DAWN-ICL: Strategic Planning of Problem-solving Trajectories for Zero-Shot In-Context Learning

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Abstract

Zero-shot in-context learning (ZS-ICL) aims to conduct in-context learning (ICL) without using human-annotated demonstrations. Existing ZS-ICL methods either use large language models (LLMs) to generate (input, label) pairs as *pseudo-demonstrations* or leverage historical pseudo-demonstrations to help solve the current problem. They assume that all problems are from the same task and traverse them in a random order. However, in real-world scenarios, problems usually come from diverse tasks, and only a few belong to the same task. The random traversing order may generate *unreliable* pseudo-demonstrations and lead to *error accumulation*. To address this problem, we reformulate ZS-**ICL** as a *planning* problem and propose a **D**emonstration-**AW**are Mo**N**te Carlo Tree Search (MCTS) approach (**DAWN-ICL**), which leverages MCTS to strategically plan the problem-solving trajectories for ZS-ICL. In addition, to achieve effective and efficient Q value estimation, we propose a demonstration-aware Q-value function and use it to enhance the *selection* phase and accelerate the *expansion* and *simulation* phases in MCTS. Extensive experiments demonstrate the effectiveness and efficiency of **DAWN-ICL** on in-domain and cross-domain scenarios, and it even outperforms ICL using human-annotated demonstrations. The code is available at https://github.com/txy77/MCTS4ZSICL.

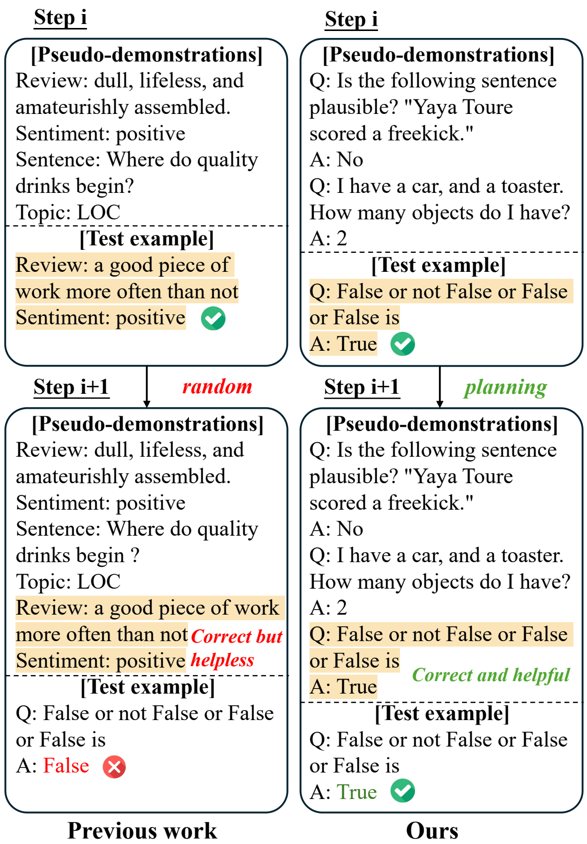

Figure 1: Comparison of our method with previous methods. Although both predictions at i-th step are correct, in previous work, the example is randomly selected and helpless. In contrast, in our method, the example is selected with planning and helpful.

1 Introduction

In-context learning (ICL) (Brown et al., 2020; Dong et al., 2023; Wang et al., 2024b) represents a significant advancement in the capabilities of large language models (LLMs). It allows LLMs to rapidly adapt to new tasks without updating the parameters by adding only a few examples as demonstrations to the input.

Although no training is required, most ICL work assumes access to large-scale external resources (*e.g.,* training dataset (Liu et al., 2022; Ye et al., 2023) or relevant corpus (Tanwar et al., 2023; Chatterjee et al., 2024)) for demonstration selection, which is usually not available in real-world scenarios. To eliminate this dependency, *zero-shot in-context learning* (ZS-ICL) (Lyu et al., 2023; Chen et al., 2023) is proposed, which uses LLMs to generate (input, label) pairs as *pseudo-demonstrations* for ICL. However, since LLMs are limited in data

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synthesis (Seddik et al., 2024; Longpre et al., 2024; Dohmatob et al., 2024), the performance of ZS-ICL usually falls behind ICL with human-annotated demonstrations. To remedy this deficiency, recent work (Su et al., 2024) employs previously predicted examples as the source of demonstrations, eliminating the need for input synthesis and reusing the predicted labels. This method assumes that test examples are from the same task and traverse them in a random order. However, in real-world scenarios, examples usually come from diverse tasks, and only a few belong to the same task. The random traversing order may cause LLMs to generate *unreliable* pseudo-demonstrations and lead to *error accumulation*, as illustrated in Figure 1.

To address the above problems, we aim to optimize the traversing order of examples in ZS-ICL and formulate it as a *planning* problem. To search the traversing order, we take inspiration from Monte Carlo Tree Search (MCTS) (Coulom, 2006), which can conduct a strategic tree search and strike a balance between exploration and exploitation. In the algorithm, MCTS maintains a state-action value function $Q(s, a)$ to estimate the expected future reward of taking action a in state s, which is updated by the simulation and back-propagation step in each iteration. However, for ZS-ICL, such an updating method is too costly to achieve accurate estimation since the state space is very large ($n!$ for n examples), and each state requires the LLM to perform one inference for reward calculation.

To this end, in this paper, we propose a novel **D**emonstration-**AW**are Mo**N**te Carlo Tree Search for ZS-**ICL**, namely **DAWN-ICL**. Our core idea is to leverage MCTS for planning the problem-solving trajectories in ZS-ICL. To achieve effective and efficient Q value estimation in MCTS, we propose to integrate the information of the pseudo-demonstration set into the Q-value function. With this demonstration-aware Q-value function, we can enhance the *selection* phase and accelerate the *expansion* and *simulation* phases of MCTS for more effective and efficient search. Furthermore, we design a calibration-enhanced aggregation method to derive the final prediction from MCTS, which aggregates results from multiple iterations and debiases the prediction with pre-trained priors. To validate the effectiveness of our approach, we conduct experiments on the in-domain and cross-domain scenarios of BBH and MMLU across various LLMs. The experimental results show that **DAWN-ICL** consistently surpasses the best ZS-ICL baseline method and even outperforms ICL using human-annotated demonstrations.

Our contributions can be summarized as follows:

• To the best of our knowledge, we are the first to formalize ZS-ICL as a planning problem, which is closer to real-world scenarios.

• We propose a demonstration-aware MCTS for ZS-ICL to achieve a more effective and efficient search for the problem-solving trajectories.

• Extensive experiments demonstrate the effectiveness of our approach on in-domain and cross-domain scenarios, and it even outperforms ICL using human-annotated demonstrations.

2 Related Work

Zero-shot In-context Learning. Zero-shot in-context learning (ZS-ICL) (Lyu et al., 2023; Chen et al., 2023; Su et al., 2024) aims to conduct in-context learning (ICL) using model-generated pseudo-demonstrations. Most ZS-ICL work separately generates pseudo-demonstrations for each example (Lyu et al., 2023; Chen et al., 2023). There is also some work that employs previously predicted examples as demonstrations and stores them in memory for future usage (Su et al., 2024). However, these methods traverse examples in a random order, which may lead to error accumulation. In this paper, we reformulate ZS-ICL as a planning problem and search for the optimal problem-solving order.

Enhancing LLMs with Planning. Recent advancements in enhancing LLMs through planning have shown promising results (Yao et al., 2023; Hao et al., 2023; Wan et al., 2024; Wang et al., 2024a). They often engage in deliberate reasoning processes by utilizing strategic planning algorithms like MCTS (Coulom, 2006) to explore intermediate steps. In this work, we aim to better utilize the in-context learning ability of LLMs by performing a novel demonstration-aware MCTS for ZS-ICL over the demonstration space.

3 Methodology

In this section, we present our demonstration-aware MCTS for ZS-ICL, namely **DAWN-ICL**. We first give an overview of our approach, then discuss how to integrate the information of demonstrations into the Q-value function, and finally present the planning approach to ZS-ICL. The overall architecture of **DAWN-ICL** is illustrated in Figure 2.

