets that cover a variety of tools and domains, rather than emerging datasets containing trajectories or tool use demonstrations.

Models. We aim to study models of various abilities, *e.g.*, natural language or code, various creators, and various sizes, ranging from single digit billions of parameters up to the edge of feasibility on consumer hardware. We include seven models available on inference service IBM watsonx³ in our study. We select three generalist natural language instruction models, LLAMA 3.1 8B, 3.2 3B, and 3.3 70B from the open-source and widely studied LLaMa family (Dubey et al. 2024). We further select three models from Mishra et al. (2024), which predate Dubey et al. (2024) by approximately 3 months. We select GRANITE 13B INSTRUCT V2 as a generalist model, and GRANITE 20B and 34B CODE INSTRUCT as code models. We select GRANITE 3.1 8B as an additional generalist model (Granite Team 2024). All of our experiments use greedy decoding, *i.e.*, no sampling, to limit the impact of hyperparameter choice. The number of models we evaluate is limited by cost in \$/token terms and execution time. By studying various models, we demonstrate the generalizability of our approach.

Alternative Setups. We evaluate two alternative experimental setups. First, to investigate lowresource scenarios, we examine whether performance on one dataset can be improved by using demonstrations D_{train} from a similar dataset, while optimizing w.r.t. D_{valid} . For this experiment, we investigate whether performance on GSM-Hard can be improved by using demonstrations from *GSM8K*, while optimizing w.r.t. GSM-Hard D_{valid} . Second, to explore saving optimization costs, we assess whether optimized prompt programs of one model can transfer well to a frontier model. The intuition is that while that might not be the best program for the frontier model, it might at least improve somewhat over the baseline. To this end, we evaluate the optimized PDL programs of LLAMA 3.1 70B on OpenAI's gpt-40-mini-2024-07-18, for each dataset.

5 Results

This section describes the results of our empirical study to evaluate our AutoPDL approach and answer the following research questions:

RQ 1: To what extent does AutoPDL improve accuracy, and how much does the best solution vary by task and model?

RQ1 asks to what degree our AutoPDL approach can improve model performance over their zero-shot baseline across a variety of commonly used benchmarks. We also seek to identify trends, if any, in optimal configurations, *e.g.*, whether more few-shots is always better, or whether certain prompt patterns are particularly suited to certain problem domains.

RQ 2: Can AutoPDL make up for a missing few-shot example bank for a given task by reusing the example bank from a similar task?

RQ2 investigates whether optimizing on one dataset using demonstrations from another, related, dataset can result in higher performance than using no demonstrations (zero-shot). This RQ addresses a low-resource scenario in which a limited pool of demonstrations exists in one dataset, but a dataset from a similar domain has a large pool.

RQ 3: Do solutions found by AutoPDL improve performance on frontier models, even when optimized for open-source models?

³https://www.ibm.com/watsonx

It can be expensive to run optimization against commercial frontier-model APIs. RQ3 assesses whether optimized prompt programs are transferable to different (and likely stronger) models than those they were optimized with.

Table 1 reports the results of our optimization and evaluation procedure. We performed three complete optimization runs for GSM8K and MBPP+, and report mean accuracy and standard deviation in percentage points (*i.e.*, absolute, *not* relative, uncertainty). We did not complete multiple runs for all model-dataset pairs due to time and resource constraints. Where multiple runs were performed, we report the pattern of the highest scoring run. Additionally, we note minor variance in certain zero-shot settings due to API non-determinism. Across models and datasets, we generally find some improvement over the zero-shot baseline with few-shot chain-of-thought, or agentic patterns ReAct or ReWOO.

