MARSBench: Evaluating Multi-Agent Multi-Turn Strategic Reasoning of Large Language Models and Beyond

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Abstract

 Current logical reasoning benchmarks of Large Language Models (LLMs) primarily focus on single-turn and static environments, such as arithmetic problems. The crucial problem of multi-turn, strategic reasoning is under- explored. We introduce *MARSBench*, a novel framework to evaluate the multi-turn strate- gic reasoning of LLMs through text-driven complete- and incomplete-information gaming, e.g., board games (*Tic-Tac-Toe*, *Connect-4*) and poker games (*Texas Hold'em Poker*). *MARS- Bench* offers two distinct scenarios: 1) *Online Racing*, featuring multiple LLMs/agents to fa- cilitate direct competition and comparison; 2) *Offline Probing*, constructing targeted questions **and verified ground truth to evaluate LLMs'** strategic behaviors. We show that existing state-of-the-art LLMs and reasoning schemes are largely ineffective for strategic reasoning tasks. For instance, GPT-3.5-turbo with ad- vanced Tree-of-Thought (ToT) is only slightly better than a Random agent in the naive Tic-Tac- Toe. Offline probing indicates that these LLMs suffer from serious hallucinations (e.g., spa- tial understanding) and weak strategic thinking (e.g., endgame). A recursively thinking-ahead agent is proposed to strengthen the strategic reasoning of LLMs. We hope *MARSBench* could spur further research and exploration in the multi-turn strategic reasoning of LLMs.

031 1 Introduction

 Large Language Models (LLMs) have witnessed re- markable advancements in logical reasoning. Mod- els such as ChatGPT are proven to be effective in solving math problems [\(Cobbe et al.,](#page-8-0) [2021\)](#page-8-0), long- term task planning [\(Huang et al.,](#page-8-1) [2022a\)](#page-8-1), etc. How- ever, these evaluations are predominantly single- turn and static. Although there are environments such as ALFWorld [\(Shridhar et al.,](#page-9-0) [2020\)](#page-9-0) that pro- vide interactive environments to evaluate the plan-ning and reasoning capabilities of LLMs, these

evaluations still focus on the linguistic capabili- **042** ties of LLMs, e.g., reading understanding, with- **043** out much strategic thinking. Therefore, beneath **044** the impressive linguistic capabilities of LLMs, a **045** critical question that has piqued the curiosity of re- **046** searchers and practitioners alike: "*what lies beyond* **047** *static logical reasoning for LLMs?*" **048**

Strategic multi-turn reasoning tasks, such as **049** board and card games, are more reflective of real- **050** world complexities and widely utilized in reinforce- **051** ment learning [\(Silver et al.,](#page-9-1) [2016,](#page-9-1) [2017\)](#page-9-2), present- **052** ing an innovative approach to assessing the logical **053** reasoning of LLMs. These environments simu- **054** late interactive and competitive scenarios, furnish- **055** ing mathematically well-structured rules and con- **056** trollable complexity, with explicit success criteria. **057** Each participant is prompted to strategically choose **058** actions when facing well-defined states to defend **059** against moves from opponents. In these environ- **060** ments, each race can extend over dozens of hands, **061** depending on the intricacy of the task, which ef- **062** fectively examines LLMs' abilities in maintaining **063** multi-turn contexts and exhibiting strategic think- **064** ing. The presence of opponents in the game envi- **065** ronment introduces additional dynamics and com- **066** plexity, posing a significant challenge to the rea- **067** soning abilities of LLMs [\(Ji et al.,](#page-8-2) [2023\)](#page-8-2).

To spur further research and exploration, we in- **069** troduce *MARSBench*, a comprehensive benchmark **070** for evaluating multi-turn strategic online and offline **071** reasoning of LLMs, encompassing complete infor- **072** mation gaming, such as *Tic-Tac-Toe*[1](#page-0-0) and *Connect-* **073** *4* [2](#page-0-1) , as well as incomplete information games, such **074** as *Texas Hold'em Poker*[3](#page-0-2) . These games have sim- **075** ple rules, clear criteria, limited action/state space, **076** and controllable difficulties, which make them suit- **077** able for current LLM evaluations. **078**

[%27em](https://en.wikipedia.org/wiki/Texas_hold_%27em)