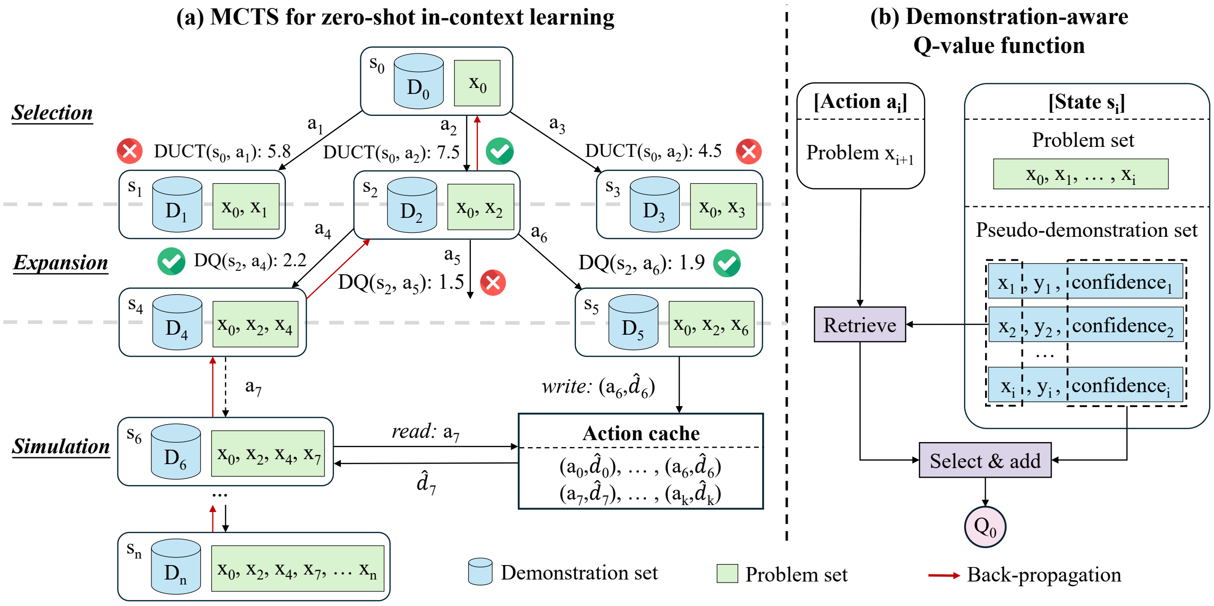


Figure 2: The overview of **DAWN-ICL**. (a) An illustration of the four phases in MCTS. We select nodes using our proposed DUCT (Eq. 3), perform expansion using our proposed DQ function (Eq. 1), accelerate simulation with an action cache supported by the DQ function, and finally back-propagate the rewards. (b) We improve the Q-value function with pseudo-demonstration information. We retrieve k pseudo-demonstrations and add the score of confidence and similarity as the initial value of the Q function.

3.1 Overview of Our Approach

Problem formulation. Zero-shot in-context learning (ZS-ICL) enables task adaptation of LLMs at test time without using human-labeled examples as the demonstration. Formally, given an LLM $\mathcal{M}$ and a set of n test examples $\mathcal{E} = \{(x_k, y_k)\}_{k=1}^{n}$, at i-th step, an example x_i is first selected from $\mathcal{E}$, and then the pseudo-demonstration $d_i = f_c(x_i, \mathcal{D}_{i-1})$ for x_i is constructed based on the existing pseudo-demonstration set $\mathcal{D}_{i-1}$. Based on this, the LLM makes the prediction $\hat{y}_i = f_p(x_i, d_i; \mathcal{M})$ and obtains a new pseudo-demonstration $\hat{d}_i = (x_i, \hat{y}_i)$. Then, the pseudo-demonstration set is updated as $\mathcal{D}_i = f_u(\mathcal{D}_{i-1}, \hat{d}_i)$. The above process is repeated until all the problems in $\mathcal{E}$ are solved.

The general planning framework. In existing work (Su et al., 2024), the test examples are assumed to belong to the same task, and the example to solve at each step (x_i) is usually randomly selected. However, in real-world scenarios, test examples come from diverse tasks, and only a few belong to the same task, limiting the performance. To solve this, one feasible way is to optimize the traversing order of test examples. This is because ICL is sensitive to the selection of demonstrations (Liu et al., 2022). Hence, the order of traversing is important for effectively leveraging historical examples as pseudo-demonstrations to help solve the current one. To this end, our idea is to formalize ZS-ICL as a planning problem using a Markov Decision Process (MDP), represented by the tuple $(\mathcal{S}, \mathcal{A}, T, r)$. In this planning framework, we define the state $s_i \in \mathcal{S}$ as the set of test examples that have been solved at i-th step, along with the pseudo-demonstration set $\mathcal{D}_i$. The action $a_i \in \mathcal{A}$ is to select the next problem x_{i+1} to solve. The transition function T from the current state s_i to the next state s_{i+1} first performs the pseudo-demonstration construction function f_c, then the prediction function f_p to solve x_{i+1}, and finally the pseudo-demonstration set updating function f_u to obtain the new state s_{i+1}. The reward function $r_i = r(s_i, a_i)$ measures the quality of the action a_i applied to the state s_i. Since ground-truth labels are not available at test time, we take the confidence of model prediction in f_p as the reward, which has been shown to be aligned with the model performance (Xiong et al., 2024; Zhang et al., 2024).

Monte Carlo Tree Search for zero-shot ICL. Our approach is inspired by the powerful planning algorithm Monte Carlo Tree Search (MCTS), which can be used to strategically conduct tree search for problem-solving trajectories in ZS-ICL and strike a balance between exploration and exploitation to find high-reward trajectories. To perform an effective search, MCTS maintains a state-action value function $Q : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$, where $Q(s, a)$ estimates the expected future reward of taking action a in state s. For ZS-ICL, the quality of the pseudo-demonstration set in the current state is also an important signal for Q values since ICL is known to be sensitive to demonstrations (Yoo et al., 2022; Liu et al., 2022). Taking this into consideration, we design specific metrics to integrate this information and propose a *demonstration-aware* Q-value function (Section 3.2). Based on this, we conduct MCTS for ZS-ICL (Section 3.3), where the proposed Q-value function is used to enhance the *selection* phase and accelerate the *expansion* and *simulation* phases. Furthermore, we design a calibration-enhanced aggregation method to derive the final prediction from MCTS, which aggregates results from multiple iterations and debiases the prediction with pre-trained priors. In what follows, we introduce these two parts in detail.

3.2 Demonstration-aware Q-value Function

The MCTS algorithm maintains a state-action value function $Q(s, a)$ to estimate the expected reward of taking the action a in the state s. Originally, this Q-value function is updated by simulating the future states (*i.e.,* simulation) and aggregating their rewards (*i.e.,* back-propagation). However, for ZS-ICL, such an updating method is too costly to achieve accurate estimation since the state space is very large, and the reward calculation of each state requires the LLM to perform one inference.

To perform effective Q value estimation, we propose to leverage the contextual information of the current state and action to initialize the Q value. The performance of ICL is known to be highly dependent on the selection of demonstrations. Inspired by this, we propose to initialize the Q value by evaluating the quality of the pseudo-demonstration set D_i in the current state s_i with respect to the problem x_{i+1} (*i.e.,* action a_i). Specifically, we first retrieve k_d demonstrations that are most semantically similar to the problem, and then evaluate their quality by aggregating their confidence and similarity scores. The demonstration-aware Q-value function DQ can be represented as follows:

$$\mathrm{DQ}(s, a) = Q_0(s, a) + w_Q \cdot Q(s, a), \quad (1)$$

$$Q_0(s, a) = \frac{1}{k_d} \sum_{i=1}^{k_d} \left(C(d_i) + S(d_i, x_{i+1})\right), \quad (2)$$

where d_i is the retrieved demonstration, $C(d_i)$ is the confidence score of the demonstration from the prediction function f_p, $S(d_i, x_{i+1})$ is the similarity score between the demonstration and the problem x_{i+1} chosen by the action measured with the BGE model (Xiao et al., 2024), and w_Q is a constant to balance the initial value ($Q_0(s, a)$) and updated value ($Q(s, a)$).

With this demonstration-aware Q-value function, the estimation of Q values can be more accurate with a limited computational budget. Based on this, we conduct MCTS for ZS-ICL, where the demonstration-aware Q-value function is used to enhance the *selection* step and accelerate the *expansion* and *simulation* step. In the next section, we will introduce this in detail.

3.3 Strategic Planning for Zero-shot In-context Learning

In this section, we first introduce the demonstration-aware MCTS to plan problem-solving trajectories for ZS-ICL, then detail the calibration-enhanced aggregation method to derive the final prediction from the searched trajectories.

3.3.1 Demonstration-aware MCTS

The reformulation of ZS-ICL as a planning problem (Section 3.1) enables us to leverage principle planning algorithms, notably the Monte Carlo Tree Search (MCTS). Specifically, MCTS iteratively constructs a tree for search, where each node represents a state and each edge represents an action and the transition from the current state to the next one by applying the action. Each iteration consists of four phases: selection, expansion, simulation, and back-propagation. For ZS-ICL, we randomly select a problem with the empty pseudo-demonstration set as the initial state and execute the algorithm until a predefined number of iterations is reached. In each iteration, we use the proposed demonstration-aware Q-value function to enhance the *selection* phase and accelerate the *expansion* and *simulation* phases. Next, we detail the four phases of MCTS for planning problem-solving trajectories in ZS-ICL. The pseudo-code is presented in Algorithm 1.

Selection. The first phase of MCTS is to select the most promising part of the existing tree for expansion. A well-known selection strategy is the Upper Confidence bounds applied to Trees (UCT) algorithm (Kocsis and Szepesvári, 2006), which can effectively balance exploration (less visited times) and exploitation (high Q values). However, as mentioned in Section 3.2, the estimation of Q values is too costly to be accurate in ZS-ICL. Therefore, we propose to integrate our DQ function (Eq. 1) into UCT. This demonstration-aware UCT function DUCT can be represented as follows:

$$\text{DUCT}(s,a) = \text{DQ}(s,a) + w_a \sqrt{\frac{\ln N(s)}{N(\mathrm{c}(s,a))}}, \quad (3)$$

where $N(s)$ is the number of times node s has been visited, $\mathrm{c}(s,a)$ is the child node for s after applying action a, and w_a is a constant to balance exploration ($U(s,a)$) and exploitation ($\text{DQ}(s,a)$). We start from the root node (*i.e.,* initial state s_0) and repeatedly select a child node with the maximum DUCT value until reaching a leaf node.