Dataset	Model	Accuracy			Dattann	Desertheres
		Zero-Shot	Optimized	Delta	Fattern	Kuittime
FEVER	Granite 3.1 8B	78.3 %	79.0 %	+0.7pp	ReWOO (5 shot)	08:55
	Granite 13B Instruct V2	6.5 %	75.4%	+68.9pp	ReWOO (3 shot)	08:12
	Granite 20B Code	39.7 %	64.2 %	+24.5pp	CoT (3 shot)	05:06
	Granite 34B Code	56.4%	65.6 %	+9.2pp	CoT (3 shot)	03:47
	LLaMA 3.1 8B	68.5%	78.0 %	+9.5pp	CoT (3 shot)	05:24
	LLaMA 3.2 3B	38.0 %	66.9 %	+28.9pp	ReWOO (5 shot)	09:08
	LLaMA 3.3 70B	67.6 %	77.5 %	+9.9pp	ReWOO (5 shot)	09:32
GSM8K	Granite 3.1 8B	74.2%	(74.2 ± 0.6) %	+0.0pp	Zero-Shot (Baseline)	08:56
	Granite 13B Instruct V2	23.0 %	(30.9 ± 1.0) %	+7.9pp	CoT (3 shot)	09:20
	Granite 20B Code	68.7 %	(68.7 ± 0.1) %	+0.0pp	Zero-Shot (Baseline)	09:27
	Granite 34B Code	72.1%	(72.1 ± 0.1) %	+0.0pp	Zero-Shot (Baseline)	08:52
	LLaMA 3.1 8B	78.4%	(85.3 ± 0.6) %	+6.9pp	CoT (5 shot)	08:48
	LLaMA 3.2 3B	71.8 %	(75.3 ± 0.4) %	+3.5pp	CoT (3 shot)	16:36
	LLaMA 3.3 70B	85.5 %	(95.4 ± 0.2) %	+9.9pp	CoT (3 shot)	07:50
MBPP+	Granite 3.1 8B	62.9 %	(62.9 ± 0.0) %	+0.0pp	Zero-Shot (Baseline)	02:14
	Granite 13B Instruct V2	10.7~%	(19.2 ± 1.2) %	+8.5pp	ReAct (5 shot)	04:02
	Granite 20B Code	51.8 %	(51.8 ± 0.4) %	+0.0pp	Zero-Shot (Baseline)	03:43
	Granite 34B Code	48.7 %	(61.3 ± 1.0) %	+12.6pp	ReAct (3 shot)	04:54
	LLaMA 3.1 8B	61.2%	(62.8 ± 4.0) %	+1.6pp	ReAct (5 shot)	01:45
	LLaMA 3.2 3B	58.0 %	(58.0 ± 0.4) %	+0.0pp	Zero-Shot (Baseline)	02:01
	LLaMA 3.3 70B	71.4%	$(71.4 \pm 0.0)\%$	+0.0pp	Zero-Shot (Baseline)	02:27

Table 1: Model accuracies across datasets for baseline (zero-shot) and optimized versions.

FEVER. We observed the minimum improvement in GRANITE 3.1 8B, with a 0.7 percentage point (pp) improvement, and a maximal improvement of 68.9pp for GRANITE 13B INSTRUCT V2. In terms of prompt pattern, CoT and ReWOO are equally represented. ReAct was not the optimal for any of the models. Interestingly, the largest model (LLAMA 3.3 70B) benefited by 9.9pp from 5-shot CoT. FEVER runtimes are generally higher than the other benchmarks, likely due to the large number of tokens involved by including Wikipedia content.

GSM8K. The highest improvement recorded (9.9pp) was for LLAMA 3.3 70B using 3-shot CoT, while the minimum improvement of 3.5pp was in LLAMA 3.2 3B using 3-shot CoT. ReAct and ReWOO were not the optimal for any model. For GRANITE 3.1 8B, GRANITE 20B CODE, and GRANITE 34B CODE, no improvement over the zero-shot baseline was identified. This was somewhat surprising, as generally including even some few-shot samples improves performance in LLMs.