¹ <https://en.wikipedia.org/wiki/Tic-tac-toe>

² https://en.wikipedia.org/wiki/Connect_Four 3 [https://en.wikipedia.org/wiki/Texas_hold_](https://en.wikipedia.org/wiki/Texas_hold_%27em)

Benchmarks	Multi-Turn Multi-Agent	Strategic	Opponent Reasoning Agents
HotpotQA (Yang et al., 2018)			
ALFWorld (Shridhar et al., 2020)			
VirtualHome (Puig et al., 2018)			
TextWorld (Côté et al., 2018)			
MINT (Wang et al., 2023)			
AgentBench (Liu et al., 2023c)			
WebArena (Zhou et al., 2023)			
<i>MARSBench</i> (ours)			

Table 1: Comparisons between *MARSBench* and existing reasoning benchmarks.

 MARSBench introduces two different evalua- tion paradigms: *Online Racing* and *Offline Prob- ing*. For online racing, *MARSBench* facilitates direct competitions among multiple LLMs, al- lowing for a straightforward comparison of their reasoning skills by pitting them against each other in a race. Apart from LLMs, *MARSBench* also evaluates advanced reasoning paradigms, 087 e.g., Chain-of-Thought (CoT) [\(Wei et al.,](#page-9-7) [2022b\)](#page-9-7), 088 **[S](#page-9-8)elf-Consistent Chain-of-Thought (CoT-SC) [\(Wang](#page-9-8)** [et al.,](#page-9-8) [2022b\)](#page-9-8), Tree-of-Thought (ToT) [\(Yao et al.,](#page-10-1) [2023\)](#page-10-1), ReAct [\(Yao et al.,](#page-10-2) [2022b\)](#page-10-2).

 In terms of offline probing, *MARSBench* sup- ports demographic analysis by constructing error- driven questions and verified ground truth, for a detailed analysis of LLMs' strategic behaviors. As a demonstration, we examine LLM races and sum- marize 9 common strategic reasoning errors for general board games: 5 for hallucination (e.g., *spatial understanding*, *pattern recognition*) and 4 for strategic thinking (e.g., *endgame*). Then we evaluate LLMs over 2.7k questions specifically designed for each error type and quantify their performances. Our experimental results suggest that existing LLMs suffer from both hallucina- tion [\(Duan et al.,](#page-8-4) [2023;](#page-8-4) [Manakul et al.,](#page-9-9) [2023\)](#page-9-9) and [r](#page-8-6)easoning errors [\(Bian et al.,](#page-8-5) [2023;](#page-8-5) [Karpinska and](#page-8-6) [Iyyer,](#page-8-6) [2023;](#page-8-6) [Gekhman et al.,](#page-8-7) [2023\)](#page-8-7), such as judg- ing *fork* (two-win moves) and assessing *priority*. At last, we propose a Recursively Thinking Ahead (ReTA) agent equipped with uncertainty quantifica- tion mechanisms, to strengthen the strategic rea- soning of LLMs, which also serve as a competitive baseline in our benchmark. Our contributions can be summarized as the following:

 • *MARSBench*: We propose *MARSBench* for evaluating the under-explored multi-turn strategic reasoning capabilities of LLMs, through a set of complete-/incomplete-information board and card games. HotpotQA [\(Yang et al.,](#page-9-3) [2018\)](#page-9-3) is a challenging **119** QA dataset, necessitating multi-hop reasoning **120** skills such as retrieval and search from LLMs. **121**

- Online LLMs Racing: *MARSBench* offers **122** online competitions among multiple LLMs **123** and reasoning agents, allowing for a straight- **124** forward comparison of their reasoning skills **125**
- Offline Reasoning Probing: *MARSBench* **126** provides targeted questions and verified **127** ground truth, regarding the common errors **128** during reasoning, for detailed demographic **129** analysis of the strategic reasoning capabilities **130** of LLMs. **131**
- Improved Strategic Reasoning: We pro- **132** pose a recursively thinking ahead agent, with **133** mechanisms such as majority vote and uncer-
134 tainty quantification for hallucination control, **135** to further strengthen the strategic reasoning of **136** LLMs. **137**