Expansion. This phase expands the tree by generating child nodes for the leaf node selected above. Since the action space of a state (*i.e.,* remaining problems to solve) can be large, we use our proposed DQ function for efficient action selection. Specifically, we first calculate the value of each action using Eq. 1, and then choose the top-k_a actions with the highest values for expansion. For each selected action a_i, we need to predict the corresponding state s_{i+1}, which is the role of the transition function T described in Section 3.1. In T, the first step is to construct the pseudo-demonstrations for the problem x_{i+1} selected by the action (*i.e.,* function f_c). To make the pseudo-demonstrations relevant and diverse, we first retrieve k most semantically similar ones with the problem x_{i+1} from the pseudo-demonstration set to increase the relevance, and then randomly select samples with different pseudo-labels from them to enhance the diversity. With the pseudo-demonstrations d_{i+1}, the second step in T is to predict the label for the problem x_{i+1} using the LLM (*i.e.,* function f_p). Here, we use greedy decoding to generate the prediction. Finally, the predicted label $\hat{y}_{i+1}$ paired with the problem x_{i+1} is added to the pseudo-demonstration set (*i.e.,* function f_u), and the new state s_{i+1} is obtained. For the expanded nodes, we choose the one with the largest reward for the next simulation phase.

Simulation. This phase simulates the future trajectories for the node selected from the previous expansion step. The simulation process typically involves a roll-out policy to reach the terminal state and calculate the future rewards. For simplicity, we follow the same procedure as the expansion phase, *i.e.,* selecting k_a candidate actions with the highest DQ values and picking the one with the largest reward. To further accelerate the simulation process, we propose a cache mechanism based on the DQ function. Specifically, we maintain the maximum DQ value for each action a_i as $\text{DQ}^{(i)}_{\max}$ and record the corresponding pseudo-demonstration $\hat{d}_i = (x_{i+1}, \hat{y}_{i+1})$. If $\text{DQ}^{(i)}_{\max}$ breaks through the threshold ϵ, we add the $(a_i, \hat{d}_i)$ pair into the cache. In the simulation process, if we take an action that exists in the cache, the pseudo-demonstration is read from the cache, and we skip the transition function T to directly obtain the new state.

Back-propagation. This phase is executed when we reach a terminal node. We back-propagate the rewards along the path from the terminal node to the root node by updating the Q-value function. Specifically, we update $Q(s_i, a_i)$ by calculating the mean rewards in all the future trajectories starting from s_i.

3.3.2 Calibration-Enhanced Aggregation

The above MCTS algorithm could produce multiple trajectories and predictions for each test example through multiple iterations. In this part, we introduce a calibration-enhanced aggregation method to produce the final answer while debiasing the answer with pre-trained priors.

Aggregation. Considering that in ICL, the unique correct answer can be derived from multiple different demonstrations, we collect the predictions from each iteration of MCTS to make the final prediction. Specifically, we calculate the average probabilities for each label and select the one with the highest probability as the final answer, which can be represented as follows:

$$y^* = \arg\max_{y_i \in \mathcal{Y}} \frac{1}{N_i} \sum_{j=1}^{N_i} \Pr(y_i | x, d_j; \mathcal{M}), \quad (4)$$

where $\mathcal{Y}$ is the label space, N_i is the number of predictions for label y_i, and $\Pr(y_i|x, d_j; \mathcal{M})$ is the probability for y_i given by the LLM $\mathcal{M}$ with problem x and pseudo-demonstration d_j as the input.

Calibration. LLMs are known to suffer from common token bias (Zhao et al., 2021), which means they are biased towards tokens common in their pre-training data. To debias the prediction of LLMs, we adopt a calibration strategy based on prior probability. Specifically, we first obtain the prior probability of each label by calculating its average probability predicted by the LLM across all the test examples. Then, we derive the calibrated probability of each prediction by dividing the prior probability. We can integrate this strategy with aggregation, which is represented as follows:

$$y^* = \arg\max_{y_i \in \mathcal{Y}} \frac{1}{N_i} \sum_{j=1}^{N_i} \frac{\Pr(y_i|x, d_j; \mathcal{M})}{\Pr(y_i|\mathcal{M})}, \quad (5)$$

$$\Pr(y_i|\mathcal{M}) = \frac{1}{|\mathcal{E}|} \sum_{j=1}^{|\mathcal{E}|} \Pr(y_i|x_j; \mathcal{M}), \quad (6)$$

where $\Pr(y_i|\mathcal{M})$ is the prior probability of the LLM $\mathcal{M}$ for y_i and $\Pr(y_i|x_j; \mathcal{M})$ is the zero-shot probability for y_i given by the LLM $\mathcal{M}$ with only the problem x_j as the input.

4 Experiments

In this section, we first set up the experiments, then report the results and conduct a detailed analysis.

4.1 Experimental Setup

Datasets. To evaluate the effectiveness of our method, following Su et al. (2024), we conduct experiments on the BIG-Bench Hard (BBH) (Suzgun et al., 2023) and Massive Multitask Language Understanding (MMLU) (Hendrycks et al., 2021) benchmarks. Specifically, we consider two scenarios: in-domain and cross-domain. For the in-domain scenario, we evaluate each task of BBH and MMLU separately. For the cross-domain scenario, we randomly select 8 samples from each task of BBH to construct a dataset called BBH-mini.

Baselines. To facilitate a systematic comparison, we select several representative methods:

• **Zero-shot**: The model directly makes predictions without any demonstration.

• **Few-shot** (Brown et al., 2020): The model makes predictions with human-annotated demonstrations. It is not entirely fair to compare it with other methods, as it uses external information.

• **Self-ICL** (Chen et al., 2023): The model makes predictions with self-generated pseudo-demonstrations.

• **DAIL** (Su et al., 2024): The model makes predictions with pseudo-demonstrations retrieved from previously predicted examples.

Models. We use representative open-source LLMs (*i.e.,* Llama3.1-8B (Dubey et al., 2024), Qwen2.5-7B (Yang et al., 2024), and Mistral-7B-v0.3 (Jiang et al., 2023) and a close-source LLM (*i.e.,* GPT-4o-mini (OpenAI, 2024)) for experiment.

Implementation Details. In MCTS, we set the number of iterations as 5. For the Q' function, we set k_d as 30 and w_Q as 1. For the selection phase, we set w_a in Eq. 3 as 5. For the expansion phase, we set k_a as 3. For the simulation phase, we set ϵ as 1.5. Following Su et al. (2024), we set the number of demonstrations in f_p to 3 for BBH and 4 for MMLU. Notably, we can not obtain the logits of GPT-4o-mini, so we do not use calibration for it. To test the full potential of our approach, we also consider removing the cache mechanism in the simulation phase, named "DAWN-ICL w/o cache".

4.2 Experimental Results

In-domain scenario. Table 1 presents the results across various LLMs on the in-domain scenario. As we can see, Self-ICL performs poorly and even worse than zero-shot prompting for some LLMs. The main reason is that LLMs are limited in data synthesis (Seddik et al., 2024) and may even have insufficient domain knowledge for specific tasks. Thus, they struggle to generate high-quality pseudo-demonstrations. In contrast, DAIL shows decent improvements and consistently outperforms zero-shot prompting. DAIL employs previously predicted examples as the source of demonstrations, eliminating the need for input synthesis to improve the quality of pseudo-demonstrations. However, DAIL still underperforms few-shot prompting sometimes, as it randomly selects examples at each step, and the historical examples may not be beneficial for the current one. Finally, **DAWN-ICL** surpasses all the ZS-ICL baselines by a large margin and even consistently outperforms few-shot prompting. We reformulate ZS-ICL as a planning problem and use MCTS to search for the optimal traversing order. Thus, the historical examples can better help the current one, as they are selected based on Q' values rather than chosen at random. In addition, we observe that integrating a cache mechanism has minimal impact on performance but can significantly speed up the expansion and simulation processes of MCTS. More detailed analysis of search efficiency are presented in Section 4.3.2.