MBPP+. Several models benefited from execution feedback, as 3 out of 7 had ReAct as the optimal prompt pattern (ReWOO was excluded as described in § 4.3). The greatest improvement of

12.6pp was in GRANITE 34B CODE, and 8.5pp in GRANITE 13B INSTRUCT V2, likely due to its poor programming performance as a generalist, non-code model. In contrast, the smaller LLAMA 3.1 8B model had high zero-shot performance of 61.2%, yet still improved by up to 6.2pp (1.6pp on average) with ReAct. No improvement was observed for GRANITE 3.1 8B, GRANITE 20B CODE, or the other LLAMA models.

Dataset	Model	Accuracy			Dattarn	Duntimo
		Zero-Shot	Optimized	Delta	Fattern	Kuntille
GSM-Hard	Granite 3.1 8B	44.0 %	44.0 %	+0.0pp	Zero-Shot (Baseline)	04:57
	Granite 13B Instruct V2	4.7 %	5.6 %	+0.8pp	CoT (3 shot)	03:30
	Granite 20B Code	28.8 %	28.8 %	+0.0pp	Zero-Shot (Baseline)	08:26
	Granite 34B Code	27.9%	30.0 %	+2.0pp	ReWOO (5 shot)	05:49
	LLaMA 3.1 8B	31.6 %	32.3 %	+0.7pp	ReWOO (5 shot)	04:44
	LLaMA 3.2 3B	26.3 %	27.4%	+1.2pp	CoT (5 shot)	16:50
	LLaMA 3.3 70B	47.3 %	53.4%	+6.1pp	CoT (5 shot)	11:07

Table 2: Model accuracies on GSM-Hard for cross optimization experiment.

Table 3: Model accurac	y for GPT-40-mini cross	experiment results
------------------------	-------------------------	--------------------

Datacet	Model	Accuracy			Dattorn	
Dataset		Zero-Shot	Optimized	l Delta	I attern	
FEVER	GPT-40-mini	83.7 %	87.7 %	+4.0pp	CoT (3 shot)	
GSM-Hard	GPT-40-mini	45.6 %	54.9 %	+9.3pp	ReAct (5 shot, Granite LLaMa)	
GSM8K	GPT-40-mini	77.8 %	90.9 %	+13.1pp	CoT (5 shot)	
MBPP+	GPT-40-mini	72.3 %	72.3 %	+0.0pp	Zero-Shot (Baseline)	

Missing Few-Shot Example Bank. We optimized the PDL program for GSM-Hard, using GSM8K demonstrations, and report results in Table 2. We found that in most cases, GSM8K demonstrations were at least not harmful for models on GSM-Hard, with up to 6.1pp improvement for LLAMA 3.3 70B using 5-shot CoT.

Commercial Frontier Model. To assess whether performance gains in one model can be achieved in another, we evaluate the optimized PDL programs of LLaMA 3.1 70B on OpenAI's gpt-4o-mini-2024-07-18 and report results in Table 3 (we did not use LLaMA 3.3 70B here because we did this experiment earlier and did not have the time and resources to repeat it for the final version of this paper). For all dataset/prompt pattern pairs that resulted in improvement for LLAMA 3.1 70B, we found a surprising improvement in GPT40-MINI of at least 4pp on FEVER using 3-shot CoT, 9.3pp on GSM-Hard (using GSM8K demonstrations) with 5-shot ReAct (Granite LLaMa instructions), and up to 13.1pp on GSM8K using 5-shot CoT. This suggests that optimizing for an open-source model can also benefit a closed-source model.

6 Related Work

The closest related work is on **prompt optimization**. APE starts with an LLM-generated set of candidate prompts, then performs rejection sampling based on evaluation on a subset of data (Zhou et al. 2023). ZOPO incorporates a Neural Tangent Kernel-based derived Gaussian process into standard zeroth-order optimization for an efficient search of a locally-optimal instruction (Hu et al. 2024). Unlike our approach, neither APE nor ZOPO optimize few-shot samples. Aviary can also jointly optimize over prompt pattern, instruction, and few-shot examples (Narayanan et al. 2024). However, it would require the definition of a custom operator. CEDAR uses a demonstration pool, from which it retrieves few-shot examples at query time (Nashid et al. 2023). Unlike our approach, these few-shot samples are retrieved on a per-inference basis, not optimized ahead-of-time.