2 Related Work **¹³⁸**

Benchmarks for LLMs Reasoning . Recently, **139** there has been a substantial amount of re- **140** search focused on evaluating the reasoning ca- **141** pabilities of LLMs and LLMs-powered agents. **142** ALFWorld [\(Shridhar et al.,](#page-9-0) [2020\)](#page-9-0) and Virtual- **143** Home [\(Puig et al.,](#page-9-4) [2018\)](#page-9-4) are popular text-driven 144 scenarios that simulate interactive house-holding 145 environments, which have been widely utilized **146** [i](#page-8-1)n evaluating the planning and reasoning [\(Huang](#page-8-1) **147** [et al.,](#page-8-1) [2022a\)](#page-8-1) of LLMs. There have been a lot **148** of benchmarks aiming to evaluate tool utiliza- **149** tion capabilities (e.g., web browsering), including **150** [M](#page-10-0)ind2Web [\(Deng et al.,](#page-8-8) [2023\)](#page-8-8), WebArena [\(Zhou](#page-10-0) **151** [et al.,](#page-10-0) [2023\)](#page-10-0), and Webshop [\(Yao et al.,](#page-10-3) [2022a\)](#page-10-3). **152** [A](#page-9-5)gentBench [\(Liu et al.,](#page-9-6) [2023c\)](#page-9-6) and MINT [\(Wang](#page-9-5) **153** [et al.,](#page-9-5) [2023\)](#page-9-5) present comprehensive evaluations **154**

Figure 1: LLMs online racing in multi-turn strategic scenarios.

155 for LLMs-as-agents, from the perspective of code, **156** web, and game.

157 The differences between *MARSBench* and exist-**158** ing benchmarks are summarized in Table [1.](#page-1-0)

 Reasoning and Planning with LLMs. LLMs have demonstrated reasoning and planning abilities by breaking down intricate questions into sequen- tial intermediate steps, known as Chain-of-Thought (CoT) [\(Wei et al.,](#page-9-7) [2022b\)](#page-9-7), prior to generating the final response. Building upon this concept, Self- Consistency [\(Wang et al.,](#page-9-10) [2022a\)](#page-9-10) samples multiple chains and selects the best answer via majority vot- ing, ToT [\(Yao et al.,](#page-10-1) [2023\)](#page-10-1) models the LLM reason- ing process as a tree structure. In addition, LLMs have achieved successful results in planning and action generation [\(Wu et al.,](#page-9-11) [2023;](#page-9-11) [Huang et al.,](#page-8-9) [2022b\)](#page-8-9). [\(Driess et al.,](#page-8-10) [2023\)](#page-8-10) proposes a multi- modal language model for embodied reasoning tasks, visual-language tasks, and language tasks. Beyond that, [\(Liu et al.,](#page-8-11) [2023a\)](#page-8-11) translates such intermediate steps into executable programming languages to conduct classical planning algorithms. Also, Autonomous Agents have driven zero/few- **177** shot LLMs to achieve complex reasoning and plan- **178** ning tasks through prompt engineering [\(Liu et al.,](#page-8-12) **179** [2023b;](#page-8-12) [Xi et al.,](#page-9-12) [2023;](#page-9-12) [Xiang et al.,](#page-9-13) [2023\)](#page-9-13). [\(Yao](#page-10-2) **180** [et al.,](#page-10-2) [2022b;](#page-10-2) [Shinn et al.,](#page-9-14) [2023\)](#page-9-14) endow agents with **181** the capability to engage in introspection regarding **182** the feedback provided by LLMs. **183**

3 *MARSBench*: Online Agents Racing **¹⁸⁴**

MARSBench facilitates online competition among **185** LLMs and agents, providing a versatile platform for **186** assessing strategic reasoning capabilities. Figure [1](#page-2-0) **187** presents the procedures of online LLMs racing and **188** the demonstration of each environment. **189**

3.1 Preliminary **190**

We present online LLMs racing among two strate- **191** gic games and seven agents in this section: **192 Tic-Tac-Toe:** We utilize the version of 3×3 grid 193 with the winning length as 3. There are two agents 194 in each match and each agent is prompted to select **195** actions when giving the current board state (e.g., **196** legal moves and the opponent's moves). We uti- **197**