Cross-domain scenario. For the cross-domain scenario, the results are shown in Table 2. Similar to the in-domain scenario, Self-ICL and DAIL (ran-

Task		BBH			MMLU				
		Binary Choice	Multiple Choice	Average	STEM	Human anities	Social Sciences	Other	Average
Llama3.1-8B	Zero-shot	52.26	38.81	42.32	48.91	52.22	68.28	65.82	58.00
	Few-shot	53.93	42.42	45.42	51.92	56.77	73.94	69.13	62.18
	Self-ICL	50.87	31.64	36.65	43.51	47.57	61.94	58.77	52.29
	DAIL	52.82	39.08	42.66	52.65	56.30	75.14	70.04	62.65
	DAWN-ICL	60.26	43.69	48.01	54.04	58.11	75.24	70.94	63.79
	DAWN-ICL w/o cache	**61.86**	**43.86**	**48.56**	**54.65**	**58.94**	**76.34**	**71.58**	**64.58**
Qwen2.5-7B	Zero-shot	59.71	46.56	49.99	64.03	59.64	80.18	74.90	68.50
	Few-shot	55.74	**50.76**	52.06	67.68	64.31	82.03	75.99	71.54
	Self-ICL	52.75	45.83	47.63	62.92	56.77	75.98	71.29	65.57
	DAIL	55.74	47.25	49.46	67.71	64.59	82.74	76.29	71.86
	DAWN-ICL	64.51	49.21	53.20	**68.41**	64.91	83.26	75.47	72.06
	DAWN-ICL w/o cache	**65.90**	50.17	**54.27**	68.03	**65.27**	**83.82**	**76.44**	**72.43**
Mistral-7B	Zero-shot	53.79	33.46	38.76	46.69	52.75	66.17	64.85	57.01
	Few-shot	60.26	40.03	45.31	51.74	54.98	71.40	68.10	60.70
	Self-ICL	56.44	33.51	39.48	40.63	48.20	58.21	58.80	51.04
	DAIL	58.39	36.43	42.15	50.62	54.54	72.44	68.59	60.69
	DAWN-ICL	61.10	41.80	46.83	51.51	57.32	72.77	**68.97**	61.98
	DAWN-ICL w/o cache	**62.14**	**42.24**	**47.43**	**52.14**	**58.51**	**73.06**	68.78	**62.54**
GPT-4o-mini	Zero-shot	52.26	37.43	41.30	40.37	52.77	59.05	56.90	52.28
	Few-shot	**65.97**	49.56	53.84	45.26	64.34	71.17	69.07	62.60
	Self-ICL	63.47	47.91	51.97	48.37	59.17	71.56	65.59	60.88
	DAIL	64.44	50.00	53.77	44.08	61.91	61.46	59.25	57.22
	DAWN-ICL	62.98	54.10	56.41	51.95	65.65	70.75	68.20	64.26
	DAWN-ICL w/o cache	64.93	**54.25**	**57.03**	**53.38**	**66.18**	**73.12**	**69.18**	**65.62**

Table 1: Performance comparison across various LLMs on the in-domain scenario using BBH and MMLU. The best method in each group is marked in **bold**, and the second-best method is marked with an underline.

Model	Llama3.1 -8B	Qwen2.5 -7B	Mistral -7B	GPT-4o -mini
Zero-shot	36.41	48.37	36.41	37.50
Few-shot	40.76	49.46	39.67	54.35
Self-ICL	40.22	47.28	35.87	51.09
DAIL (random)	35.33	44.02	39.13	50.00
DAIL (sequential)	39.13	47.28	40.22	54.89
DAWN-ICL	43.48	**51.09**	**47.83**	55.43
DAWN-ICL w/o cache	**44.57**	50.54	44.57	**59.24**

Table 2: Performance comparison across various LLMs on the cross-domain scenario using BBH-mini. The best method in each group is marked in **bold**, and the second-best method is marked with an underline.

dom) with the random traversing order perform poorly. In contrast, if DAIL sequentially deals with each task (*i.e.,* DAIL (sequential)), the performance improves greatly, which means that traversing order is important, especially in the cross-domain scenario. Finally, **DAWN-ICL** achieves the best performance and even surpasses the few-shot prompting. It demonstrates that our approach is generally applicable to various scenarios in ZS-ICL.

Task	BBH		MMLU	
Model	Llama3.1 -8B	Qwen2.5 -7B	Llama3.1 -8B	Qwen2.5 -7B
DAWN-ICL	48.01	53.20	63.79	72.06
w/o Q_0 function	47.12	52.53	63.20	71.88
w/o aggregation	45.94	53.08	63.15	71.98
w/o calibration	44.96	51.12	63.11	71.91

Table 3: Ablation study on BBH and MMLU.

4.3 Detailed Analysis

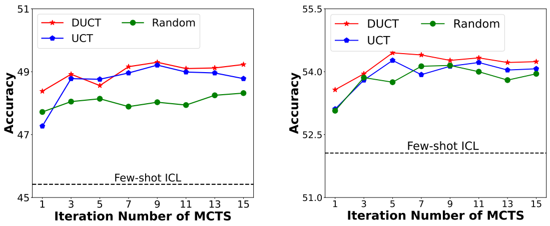
In this part, we construct a detailed analysis of the effectiveness of our approach.

4.3.1 Ablation Study

Our approach incorporates several important components to improve search quality and performance. To validate the effectiveness of each component, we conduct the ablation study by removing demonstration-aware initial Q_0 value function, aggregation, and calibration strategies, respectively. The results are shown in Table 3. We can see that removing any component would lead to performance

Task	MC	Greedy	Beam	MCTS	MCTS w/o cache
Boolean	75.20	79.20	82.00	80.40	**83.20**
Formal	50.40	52.40	52.40	52.00	**54.00**
Geometric	28.80	33.60	40.80	**43.60**	42.40
Hyperbaton	70.40	71.60	78.00	78.80	**80.40**
Movie	72.40	78.80	81.60	76.00	**83.60**
Reasoning	37.60	41.60	45.60	**50.00**	48.40
Snarks	57.30	57.30	59.55	58.43	**61.80**
Accuracy	56.01	59.21	62.85	62.75	**64.83**
Time	$\times$1.0	$\times$1.0	$\times$14.8	$\times$4.8	$\times$14.8

Table 4: Average performance and inference time of different search methods on the selected tasks of BBH.



(a) Llama3.1-8B (b) Qwen2.5-7B

Figure 3: Accuracy on BBH with increasing numbers of iterations using the selection strategy of random, UCT, and our proposed DUCT.

degradation. It indicates that all the components in our model are helpful. Among them, performance decreases the most after removing the calibration strategy. This indicates the importance of calibration in our approach since it can effectively mitigate the inherent biases of LLMs.

4.3.2 The Impact of Search Strategy

To systematically investigate the MCTS-based planning method in our approach, we conduct a comprehensive ablation study by comparing it with several alternative search methods on Llama3.1-8B, including a single Monte Carlo (MC) search, greedy search, and beam search. To ensure a fair comparison, we replace MCTS with other search methods while keeping other factors unchanged. Specifically, MC search is a directionless method, which randomly selects one action at each step. Greedy search selects the action with the highest DUCT score at each step. Both methods perform a single pass through the problem space, meaning that LLMs generate one answer for each sample, which we use as the final answer. Beam search maintains multiple promising paths by selecting the top beam-size paths with the maximum mean DUCT values at each step. To keep a similar exploration space with MCTS, we set the expansion number for each node (beam size) to 3 and keep the best 5 nodes for the next iteration to obtain the same number of trajectories. In addition, we use the same calibration-enhanced aggregation method in Section 3.3.2 to obtain the prediction results.

The results are shown in Table 4. Greedy search is better than MC, which suggests the importance of a structured search strategy. Beam search further improves the performance by maintaining multiple paths and exploring them in parallel. However, these methods cannot strategically explore the problem space since they cannot look ahead and backtrack. Thus, they are short in either performance or efficiency. In contrast, our demonstration-aware MCTS can perform better with less inference budget. Our approach explores the problem space with DCUT and efficiently looks ahead through memory-augmented simulation, making it more powerful for the complex search space in ZS-ICL.

4.3.3 Exploration Efficiency Analysis

In this section, we conduct an exploration efficiency analysis of our approach. Due to limited computational resources, we run MCTS with up to 15 iterations and conduct experiments on BBH using Llama3.1-8B and Qwen2.5-7B. To keep the same number of inference times across different strategies, we do not use the cache method to ensure a fair comparison. The results are presented in Figure 3. As the number of iterations increases, the performance of our approach (DUCT) quickly improves and reaches the plateau with about 9 iterations, showing its effectiveness and efficiency. Compared with the original selection strategy UCT in MCTS, our proposed DUCT strategy achieves faster convergence and better performance. The main reason is that it uses the demonstration information to initialize Q values, achieving a more reliable estimation of the expected future reward.

4.4 The Effect of Demonstration Selection Strategy

In this part, we explore the effect of various demonstration selection methods (*i.e.,* random selection, BM25 (Robertson and Zaragoza, 2009), TopK (Liu et al., 2022), and TopK+DPP (Ye et al., 2023)). Specifically, the random selection method refers to randomly selecting the demonstrations for each sample. BM25 selects demonstrations by computing the BM25 relevance score, which is a popular ranking function in information retrieval. TopK se-

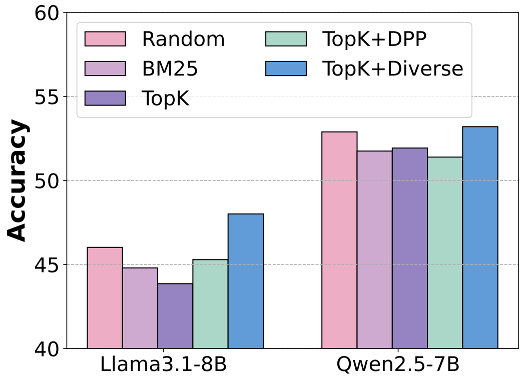


Figure 4: The Accuracy (%) of BBH with different demonstration selection methods.