EASE leverages embeddings to represent few-shot examples, and uses a neural bandit algorithm to find an ordered set that performs well for test queries from a given task (Z. Wu et al. 2024). An extension of their approach jointly optimizes demonstrations and instructions. However, the approach requires both an additional embedding model, and the training of a new model to predict validation scores from embeddings. Unlike our approach, EASE does not optimize over agentic patterns.

DSPy optimizes instructions and few-shot samples for a chain of LLM calls (Khattab et al. 2024) (not just a single call like APE or CEDAR). Also, DSPy takes away control over the exact prompt from the programmer, which our approach preserves. Similarly to DSPy, TextGrad also optimizes a chain of LLM calls, by using LLMs to back-propagate modifications to instructions in prompts (Yuksekgonul et al. 2025). However, unlike our approach, neither of these optimize agentic patterns.

BPO trains a sequence-to-sequence model on prompts augmented by an LLM incorporating human preferences, producing a model that improves given input prompts (Cheng et al. 2024). APOHF introduce a strategy to select a pair of prompts to query the user for preference feedback, which they use to optimize LLM-generated instructions on a validation set (Lin et al. 2024). However, neither of these approaches explicitly optimize demonstrations or agentic patterns. EvoAgent optimizes the instructions of a population of agents via crossover, mutation, and selection (Yuan et al. 2024). It then forms an ensemble from the final, fittest, population. GPTSwarm represents each agent as a graph, then freezes intra-agent edges and optimizes the placement of additional inter-agent edges (Zhuge et al. 2024). Unlike our approach, neither EvoAgent nor GPTSwarm optimize the agentic pattern inside individual agents, nor do they optimize few-shot samples.

Another closely related field of study is **AutoML**. Auto-sklearn (Feurer et al. 2015) used Bayesian optimization to jointly perform both algorithm selection and hyperparameters of a scikitlearn pipeline (Buitinck et al. 2013). While different, we see some analogy between algorithms and agentic patterns, and between hyperparameters and few-shot samples. DAUB first evaluates many candidate models on a small amount of data, then successively reduces candidates and increases data to ultimately pick a strong model (Sabharwal et al. 2016). The successive-halving algorithm takes a similar approach (Jamieson et al. 2016). Our approach is inspired by the same incremental data allocation idea. While both randomized search and Bayesian optimization are popular in AutoML, there are also more intricate approaches. For instance, TPOT uses genetic algorithms (Olson et al. 2016), and AlphaD3M uses Monte-Carlo tree search (Drori et al. 2018). We chose to start with a simpler technique that depends less on a well-behaved optimization space. That said, exploring more advanced AutoML optimizers could be fruitful future work for AutoPDL. Lale (Baudart et al. 2021) treats AutoML as a source-to-source optimization, similar to this paper, but unlike AutoPDL, it has not been used to optimize agentic patterns or prompts.

7 Conclusion

We present our AutoPDL approach for jointly optimizing prompting patterns and textual prompts for large language models, addressing the challenges associated with manual prompt engineering. By formulating the optimization as a discrete search over both agentic and non-agentic patterns, combined with instructions and few-shot samples, we leveraged successive halving to efficiently navigate this search space. Our evaluation across various datasets (FEVER, GSM8K, GSM-Hard, and MBPP+) and multiple models (from the LLaMA, Granite, and GPT families) demonstrates substantial accuracy improvements, up to 68.9 percentage points, and affirms that no single prompting strategy universally outperforms others across tasks and models. Additionally, generating code in a YAML-based prompt programming language (PDL) makes it executable, easy to modify, and readable by humans, supporting practical adoption and adaptation.