Agent v.s. Agent	Random	MinMax	Prompt	CoT	$CoT-SC$ ТоТ		ReAct	Avg. Win Ratio (\uparrow)
Random		4.50%	40.00%	36.50%	37.50%	33.50%	37.50%	31.58%
MinMax	86.00%	$\overline{}$	92.00%	83.50%	85.00%	81.50%	76.00%	84.00%
Prompt	54.50%	5.00%	$\overline{}$	24.00%	20.00%	24.00%	24.50%	25.33%
CoT	54.00%	4.50%	43.50%	$\overline{}$	36.00%	42.50%	39.00%	36.58%
$CoT-SC$	52.50%	7.00%	38.00%	36.00%	$\overline{}$	31.50%	36.00%	33.50%
ToT	55.00%	8.00%	52.00%	30.00%	29.00%	$\overline{}$	48.00%	37.00%
ReAct	54.00%	6.00%	38.50%	39.00%	33.50%	38.50%	۰	34.92%
Avg. Loss Ratio (\downarrow)	59.33%	5.83%	50.67%	41.50%	40.17%	41.92%	43.50%	-

Table 2: Benchmarking reasoning agents in the Tic-Tac-Toe environment. Each cell (**Row, Col**) means the **win** ratio of the Row agent when against the Col agent. Note that the game result can be a draw, so the sum of the win ratios of a pair of two agents is not 100%. It is shown that only ToT and CoT outperform the Random agent with moderate margins and all other agents are just slightly better or even worse than Random.

Figure 2: Remaining chips of reasoning agents at each hand in the Texas Hold'em Poker environment. Standard deviations over 20 trials are shown as the shadowed areas. Agents with more remaining chips at last mean better performance. Among these agents, the naive Prompt agent works better than other methods.

198 lize the symbol $\langle CxRy \rangle$ to represent each move on the Tic-Tac-Toe board where x and y represent the column index and row index respectively. Sym- bolic representations have been widely adopted by other board games, e.g., FEN [\(Wikipedia,](#page-9-15) [2023b\)](#page-9-15) and Algebraic notation [\(Wikipedia,](#page-9-16) [2023a\)](#page-9-16). All the prompt templates can be found in Appendix [A.1.](#page-11-0) Since the first-go player obtains significant advan- tages in this game, we execute 200 matches with each agent going first for 100 matches. We use the 208 average *win ratio*, i.e., $\frac{\text{win match}}{\text{total match}}$ and *loss ratio*, i.e., 209 boss match, to evaluate performance.

Texas Hold'em Poker^{[4](#page-3-0)}: Each agent is assigned \$200 chips initially. The agent is prompted to se- lect an action from the action set: FOLD, CHECK, CALL, RAISE_3BB, RAISE_HALF_POT, RAISE_POT,

RAISE_2POT, ALL_IN, SMALL_BLIND, BIG_BLIND. **214** The utilized prompts can be found in Appendix [A.2.](#page-11-1) **215** Detailed explanations of these actions can be found **216** in Appendix [B.](#page-12-0) There are dozens of hands within **217** each match. We utilize the hand win ratio, e.g., 218 win hands total hands to evaluate performance. **²¹⁹**

Reasong Agents: We consider 7 agents (5 LLMs- **220** powered agents and 2 baseline agents): ➊ Random: **²²¹** the agent that randomly selects action at each step; **222** ➋ MinMax: the agent that selects action based on **²²³** conventional min-max gaming strategy (only com- **224** patible with Tic-Tac-Toe); ➌ Prompt: the agent **²²⁵** that directly prompts LLMs to return answers; \bullet 226 Chain-of-Thought (CoT): the agent that reasons **227** through thinking step by step; \bullet Self-Consistent 228 CoT (CoT-SC): the agent that utilizes multiple step- **229** by-step-thinking trajectories during reasoning; θ 230 Tree-of-Thought (ToT): the agent that augmented **231**

⁴ https://github.com/dickreuter/neuron_poker

	1, and you have finished moves Column 1, Row 1 and Column 2, Row 2. Assume the opponent will take Column 2, Row 3 as the next move, what's the advantage for this move?
	GPT-3.5-turbo: The opponent's next move completes a vertical line of O's in the second column. This means the opponent will have three O's in a row vertically, which is a winning combination.
current situation	Miss Identified Ownership

(b) *hallucination*: LLMs failed to recognize the identity of pieces.