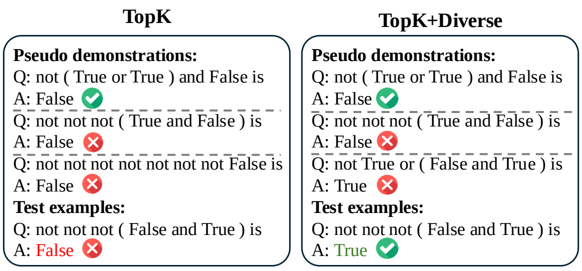


Figure 5: The error accumulation phenomenon of the similarity-based demonstration selection method.

lects demonstrations that are semantically relevant to each sample. TopK+DPP employs a two-stage demonstration selection strategy. In the first stage, this method retrieves k_d candidates that are semantically similar to the input sample. In the second stage, Determinantal Point Processes (DPP) are applied to simulate interactions between the query and the candidate samples to select a diverse set of demonstrations.

The experimental results are illustrated in Figure 4. It can be observed that the similarity-based demonstration selection methods (*i.e.,* BM25 and TopK) perform worse than the random selection method. This can be attributed to the fact that these methods tend to use samples with the same label as demonstrations, which can lead to incorrect predictions and subsequent error accumulation. As shown in Figure 5, selecting semantically similar samples typically results in demonstrations that have the same label. Due to the copying phenomenon of ICL (Olsson et al., 2022), LLMs can exhibit majority bias (Zhao et al., 2021), which results in generating answers that are frequent in the demonstrations. Furthermore, these incorrectly predicted demonstrations can mislead subsequent predictions made by the LLMs. To address this issue, we select samples with more diverse labels, allowing LLMs to make predictions without being influenced by the labels of the demonstrations. Experimental results indicate that our proposed TopK+Diverse demonstration selection method consistently achieves the best performance across different LLMs, confirming the effectiveness of incorporating label diversity into the demonstration selection process for ZS-ICL.

5 Conclusion

In this paper, we introduce **DAWN-ICL**, a strategic *planning* approach for ZS-ICL that utilizes MCTS to search for the optimal problem-solving sequence. To achieve effective and efficient Q value estimation, we propose a novel demonstration-aware Q-value function that aims to enhance the *selection* phase and accelerate the *expansion* and *simulation* phases in MCTS. Experimental results demonstrate that our approach consistently outperforms existing ZS-ICL methods and even performs better than ICL with human-annotated demonstrations. Overall, our work highlights the importance of planning for ZS-ICL in real-world scenarios, paving the way for more effective deployment of LLMs.

6 Limitations

In this work, we employ the MCTS algorithm for planning the problem-solving path in ZS-ICL. More advanced planning algorithms remain to be explored. We estimate the expected future rewards by simulation and back-propagation. This is quite time-consuming for ZS-ICL since each simulated state requires the LLM to perform one inference for reward calculation. A promising direction for future work is to train a value model for efficient evaluation (Wang et al., 2024a). In addition, due to limitations in computational resources, we only conduct experiments on several representative LLMs.

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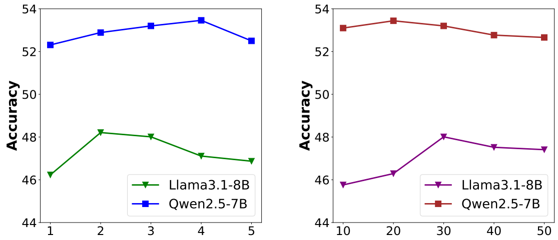
Model	Gemma2-9B	Qwen2.5-14B	Qwen2.5-32B
Zero-shot	47.58	56.61	59.74
Few-shot	53.87	59.37	64.80
Self-ICL	45.22	54.35	57.30
DAIL	38.89	57.88	62.13
DAWN-ICL	55.89	61.37	66.72
DAWN-ICL w/o cache	**57.01**	**63.35**	**68.44**

Table 5: Performance comparison across larger open-source LLMs on BBH. The best method in each group is marked in **bold**, and the second-best method is marked with an underline.

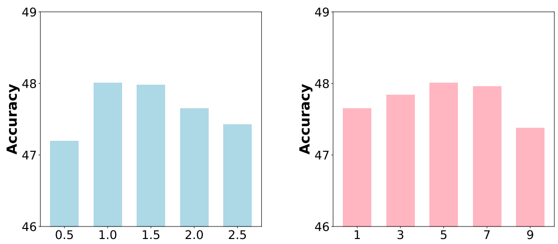
Method	MultiArith	Last Letter
Zero-shot	94.44	86.00
Few-shot	94.44	88.00
Self-ICL	96.67	86.67
DAIL	96.11	89.33
DAWN-ICL	97.22	91.33
DAWN-ICL w/o cache	**98.33**	**92.00**

Table 6: Performance comparison on generation tasks using GPT-4o-mini. The best method in each group is marked in **bold**, and the second-best method is marked with an underline.



(a) The Number of Node Expansion on BBH.

(b) The Number of the Retrieved Candidates on BBH.



(c) Analysis of the Hyper-parameter w_a on BBH using Llama3.1-8B.

(d) Analysis of the Hyper-parameter w_Q on BBH using Llama3.1-8B.

Figure 6: Performance comparison *w.r.t.* the number of expansion nodes, retrieved candidates, balance constant between exploration and exploitation, and balance constant of the initial and updated Q-value of **DAWN-ICL**.

A More experiments

A.1 The Effect of Larger Models

In this part, we conduct experiments on larger open-source LLMs (*i.e.,* Gemma2-9B, Qwen2.5-14B, and Qwen2.5-32B) on BBH. As illustrated in Table 5, **DAWN-ICL** can outperform other competitive ZS-ICL baselines and even surpass few-shot prompting with human-labeled demonstrations on larger LLMs. This further demonstrates the effectiveness of our proposed method.

A.2 Experiments on Generation Tasks

To confirm the effectiveness of our proposed method on generation tasks, we conduct experiments on two types of generation tasks (*i.e.,* math reasoning and symbolic reasoning) using GPT-4o-mini. Specifically, for the math reasoning problem, we use Multiarith (Roy and Roth, 2015) for evaluation. For the symbolic reasoning problem, we use Last Letter Concatenation (Wei et al., 2022) for evaluation. As shown in Table 6, **DAWN-ICL** consistently outperforms other methods on these generation tasks. This further highlights the importance of strategically planning problem-solving trajectories and demonstrates the effectiveness of **DAWN-ICL**.

A.3 Hyper-parameters Analysis

DAWN-ICL includes a few hyper-parameters to tune. In this section, we report the tuning results of four hyper-parameters on BBH: the expansion size (*i.e.,* k_a), the number of retrieved candidates (*i.e.,* k_d), the balance constant between exploration and exploitation (*i.e.,* w_a), and the balance constant between the initial and updated Q value (*i.e.,* w_Q). The results are presented in Figure 6. We observe that **DAWN-ICL** achieves the best performance when the expansion size is set to 3. If the expansion size is too large, it may introduce suboptimal states which can lead to a shift in the exploration direction. Conversely, if the expansion size is too small, the tree will not expand sufficiently due to the absence of some important nodes. On the other hand, we find that the number of retrieved candidates cannot be too small or too large. If the number is too small, some important examples can be overlooked, which results in performance degradation. In contrast, if the number is too large, irrelevant examples can be introduced during the calculation of Q_0, leading to a deviation in the exploration direction. For w_a and w_Q, we

Method	Input Tokens	Output Tokens	Cost
	BBH		
Zero-shot	764K	15K	0.12
Few-shot	2324K	15K	0.36
Self-ICL	3537K	1197K	1.25
DAIL	2567K	15K	0.39
DAWN-ICL	3418K	20K	0.52
DAWN-ICL w/o cache	37836K	220K	5.81
	MMLU		
Zero-shot	1491K	14K	0.23
Few-shot	7761K	14K	1.17
Self-ICL	12364K	3435K	3.92
DAIL	7728K	14K	1.17
DAWN-ICL	28881K	52K	4.36
DAWN-ICL w/o cache	114446K	207K	17.29

Table 7: The number of consumed tokens and the cost (in US dollars) on BBH and MMLU using GPT-4o-mini.

find that they have minimal effect on performance, with the best results achieved when w_a is set to 5 and w_Q is set to 1.

B Details of Experimental Cost

In this section, we present detailed information on the experimental costs of GPT-4o-mini in Table 7.

C Detailed Results

In this part, we report the detailed experimental results on BBH and MMLU across four LLMs in Table 8, 9, 10, and 11.

D Example Prompts

In this part, we present the example prompt for BBH and MMLU.