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8 Supplemental Material

8.1 Concrete Prompt Example

```
1 defs:
     prompt_pattern: cot
2
     num_demonstrations: 2
     demonstrations:
       data:
5
       - question: Tricia is a third of Amilia's age and Amilia is a quarter of Yorick's age. Yorick is twice
           Eugene's age and Khloe is a third of Eugene's age. Rupert is 10 years older than Khloe but 2 years
           younger than Vincent who is 22 years old. How old, in years, is Tricia?
         reasoning: |-
10
           Rupert is younger than Vincent by 2 years, so he is 22 years old - 2 years = <<22-2=20>>20 years old.
           Khloe is 10 years younger than Rupert so she is 20 years old - 10 years = 10 years old.
           Eugene is 3 times older than Khloe so he is 10 years old * 3 = <<10*3=30>>30 years old.
12
           Yorick is twice Eugene's age so he is 30 years old * 2 = <<30*2=60>>60 years old.
14
           Amilia is a quarter of Yorick's age so she is 60 years old / 4 = \langle 60/4=15 \rangle 15 years old.
           Tricia is a third of Amilia's age so she is 15 years old / 3 = <<15/3=5>>5 years old.
16
        answer: '5'
       - question: Emmalyn decided to paint fences in her neighborhood for twenty cents per meter. If there were
           50 fences in the neighborhood that she had to paint and each fence was 500 meters long, calculate
18
           the total amount she earned from painting the fences.
19
         reasoning: |-
20
           The total length for the fifty fences is 50*500 = <<50*500=25000>>25000 meters.
22
           If Emmalyn charged twenty cents to paint a meter of a fence, the total income she got from painting
           the fences is $0.20*25000 =$5000
23
         answer: '5000'
24
    instruction: Answer the questions to the best of your abilities.
25
26 text:
    - include: CoT.pdl
27
    - "${ instruction }\n\n"
28
    - call: ${ chain_of_thought }
29
30
      args:
         examples: ${ demonstrations }
31
32
         question: ${ question }
         model: ${ model }
33
```

Figure A1: Basic example of a concrete prompt configuration in PDL, using CoT pattern and two demonstrations.

1 Answer the questions to the best of your abilities. 3 Question: Tricia is a third of Amilia's age and Amilia is a quarter of Yorick's age. Yorick is twice Eugene's $_{\rm 4}$ age and Khloe is a third of Eugene's age. Rupert is 10 years older than Khloe but 2 years 5 younger than Vincent 6 who is 22 years old. How old, in years, is Tricia? 7 Answer: Let's think step by step. Rupert is younger than Vincent by 2 years, so he is 22 years 8 old - 2 years = <<22-2=20>>20 years old. 9 Khloe is 10 years younger than Rupert so she is 20 years old - 10 years = 10 years old. 10 Eugene is 3 times older than Khloe so he is 10 years old * 3 = <<10*3=30>>30 years old. 11 Yorick is twice Eugene's age so he is 30 years old * 2 = <<30*2=60>>60 years old. $_{\rm 12}$ Amilia is a quarter of Yorick's age so she is 60 years old / 4 = <<60/4=15>>15 years old. $\scriptstyle 13$ Tricia is a third of Amilia's age so she is 15 years old / 3 = <<15/3=5>>5 years old. 14 The answer is 5 15 ${\scriptstyle 16}$ Question: Emmalyn decided to paint fences in her neighborhood for twenty cents per meter. If there were 50 17 fences in the neighborhood that she had to paint and each fence was 500 meters long, calculate the total 18 amount she earned from painting the fences. 19 Answer: Let's think step by step. The total length for the fifty fences is 50*500 = <<50*500=25000>>25000 meters. 20 If Emmalyn charged twenty cents to paint a meter of a fence, the total income she got from painting the 21 fences is \$0.20*25000 =\$5000 22 The answer is 5000

```
24 Question: ${ question }
```

```
25 Answer: Let's think step by step.
```

Figure A2: Corresponding rendered prompt configuration for Figure A1. With the exception of the non-rendered \${ question } variable, this is the input to the language model.