Figure 3: Some representative error patterns of CoT GPT-3.5-turbo in Tic-Tac-Toe.

 with exploration and deliberate decision-making, **i.e., self-evaluation. O** ReAct: the agent that fol- lows reasoning-before-acting policy. All the agents are driven by ChatGPT (GPT-3.5-turbo-0613).

 It is worth noting that some agents are not orig- inally designed for strategic gaming tasks. In Ap- pendix [C,](#page-12-1) we provide details on how we make them applicable to *MARSBench*.

240 3.2 Evaluation Results

 In Table [2,](#page-3-1) we report the average win ratios and loss ratios in the *MARSBench* Tic-Tac-Toe envi- ronment. The optimization-based MinMax agent significantly outperforms all other methods, which is expected as we just use it as a reference base- line. Surprisingly, we found that most advanced reasoning agents work only slightly better than the Random agent. The Prompt agent works even worse than the Random agent. Among these methods, ToT achieves the highest average win ratio (37%) and CoT-SC achieves the lowest loss ratio (40.17%).

 In Figure [2,](#page-3-2) we present the performance of rea- soning agents when playing Texas Hold'em Poker. We found that the Prompt agent works better than other agents. Advanced reasoning agents work slightly better than the Random agent.

257 3.3 Analytical Insights

258 We summarize the following insights according to **259** the obtained experimental results in *MARSBench*:

260 Serious Hallucination and Reasoning Errors. **261** We found that LLMs suffer from serious halluci-**262** nations and reasoning errors. Figure [3](#page-4-0) provides

demonstrations of how LLMs failed in perceiving **263** board states and endgames. **264**

Advanced Reasoning Not Always Help. Al- **265** though advanced reasoning agents (e.g., CoT, **266** CoT-SC, ReAct, ToT) all work better than directly **267** prompt LLMs in Tic-Tac-Toe, this trend reverses **268** in Texas Hold'em Poker, where directly prompted **269** LLMs actually perform better than all the advanced **270** reasoning agents. One potential reason is the na- **271** ture of incomplete games, where only partial infor- **272** mation is available, hindering effective reasoning **273** by LLMs. Additionally, Texas Hold'em Poker de- **274** mands strong Theory-of-Mind (ToM) skills like **275** [b](#page-9-17)luffing, which are challenging for LLMs [\(Stepput-](#page-9-17) **276** [tis et al.,](#page-9-17) [2023\)](#page-9-17). **277**

4 *MARSBench*: Offline In-Depth Probing **²⁷⁸**

The limited success of state-of-the-art LLMs when **279** against random agents as opponents raises a critical **280** question: *What specific vulnerabilities and limita-* **281** *tions are being exposed by MARSBench?* **282**

4.1 Preliminary **283**

To answer this question, *MARSBench* provides tar- **284** geted questions and verified answers for detailed **285** offline demographic analysis. As a demonstration, **286** we show how *MARSBench* characterizes LLMs' **287** strategic behaviors over board games (e.g., Tic- **288** Tac-Toe and Connect-4). We first examine LLMs' **289** behaviors from online races obtained in Section [3](#page-2-1) **290** and summarize two main error categories: *halluci-* **291** *nation* and *strategic reasoning*, that result in loss. **292**

Hallucination. We probe hallucinations by ex- **293** amining whether LLMs are capable of **O** Spatial 294 Understanding, i.e., spatial relationship given any **295** two pieces; ➋ Pattern Recognition, i.e., discovering **²⁹⁶**

Figure 4: Error profiles in *MARSBench* offline dataset.

 consecutively connected pieces; ➌ Counting, i.e., counting finished pieces; ➍ Memory, i.e., identify-299 ing the ownership of each piece; \bullet Legality, i.e., recognizing legal and illegal moves.

 Strategic Reasoning. We probe four common abilities in general board games: ➊ Action Prior- ity, i.e., winning moves should be prioritized; ➋ Endgame, i.e., recognizing immediate win/loss sit- uations; ➌ Blocking, i.e., blocking the winning of the opponent; ➍ Fork, i.e., constructing moves that lead to two potential winning moves.

 We provide demonstrations for each type of er- ror in Figure [4.](#page-5-0) It is worth noting that these errors, e.g., fork, blocking, endgame, are also prevalent in general board games [\(Dixit and Nalebuff,](#page-8-13) [2010\)](#page-8-13). Although we only provide demonstrations over Tic- Tac-Toe and Connect-4, this can be easily general-ized to other board games such as Chess and Go.