Example Prompt for BBH

Pseudo demonstrations:
Q: Which statement is sarcastic?
Options:
(A) But his eyes were on the ball, shouldn't be a red
(B) But his cleats were on the ball, shouldn't be a red
A: (B)
Q: Is the following sentence plausible? "John Carlson scored in the third period."
A: yes
Q: Is the following sentence plausible? "Elias Lindholm beat the buzzer."
A: no
Test example:
Q: Is the following sentence plausible? "Marcelo got on the end of a through ball."
A: yes

Example Prompt for MMLU

Pseudo demonstrations:
Question: Objects that absorb light appear A.black B.white C.dark D.bright
Answer: A
Question: Of the following, most children will develop which skill first?
A.write with a pencil B.cut with a knife C.say a sentence D.clap their hands
Answer: D
Question: Which of the following most accurately explains why a pool with water temperature of 82 degrees may feel cool to a person who has been sunbathing, yet warm to a person who has been inside in the air conditioning?
A.Sensory restriction B.Perceptual constancy C.Relative clarity D.Sensory adaptation
Answer: B
Question: What part of the human body does a gastroenterologist examine?
A.Brain B.Skeleton C.Stomach D.Nose
Answer: A
Test example:
Question: Paper will burn at approximately what temperature in Fahrenheit?
A.986 degrees B.2125 degrees C.3985 degrees D.451 degrees
Answer: D

Algorithm 1 **DAWN-ICL**$(\mathcal{X}, s_0, t_\theta, r_\theta, k_a, \tau, \epsilon)$

Inputs:
  Problem set $\mathcal{X} = \{x_i\}_{i=1}^n$, Initial state s_0, deterministic state transition function t_θ,
  reward function r_θ, action expansion number k_a, iteration number τ, action cache threshold ϵ
Initialize:
  State to action mapping $A : \mathcal{S} \mapsto \mathcal{A}$, children mapping ch : $\mathcal{S} \times \mathcal{A} \mapsto \mathcal{S}$, rewards $r : \mathcal{S} \times \mathcal{A} \mapsto \mathbb{R}$,
  visited counter $\mathcal{N} : \mathcal{S} \mapsto \mathbb{N}$, action cache ac : $\varnothing$, State-action value function $Q : \mathcal{S} \times \mathcal{A} \mapsto \mathbb{R}$,
  Demonstration-aware state-action value function DQ : $\mathcal{S} \times \mathcal{A} \mapsto \mathbb{R}$
for $n \leftarrow 0, \dots, \tau - 1$ **do**
  $t \leftarrow 0$
  while $\mathcal{N}(s_t) > 0$ **do** ▷ selection
    Select a_t from $A(s_t)$ with the highest DUCT score based on Equation 3
    $s_{t+1} \leftarrow \text{ch}(s_t, a_t), \mathcal{N}(s_t) \leftarrow \mathcal{N}(s_t) + 1$
    $t \leftarrow t + 1$
  end while
  while s_t is not a terminal state **do** ▷ expansion and simulation
    Select a_t from $A(s_t)$ with the top-k_a DQ score based on Equation 1
    for $i \leftarrow 1, \dots, k_a$ **do**
      if a_t^i in Ac **then**
        Read $(x_i, \hat{y}_i)$ from Ac
      else
        Perform zero-shot in-context learning for x_i to generate $\hat{y}_i$
        $r_t^i \leftarrow r_\theta(s_t^i, a_t^i)$
        if $\text{DQ}_t^i > \epsilon$ **then**
          Write $(a_i, (x_i, \hat{y}_i))$ to Ac
        end if
      end if
      $s_{t+1}^i \leftarrow t_\theta(s_t, a_t^i)$
    end for
    $a_t^* \leftarrow \arg\max_{a_t^i \in A(s_t)} r_t^i(s_t^i, a_t^i)$
    $s_{t+1} \leftarrow \text{ch}(s_t, a_t^*), \mathcal{N}(s_t) \leftarrow \mathcal{N}(s_t) + 1$
    $t \leftarrow t + 1$
  end while
  $T \leftarrow$ the actual number of simulation steps
  for $t \leftarrow T - 1, \dots, 0$ **do** ▷ back-propagation
    Update $Q(s_t, a_t)$ with $\{r_t, r_{t+1}, \dots, r_T\}$.
  end for
end for

BBH Tasks	Llama3.1-8B						Qwen2.5-7B					
	ZS	FS	Self-ICL	DAIL	**DAWN-ICL**	**DAWN-ICL** w/o cache	ZS	FS	Self-ICL	DAIL	**DAWN-ICL**	**DAWN-ICL** w/o cache
Boolean Expressions	71.60	80.40	62.40	75.20	80.40	83.20	85.20	87.60	78.00	84.80	90.00	89.20
Causal Judgement	51.87	52.94	51.87	51.87	51.87	54.55	52.41	51.87	52.41	53.48	59.89	61.50
Date Understanding	50.00	51.20	36.80	59.20	53.20	54.40	61.20	56.80	54.40	59.20	58.40	61.60
Disambiguation QA	40.00	57.20	46.80	39.20	66.40	54.80	59.60	65.60	64.80	62.00	66.80	69.20
Formal Fallacies	53.20	53.20	54.40	52.80	52.00	54.00	56.80	57.20	49.20	58.40	59.60	57.60
Geometric Shapes	9.20	40.00	18.00	28.40	43.60	42.40	25.20	53.60	31.20	30.80	38.80	41.60
Hyperbaton	75.20	60.80	57.60	67.20	78.80	80.40	68.40	63.60	79.20	71.20	82.40	82.80
Logical Deduction(five objects)	38.00	37.60	29.20	37.60	38.80	40.00	50.00	50.00	47.60	45.60	50.00	50.80
Logical Deduction(seven objects)	37.60	30.40	21.60	42.00	47.20	48.00	48.40	51.20	43.60	49.20	50.80	52.80
Logical Deduction(three objects)	52.40	50.80	36.80	48.40	53.60	56.40	75.20	76.40	74.40	73.60	74.00	77.20
Movie Recommendation	77.60	84.40	47.20	78.80	76.00	83.60	74.40	74.80	63.60	74.40	76.00	77.20
Navigate	42.00	42.00	42.00	42.00	53.20	53.20	48.00	42.00	42.00	42.40	61.20	65.20
Penguins in a Table	40.41	43.15	32.19	39.04	50.68	46.58	57.53	58.22	52.74	54.79	56.16	54.79
Reasoning about Colored Objects	45.60	44.00	12.80	40.00	50.00	48.40	56.00	56.80	34.40	54.40	53.20	57.20
Ruin Names	40.00	58.80	40.40	44.40	42.40	44.00	46.40	57.20	50.80	50.80	53.20	52.80
Salient Translation Error Detection	20.40	35.20	20.80	30.00	36.00	36.40	34.40	46.80	36.40	45.20	48.00	49.60
Snarks	51.69	57.30	48.88	53.93	58.43	61.80	66.85	77.53	73.03	74.16	76.97	75.84
Sports Understanding	46.00	46.00	46.00	46.00	67.60	70.80	65.20	46.00	46.00	46.00	62.40	67.20
Temporal Sequences	33.60	11.20	34.40	5.60	2.80	2.00	17.60	21.60	22.80	13.20	18.80	16.40
Tracking Shuffled Objects(five objs)	16.00	15.60	14.00	13.60	12.40	12.40	16.80	19.20	19.20	14.00	10.80	12.00
Tracking Shuffled Objects(seven objs)	10.80	12.80	15.60	9.20	10.00	8.80	14.80	17.20	16.80	13.20	12.80	10.40
Tracking Shuffled Objects(three objs)	25.60	35.20	30.00	32.00	29.60	31.60	29.20	27.20	24.80	28.40	20.40	20.00
Web of Lies	48.80	48.80	48.80	48.80	54.40	53.60	48.80	48.80	48.80	48.80	52.80	53.60
All Tasks (avg)	42.32	45.42	36.65	42.66	48.01	**48.56**	49.99	52.06	47.63	49.46	53.20	**54.27**

Table 8: Detailed Results on BBH for Llama3.1-8B and Qwen2.5-7B. “ZS” and “FS” denote zero-shot and few-shot prompting, respectively.