See Figure A1 and Figure A2.

8.2 Tool Calling Code

```
description: tool use
   defs:
 2
     tools:
       data:
       - name: calc
         description: Calculator function
         arguments:
           expr:
             type: string
9
             description: Arithmetic expression to calculate
10
11 text:
12 - role: system
13 text: You are Granite, developed by IBM. You are a helpful AI assistant
       with access to the following tools. When a tool is required to answer
14
       the user's query, respond with < |tool_call|> followed by a JSON list of
15
       tools used. If a tool does not exist in the provided list of tools,
16
      notify the user that you do not have the ability to fulfill the request.
17
18
     contribute: [context]
19 - role: tools
   text: ${ tools }
20
21
     contribute: [context]
_{\rm 22} - "Out of 1400 participants, 400 passed the test. What percentage is that?\n"
23 - def: actions
     model: replicate/ibm-granite/granite-3.1-8b-instruct
24
     parser: json
25
26
    spec: [{ name: str, arguments: { expr: str }}]
27 - "\n"
28 - if: ${ actions[0].name == "calc" }
29
     then:
       lang: python
30
31
       code: result = ${ actions[0].arguments.expr }
```

Figure A3: Basic example of a PDL program.

See Figure A3.

8.3 Optimization

Algorithm 1 Successive Halving for PDL Optimization

Require: Program candidate set C, validation dataset D_{valid} , initial validation subset size v_{\min} , maximum validation subset size v_{\max}

```
1: v \leftarrow v_{\min}
```

```
2: while |C| > 1 do
```

- 3: $d_{\text{valid}} \leftarrow \text{first } v \text{ elements of } D_{\text{valid}} \text{ s.t. } d_{\text{valid}} \subseteq D_{\text{valid}} \text{ and } |d_{\text{valid}}| = v$
- 4: **for** each candidate $c_i \in C$ **do**
- 5: Compute loss $\ell_i \leftarrow \mathcal{L}(c_i, d_{\text{valid}})$
- 6: end for
- 7: $\mathcal{C} \leftarrow \text{top} \lfloor |\mathcal{C}|/2 \rfloor$ candidates with lowest loss
- 8: $v \leftarrow \min(v_{\max}, 2 \cdot v)$

```
9: end while
```

10: **return** Candidate in C with lowest loss

Figure A4: Illustration of the Successive Halving algorithm used to optimize the PDL program by pruning poor candidates on progressively larger validation subsets.

Figure A4 describes our optimization algorithm, based on successive halving (Jamieson et al. 2016). The algorithm accepts a candidate set sampled from possible configurations and demonstrations, a validation dataset to optimize against, an initial validation subset size, and a maximum validation subset size. AutoPDL allows the user to specify these options in a YAML configuration file, and ultimately saves its result as a PDL program. This source-to-source transformation enables the user to modify both the search space and the resulting optimized PDL program, allowing further modification and execution.

8.4 Search Space

The search space is the Cartesian product of the following discrete variables, each taking one value per candidate:

- (1) $A \in \mathcal{A} = \{$ Zero-Shot, CoT, ReWOO, ReAct $\}$, *i.e.*, the overall prompting pattern to apply.
- (2) Number of demonstrations $n \in \{0, 3, 5\}$. We selected these options as a representative sweep across no supervision, moderate few-shot use, and an upper-end case (in terms of token window). We limited the search space to three options to avoid combinatorial explosion and limit experiment cost.
- (3) If A = ReAct, System prompt ∈ {Granite Tools, LLaMa 3, Granite LLaMa}. As the system prompt instructs the model how to format tool calls, it only has an effect on benchmarks with JSON tool calling (FEVER, GSM8K, and GSM-Hard) for candidates with the ReAct prompt pattern. We note that only for MBPP+, ReWOO is not included as a prompt pattern, and that we always include two trajectories displaying iterative refinement, *i.e.*, an example of a solution failing the example test case, followed by a passing solution, in line with Wang et al. (2024). This effectively increases the number of trajectories to |*traj*| + 2.