315 4.2 Offline Dataset Generation

316 Utilizing structured symbols for each move, such **317** as <CxRy>, *MARSBench* can generate unlimited **318** legal board states with adjustable complexities. For dataset creation, we crafted prompt templates for **319** each error type and traversed all occupied/legal **320** moves to populate these templates. We also im- **321** plement verifiers for each error type to establish **322** ground truth. We then sampled balanced questions **323** based on complexity and labels, e.g., Yes and No. **324** The statistics of the offline probing dataset for Tic- **325** Tac-Toe and Connect-4 are detailed in Table [3.](#page-4-1) **326**

4.3 Evaluation and Error Analysis **327**

We evaluate strategic reasoning for both commer- **328** cial LLMs, e.g., GPT-3.5-turbo and GPT-4, and **329** [o](#page-9-18)pen-source LLMs, e.g., Llama-2-chat [\(Touvron](#page-9-18) **330** [et al.,](#page-9-18) [2023\)](#page-9-18), Mistral-Instruct [\(Jiang et al.,](#page-8-14) [2023\)](#page-8-14). **331** Results are summarized in Table [4.](#page-6-0) **332**

For hallucinations, we show that GPT-4 with CoT **333** reasoning achieves significant accuracy (90.7%), **334** suggesting that LLMs are capable of effectively **335** perceiving board states through symbolic represen- **336** tations. However, other LLMs demonstrated signif- **337** icant hallucination issues, indicating challenges in **338** understanding board states. For strategic reasoning, **339** we show that even the most state-of-the-art GPT- **340**

		Hallucination (Perception)				Strategic Reasoning						
Model and Reasoning	All Avg.	spatial	pattern	counting	memory	legalty	avg.	priority	endgame	blocking	fork	avg.
Random	0.444	0.500	0.500	0.000	0.500	0.500	0.400	0.500	0.500	0.500	0.500	0.500
GPT-4	0.665	0.843	0.597	0.746	0.777	0.837	0.760	0.567	0.560	0.523	0.533	0.546
GPT-4 w/ CoT	0.750	0.947	0.817	0.997	0.940	0.833	0.907	0.540	0.597	0.560	0.518	0.554
GPT-3.5-turbo	0.554	0.503	0.537	0.707	0.643	0.627	0.603	0.503	0.475	0.498	0.497	0.493
GPT-3.5-turbo w/ CoT	0.641	0.763	0.577	0.903	0.766	0.669	0.736	0.505	0.519	0.557	0.505	0.522
Mistral-7B-Instruct-y0.1	0.494	0.545	0.520	0.225	0.515	0.524	0.466	0.545	0.551	0.543	0.476	0.529
Mistral-7B-Instruct-y0.1 w/CoT	0.486	0.523	0.527	0.263	0.604	0.477	0.479	0.482	0.461	0.530	0.505	0.495
Llama-2-70b-chat	0.476	0.483	0.493	0.120	0.590	0.553	0.448	0.517	0.503	0.520	0.500	0.510
Llama-2-70b-chat w/ CoT	0.568	0.537	0.530	0.763	0.573	0.613	0.603	0.513	0.530	0.533	0.520	0.524
CodeLlama-34b-Instruct	0.477	0.547	0.560	0.070	0.550	0.540	0.453	0.550	0.482	0.513	0.477	0.505
CodeLlama-34b-Instruct w/ CoT	0.559	0.667	0.535	0.593	0.638	0.577	0.602	0.512	0.530	0.490	0.493	0.506

Table 4: Evaluation results of *MARSBench* offline datasets. State-of-the-art LLMs (e.g., GPT-4) with CoT reasoning are capable of perceiving board states (90.7% accuracy in hallucination scenarios). However, it only works slightly better than random guesses in strategic thinking scenarios, even with the help of CoT reasoning.

Figure 5: Correlations between board complexities and model performances. It indicates that complex board situations result in a significant performance drop for state-of-the-art LLMs.

 4 can only achieve 54.6% accuracy on average, which is only slightly better than random guessing. It suggests the vulnerabilities and limitations in strategic reasoning for LLMs. The CoT reasoning only marginally improves performance (+0.8%) in this scenario.