BBH Tasks	Mistral-7B						GPT-4o-mini					
	ZS	FS	Self-ICL	DAIL	**DAWN-ICL**	**DAWN-ICL** w/o cache	ZS	FS	Self-ICL	DAIL	**DAWN-ICL**	**DAWN-ICL** w/o cache
Boolean Expressions	76.00	82.40	73.20	74.40	79.20	84.80	51.20	63.20	59.20	57.20	49.20	57.20
Causal Judgement	50.80	55.08	52.94	53.48	53.48	52.41	59.89	66.31	62.57	60.96	64.17	64.71
Date Understanding	50.00	52.00	44.80	54.00	57.60	60.80	22.00	56.00	48.40	62.40	61.60	61.20
Disambiguation QA	49.20	60.80	57.60	54.40	62.00	68.40	37.60	50.00	51.20	50.80	52.00	53.20
Formal Fallacies	53.60	47.20	48.00	50.00	48.80	52.40	52.80	63.20	58.00	60.80	60.00	60.80
Geometric Shapes	9.20	38.40	10.80	27.60	41.20	40.00	31.20	34.00	30.80	38.00	40.80	40.00
Hyperbaton	74.80	76.40	70.00	54.40	74.80	76.40	51.60	61.60	68.80	69.60	86.00	88.00
Logical Deduction(five objects)	27.60	34.40	27.60	31.20	36.00	37.20	18.40	24.80	22.40	29.60	34.00	32.40
Logical Deduction(seven objects)	20.40	26.00	21.60	28.00	36.00	34.80	15.20	17.20	18.00	17.20	19.60	20.00
Logical Deduction(three objects)	43.20	46.00	47.60	42.80	52.80	52.80	35.20	76.00	69.20	67.20	75.60	74.40
Movie Recommendation	39.20	67.60	46.40	66.40	78.80	80.80	31.20	70.40	56.00	69.20	77.20	77.20
Navigate	45.60	50.40	52.00	48.80	55.60	54.00	50.80	68.80	69.60	68.40	65.60	67.60
Penguins in a Table	32.88	34.25	32.88	41.10	38.36	40.41	48.63	58.22	54.79	58.22	53.42	54.79
Reasoning about Colored Objects	35.20	31.60	27.20	28.00	28.00	27.60	62.80	68.00	69.60	67.20	71.60	72.80
Ruin Names	40.00	43.60	35.20	31.20	54.80	53.60	81.60	85.20	84.80	83.20	87.20	87.20
Salient Translation Error Detection	14.80	32.40	21.20	32.80	34.80	30.40	59.20	58.40	55.20	56.00	58.40	59.60
Snarks	50.00	55.62	43.26	47.75	53.93	52.81	64.04	59.55	53.93	67.42	71.91	70.79
Sports Understanding	47.20	72.80	60.40	66.00	72.40	75.20	51.60	84.00	78.00	82.00	86.40	87.20
Temporal Sequences	21.20	18.80	19.20	14.40	8.40	8.40	27.60	77.60	74.00	71.20	83.20	83.60
Tracking Shuffled Objects(five objs)	19.20	19.20	22.00	23.20	16.00	12.00	16.00	14.00	17.20	12.80	14.40	14.00
Tracking Shuffled Objects(seven objs)	13.20	13.20	11.60	11.60	8.00	9.60	10.80	9.20	11.60	11.20	8.00	7.60
Tracking Shuffled Objects(three objs)	33.20	32.40	33.20	35.60	31.20	34.40	35.60	28.80	33.20	27.20	29.60	30.40
Web of Lies	48.80	52.40	51.20	56.40	55.20	51.60	49.20	50.40	53.20	56.40	52.80	52.00
All Tasks (avg)	38.76	45.31	39.48	42.15	46.83	**47.43**	41.30	53.84	51.97	53.77	56.41	**57.03**

Table 9: Detailed results on BBH tasks for Mistral-7B and GPT-4o-mini. “ZS” and “FS” denote zero-shot and few-shot prompting, respectively.

MMLU Tasks	Llama3.1-8B						Qwen2.5-7B					
	ZS	FS	Self-ICL	DAIL	**DAWN-ICL**	**DAWN-ICL** w/o cache	ZS	FS	Self-ICL	DAIL	**DAWN-ICL**	**DAWN-ICL** w/o cache
abstract algebra	30.00	29.00	25.00	34.00	32.00	34.00	45.00	50.00	42.00	44.00	53.00	50.00
anatomy	57.78	58.52	53.33	60.74	60.00	62.96	70.37	70.37	68.15	68.89	68.89	68.89
astronomy	62.50	63.82	55.26	62.50	68.42	67.11	80.26	83.55	77.63	82.24	84.87	84.87
business ethics	55.00	67.00	58.00	66.00	72.00	68.00	71.00	74.00	66.00	75.00	72.00	76.00
clinical knowledge	64.53	69.81	57.74	70.19	72.08	73.96	79.25	78.11	74.72	79.25	78.49	80.38
college biology	70.14	77.78	59.72	74.31	78.47	79.86	88.19	84.72	79.86	86.11	84.72	85.42
college chemistry	41.00	44.00	37.00	48.00	45.00	46.00	51.00	55.00	53.00	53.00	54.00	48.00
college computer science	47.00	53.00	42.00	53.00	49.00	53.00	61.00	67.00	58.00	66.00	64.00	62.00
college mathematics	38.00	39.00	26.00	32.00	39.00	36.00	38.00	47.00	44.00	49.00	49.00	43.00
college medicine	57.23	61.85	49.71	65.32	63.58	64.74	69.94	66.47	65.90	68.79	69.36	70.52
college physics	42.16	38.24	37.25	49.02	46.08	41.18	45.10	50.98	41.18	49.02	50.00	47.06
computer security	66.00	77.00	64.00	77.00	70.00	76.00	81.00	84.00	78.00	83.00	80.00	79.00
conceptual physics	51.91	53.62	44.68	53.62	55.32	56.17	71.06	71.06	66.81	70.64	70.21	69.79
econometrics	34.21	43.86	34.21	45.61	47.37	45.61	55.26	57.89	55.26	63.16	62.28	65.79
electrical engineering	44.83	58.62	50.34	61.38	66.21	65.52	67.59	73.10	62.76	71.72	71.72	71.72
elementary mathematics	34.66	37.30	30.42	36.77	40.21	41.80	56.08	67.72	62.96	70.11	68.52	70.90
formal logic	38.89	47.62	34.92	48.41	44.44	44.44	49.21	57.14	50.00	58.73	60.32	60.32
global facts	24.00	29.00	21.00	27.00	34.00	35.00	51.00	40.00	45.00	45.00	44.00	47.00
high school biology	76.77	77.74	69.35	82.26	78.39	81.61	84.52	87.42	83.23	87.10	90.00	88.39
high school chemistry	46.80	48.77	37.93	49.26	52.71	53.69	67.98	67.49	61.58	69.46	65.02	69.95
high school computer science	56.00	63.00	54.00	62.00	62.00	63.00	80.00	81.00	80.00	82.00	84.00	83.00
high school european history	70.91	75.15	70.91	73.94	75.76	78.18	81.82	81.82	80.61	79.39	80.61	81.82
high school geography	76.26	78.28	64.65	80.81	82.32	83.84	85.86	87.37	80.81	84.34	90.91	90.91
high school government and politics	80.83	88.08	71.50	91.71	89.64	90.67	92.23	92.75	87.56	95.34	94.82	95.85
high school macroeconomics	55.64	61.03	46.41	64.36	62.05	64.10	75.38	77.69	72.05	80.00	78.72	79.74
high school mathematics	31.85	35.56	25.19	34.44	41.11	38.89	43.33	50.74	45.19	48.52	53.70	53.70
high school microeconomics	62.18	73.95	59.24	73.11	72.69	72.69	84.45	88.24	82.77	88.66	88.24	88.24
high school physics	37.75	33.11	31.13	32.45	38.41	39.07	52.32	51.66	47.02	53.64	56.95	56.29
high school psychology	81.28	83.85	74.50	83.85	83.49	84.22	88.99	89.91	84.95	91.74	90.28	90.83
high school statistics	53.24	55.09	43.98	55.09	53.70	52.31	68.06	69.44	68.06	71.76	70.83	69.91
high school us history	75.00	77.94	68.63	79.41	77.94	77.45	85.78	86.27	81.86	87.25	85.78	87.75
high school world history	80.17	80.17	76.79	80.17	79.32	82.28	84.39	84.81	81.86	86.50	85.65	86.08
human aging	60.09	68.61	55.16	63.23	67.71	68.61	72.20	76.23	62.33	75.34	73.99	73.09
human sexuality	70.23	76.34	65.65	77.86	77.86	77.86	76.34	77.86	75.57	81.68	82.44	82.44
international law	74.38	85.12	68.60	80.17	83.47	83.47	77.69	80.99	74.38	80.99	80.17	78.51
jurisprudence	70.37	68.52	66.67	75.00	73.15	75.00	77.78	78.70	75.93	80.56	80.56	80.56
logical fallacies	59.51	69.94	59.51	72.39	78.53	82.21	80.37	80.98	76.07	81.60	84.05	85.28
machine learning	33.93	42.86	43.75	44.64	43.75	41.96	47.32	46.43	47.32	47.32	49.11	48.21
management	76.70	80.58	64.08	81.55	80.58	79.61	80.58	86.41	80.58	89.32	86.41	86.41
marketing	85.04	86.32	81.62	86.75	86.32	87.61	87.61	91.45	83.76	91.88	90.60	92.31
medical genetics	75.00	78.00	69.00	75.00	78.00	82.00	81.00	80.00	77.00	79.00	78.00	80.00
miscellaneous	75.86	77.78	71.14	78.54	79.18	80.08	83.91	85.70	81.23	85.31	85.31	85.70
moral disputes	65.03	64.16	58.09	70.23	69.94	72.25	73.99	75.43	69.36	78.90	75.43	77.46
moral scenarios	32.63	35.08	24.80	27.82	33.07	32.07	31.73	47.82	25.70	46.59	48.49	47.60
nutrition	70.59	73.20	61.11	75.82	75.82	77.78	79.41	80.72	75.49	80.39	80.72	80.72
philosophy	59.81	71.38	56.91	72.99	71.38	74.60	72.67	78.46	74.60	79.10	79.42	79.74
prehistory	64.20	69.75	61.11	71.91	70.99	73.46	79.94	81.79	74.07	83.02	80.56	82.41
professional accounting	43.97	43.97	39.72	46.45	48.94	48.94	53.19	56.03	51.06	57.45	55.67	57.45
professional law	41.85	47.13	38.59	47.59	49.93	50.20	49.09	51.04	48.04	50.98	51.83	52.09
professional medicine	69.12	72.43	45.22	75.74	72.79	72.43	77.57	77.94	74.63	75.37	73.16	74.63
professional psychology	64.54	66.99	55.39	69.77	71.24	72.88	75.16	75.98	66.50	76.47	76.47	76.96
public relations	63.64	72.73	50.00	70.00	71.82	71.82	67.27	72.73	62.73	68.18	70.91	71.82
security studies	67.35	73.06	64.08	72.24	71.84	73.88	74.69	79.18	71.84	75.92	80.82	80.82
sociology	72.14	85.57	77.61	84.58	87.06	87.06	86.57	87.06	83.08	87.56	88.56	88.56
us foreign policy	80.00	88.00	80.00	88.00	87.00	91.00	85.00	87.00	87.00	88.00	89.00	89.00
virology	52.41	54.22	48.19	58.43	57.23	54.82	50.00	50.60	50.00	52.41	51.81	51.81
world religions	77.19	81.87	66.08	79.53	83.04	83.04	85.96	85.38	81.29	85.38	86.55	86.55
All Tasks (avg)	58.00	62.18	52.29	62.65	63.79	**64.58**	68.50	71.54	65.57	71.86	72.06	**72.43**

Table 10: Detailed Results on MMLU for Llama3.1-8B and Qwen2.5-7B. "ZS" and "FS" denote zero-shot and few-shot prompting, respectively.