8.5 Agent Trajectory Construction

To optimize over agentic patterns and trajectories, we require a set of example trajectories to use during optimization. For this purpose, we create a basic agentic trajectory $traj_i$ for each training example $\langle x_i, y_i \rangle$, following a rule-based transformation outlined below.

GSM8K. To demonstrate tool use in ReAct, we instead derive a trajectory *traj* as follows. We exploit the fact that there is at most one expression per reasoning step, by iterating through the steps. At each step, we append a 'thought' to the trajectory, consisting of the text leading up to the math expression, concatenated with a reflection 'I need to calculate'. We append a calculator tool call with the expression, and an 'observation', *i.e.*, the result of the expression. Finally, we append a thought 'The answer is ...', containing the ground truth answer, followed by the *finish* action with the answer. We follow the same procedure to create ReWOO trajectories, except we use slightly different wording, *e.g.*, 'Calculate xyz' in place of 'I need to calculate xyz', and omit the final thought and action. Additionally, we use string substitution to replace any assumed expression results in the trajectory with the corresponding variable.

FEVER. To produce agent trajectories, we iterate over each article associated with a claim, append a thought 'I need to search for ...', followed by the action, an observation containing the article summary, and finally a thought containing all the relevant sentences associated with that article for that claim, which we repeat for each article associated with a claim. This procedure is not ideal as there is no inherent order to the articles or sentences, even though there may be a natural ordering following the annotator's Wikipedia navigation. Finally, we append a thought 'The claim is true/false' and the finish action, both with the ground truth answer. For chain-of-thought, we perform the same procedure except we only include the concatenated evidence sentences, as there is no tool use. **MBPP+.** To generate sample agent trajectories from the training set, we follow the agent pattern (without feedback) in-context examples by Wang et al. (2024), which consists of the problem x, a thought such as "The intersection is elements that are in both lists", an execute action that contains proposed code *and* an assertion calling the proposed method with the test case input from the prompt and comparing its output. This is then followed by an observation containing the execution result, *i.e.*, either "[Executed Successfully with No Output]" or a stack traceback. This allows the agent to iterate on solutions (up to five times in our implementation). We use the full MBPP train set of 374 problems as D_{train} , and split the MBPP+ dataset into D_{valid} and D_{test} based on problem id membership in MBPP, leaving 39 and 224 validation and test problems respectively.

To generate synthetic trajectories from the training set, we start with the natural language specification and single test case (the prompt), append the thought "I should run a solution on the test case before proposing a solution.", followed by the ground truth solution and substitute in the prompt test case following the pattern [solution]res = ...; assert res == ..., "Expected ... but got ".format(res). Subsequently, we append the observation "[Executed Successfully with No Output]", the thought "There is no more AssertionError. I can now submit the solution.", and finally the solution action with the ground truth solution. This naive approach allows us to provide demonstration trajectories, albeit simplistic ones that assume the first solution is correct. Sampling a reflection or thought from a strong model may be beneficial (Li et al. 2025), but we restrict our trajectories to rule based transformations. As ReWOO is not reactive, *i.e.*, without execution feedback, it does not make sense for MBPP. Hence, we exclude it from our experiments.

8.6 Results Plot



Figure A5: Comparison of optimized prompt program performance across models and datasets. Each barbell shows the accuracy improvement, if any, over the zero-shot baseline.

In Figure A5, we visualize the results from Table 1 and Table 2.

8.7 Accuracy vs. iterations

In Figure A6, we visualize the accuracy across candidates versus the iterations of the optimization process, including a 95% confidence interval depicting the spread in accuracy across candidates. The confidence interval is computed using mean and 1,000 bootstraps. As the iterations increase, the number of candidates decreases, while the size of the validation set D_v increases.



Figure A6: Accuracy vs. iterations with 95% confidence interval.