MMLU Tasks	Mistral-7B						GPT-4o-mini					
	ZS	FS	Self-ICL	DAIL	**DAWN-ICL**	**DAWN-ICL** w/o cache	ZS	FS	Self-ICL	DAIL	**DAWN-ICL**	**DAWN-ICL** w/o cache
abstract algebra	26.00	31.00	26.00	31.00	30.00	30.00	24.00	30.00	31.00	26.00	36.00	35.00
anatomy	56.30	57.78	49.63	58.52	60.74	62.22	53.33	62.22	61.48	44.44	53.33	56.30
astronomy	55.26	63.16	51.32	65.79	63.82	61.84	61.84	48.03	73.68	57.89	75.66	79.61
business ethics	59.00	57.00	48.00	54.00	58.00	54.00	62.00	51.00	69.00	57.00	59.00	66.00
clinical knowledge	67.55	67.55	53.21	70.57	72.08	72.08	50.94	67.92	66.79	55.47	64.91	62.64
college biology	66.67	67.36	59.72	68.75	68.06	70.83	52.78	67.36	72.22	70.83	80.56	79.17
college chemistry	34.00	46.00	30.00	50.00	45.00	47.00	34.00	30.00	30.00	35.00	39.00	45.00
college computer science	46.00	44.00	38.00	45.00	49.00	47.00	40.00	42.00	45.00	47.00	52.00	61.00
college mathematics	34.00	37.00	33.00	40.00	39.00	41.00	27.00	25.00	28.00	31.00	29.00	38.00
college medicine	58.38	60.12	49.13	62.43	62.43	63.58	39.88	50.87	53.76	52.02	60.69	58.38
college physics	37.25	37.25	32.35	34.31	34.31	36.27	33.33	35.29	35.29	39.22	43.14	52.94
computer security	75.00	79.00	70.00	82.00	78.00	79.00	62.00	65.00	68.00	60.00	66.00	67.00
conceptual physics	47.23	54.89	44.26	51.91	55.74	55.74	51.06	40.43	56.60	45.11	47.23	48.51
econometrics	37.72	44.74	31.58	44.74	41.23	42.98	28.95	42.11	50.88	48.25	58.77	57.89
electrical engineering	53.79	60.00	51.03	55.17	59.31	59.31	38.62	44.14	50.34	40.00	47.59	51.72
elementary mathematics	34.66	38.89	28.31	39.15	38.89	41.01	28.31	36.77	34.92	34.39	40.48	43.65
formal logic	38.10	36.51	36.51	38.10	41.27	37.30	27.78	30.16	38.89	39.68	34.92	32.54
global facts	37.00	34.00	20.00	34.00	38.00	33.00	39.00	27.00	37.00	28.00	29.00	28.00
high school biology	70.97	73.55	61.94	74.52	76.13	77.74	54.19	65.48	74.52	58.06	69.68	69.68
high school chemistry	47.29	48.28	35.47	48.77	50.25	48.77	30.05	48.28	45.32	39.41	50.74	48.77
high school computer science	63.00	65.00	55.00	65.00	64.00	67.00	44.00	70.00	53.00	57.00	75.00	74.00
high school european history	72.12	72.73	69.70	75.76	70.30	74.55	72.12	86.06	81.82	86.06	86.06	87.27
high school geography	73.74	77.27	61.11	77.78	78.28	80.30	76.26	78.28	71.21	60.61	73.23	72.73
high school government and politics	81.35	86.53	70.47	87.56	86.53	86.53	76.17	85.49	88.08	77.72	87.56	91.19
high school macroeconomics	56.15	62.82	45.64	62.82	64.36	64.62	45.90	61.79	65.64	47.44	50.26	53.08
high school mathematics	27.78	35.93	23.70	31.11	31.48	33.70	27.78	22.96	21.11	26.30	27.78	22.59
high school microeconomics	59.24	65.55	48.32	66.81	67.23	65.13	48.74	55.88	65.55	47.06	65.97	69.75
high school physics	34.44	39.07	22.52	34.44	40.40	43.05	32.45	47.02	41.06	42.38	53.64	49.01
high school psychology	77.98	77.98	64.77	80.92	79.82	80.92	65.87	74.86	78.72	62.57	73.58	76.33
high school statistics	42.59	51.39	33.33	44.44	46.30	43.98	36.57	44.44	50.93	47.22	57.41	59.26
high school us history	75.49	81.37	74.02	81.86	82.35	82.84	78.92	91.18	83.33	89.22	93.14	92.65
high school world history	74.68	75.11	73.84	75.95	75.95	75.95	74.26	89.45	86.50	89.03	88.61	89.45
human aging	66.82	69.06	62.33	69.06	68.16	70.40	66.37	64.13	61.88	57.40	69.51	64.57
human sexuality	68.70	74.81	63.36	78.63	77.86	77.10	60.31	61.07	69.47	58.02	61.83	64.12
international law	68.60	76.03	66.94	78.51	80.17	77.69	70.25	87.60	85.95	79.34	90.08	90.08
jurisprudence	68.52	74.07	62.04	72.22	74.07	75.00	62.96	69.44	75.93	57.41	70.37	72.22
logical fallacies	71.17	74.85	65.03	74.23	76.07	80.98	55.21	60.12	69.33	60.12	66.87	64.42
machine learning	40.18	50.00	41.07	51.79	52.68	47.32	45.54	41.96	40.18	47.32	55.36	58.93
management	66.02	77.67	64.08	78.64	79.61	78.64	73.79	75.73	71.84	60.19	66.02	71.84
marketing	82.91	86.75	79.06	88.46	86.75	88.46	73.50	88.03	79.91	79.91	85.90	89.32
medical genetics	64.00	70.00	57.00	70.00	68.00	70.00	55.00	70.00	67.00	57.00	69.00	69.00
miscellaneous	75.35	80.33	70.63	79.95	80.08	79.82	77.65	89.53	83.40	68.71	82.25	82.38
moral disputes	65.03	69.65	60.69	70.23	70.52	72.54	69.08	66.47	69.36	69.94	79.19	78.90
moral scenarios	27.93	31.84	22.57	25.47	38.55	41.79	36.09	47.15	36.31	44.25	48.49	48.27
nutrition	66.34	71.24	62.09	71.57	74.18	72.22	51.96	66.34	62.09	54.58	66.01	63.73
philosophy	65.27	70.10	61.74	71.06	69.77	71.06	55.63	62.70	64.63	67.20	73.63	75.56
prehistory	66.67	64.81	62.35	68.52	68.83	69.44	66.98	83.64	68.52	62.96	66.98	71.91
professional accounting	46.45	43.97	38.30	48.23	46.10	45.74	38.30	52.13	49.65	51.42	57.09	58.51
professional law	44.26	44.98	38.33	45.63	46.54	46.54	43.48	59.65	52.80	59.00	59.78	60.10
professional medicine	58.46	65.44	57.72	63.60	63.97	63.24	23.90	61.03	51.84	61.40	67.65	83.46
professional psychology	58.33	65.52	54.41	67.32	68.46	67.65	50.16	78.43	65.85	66.01	75.98	78.76
public relations	61.82	68.18	60.00	67.27	69.09	70.91	67.27	62.73	61.82	52.73	55.45	60.91
security studies	61.22	71.02	55.92	68.16	71.02	73.88	63.67	77.14	74.69	68.57	75.92	75.51
sociology	79.60	83.08	76.12	85.57	83.58	83.58	68.16	72.64	78.61	74.63	82.09	86.07
us foreign policy	80.00	85.00	80.00	82.00	85.00	83.00	79.00	76.00	89.00	72.00	84.00	84.00
virology	48.80	51.81	46.99	49.40	51.20	52.41	43.37	51.81	43.37	40.96	42.17	47.59
world religions	80.70	81.29	77.78	80.70	80.12	83.04	76.02	80.12	74.85	67.84	80.70	82.46
All Tasks (avg)	57.01	60.70	51.04	60.69	61.98	**62.54**	52.28	62.60	60.88	57.22	64.26	**65.62**

Table 11: Detailed results on MMLU tasks for Mistral-7B and GPT-4o-mini. “ZS” and “FS” denote zero-shot and few-shot prompting, respectively.