347 4.4 States Complexity Effects

 As races progress and the complexity of the board state increases significantly, we quantify the corre- lation between this complexity and model perfor- mance. In Figure [5,](#page-6-1) we demonstrate how model performances are impacted in scenarios where com- plexity is directly influenced by the number of com- pleted turns, including Counting, Pattern, Priority, Endgame, Blocking, and Fork. We normalize the complexity derived from the number of turns to a range of (0,1) and calculate the accuracy at each

Figure 6: The emergent abilities in strategic reasoning. Increasing model parameter sizes effectively mitigate hallucination and perception errors, while it does not yield similar improvements in strategic.

specific number of turns. It is shown that as the 358 board becomes more complex, there is a significant **359** drop in the strategic reasoning performances, e.g., **360** the accuracy of GPT-4 drops from 68.8% to 46.1% .

4.5 Emergent Abilities in Strategic Reasoning **362**

Following emergent abilities of LLMs [\(Wei et al.,](#page-9-19) **363** [2022a\)](#page-9-19), we study how LLM parameter sizes affect **364** strategic reasoning. In Figure [6,](#page-6-2) we compare the **365** popular Llama models at 7b, 13b, 34b (CodeL- **366** lama), and 70b parameter sizes. For hallucination, **367** increasing parameter sizes significantly improves **368** accuracy from 43.4% to 60.3%, suggesting the **369** emergent abilities in strategic linguistic understand- **370** ing. **371**

However, there is no such trend in those strate- **372** gic thinking evaluation. We show that Llama-2-7b- **373**

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Setting		ReTA Win Ratio Others Win Ratio				
ReTA Agent vs. ToT Agent						
ReTA $(k = 2, n = 2)$	37%	59%				
ReTA $(k = 2, n = 4)$	48%	37%				
+ majority vote $(k_{mv} = 3)$	62%	35%				
+ P-UQ $(k_{pert} = 2)$	60%	34%				
+ majority vote + P-UQ	61%	31%				
GPT-3.5-turbo as LLMs: ReTA Agent vs. Other Agents						
ReTA v.s. ToT	61\% $(+30\%)$	31%				
ReTA v.s. CoT-SC	52% (+17%)	35%				
ReTA v.s. ReAct	50\% $(+10\%)$	40%				
ReTA v.s. Prompt	60\% $(+26\%)$	34%				
ReTA v.s. CoT	59% $(+29%)$	30%				
<i>Llama-2-13b-chat as LLMs</i> : ReTA Agent vs. Other Agents						
ReTA v.s. ToT	51\% $(+11\%)$	40%				
ReTA v.s. CoT	55\% $(+11\%)$	44%				
ReTA v.s. ReAct	56\% $(+13\%)$	43%				
ReTA v.s. Prompt	62\% $(+26\%)$	36%				

Table 5: Ablation study and evaluations of ReTA in the Tic-Tac-Toe environment.

 chat has similar performances as Llama-2-70b-chat model, i.e. 50.6% to 52.4%. This raises new chal- lenges regarding how to equip LLMs with the capa- bility for effective strategic reasoning when simply increasing parameter size proves ineffective.

379 5 Improved Multi-Turn Reasoning

380 We propose preliminary mechanisms for improved **381** strategic reasoning agents in this section, which **382** serve as competitive baselines for *MARSBench*.

383 5.1 Improved Reasoning

 We introduce three mechanisms: Recursively Think Ahead (ReTA), Majority Vote, and Perturbation-based Uncertainty Quantification to improve the strategic reasoning:

 Recursively Thinking Ahead (**ReTA**). It is in- spired by the conventional min-max gaming the- ory where the MinMax agent aims to maximize its own advantage while minimizing the opponent's potential gains. Following that, we introduce an imaginary enemy concept during reasoning and prompt LLMs to play ahead against this imaginary opponent for up to k steps and select n moves for each step. This process involves the agent system- atically analyzing potential moves and outcomes, both of its own and of the imaginary enemy. After this thinking-ahead process, the agent is prompted to choose the best move considering the actions of the imaginary enemy as the next move. Detailed architecture of ReTA can be found in Appendix [E.](#page-13-0)

Setting	ReTA Hand Win Ratio	Others Hand Win Ratio
ReTA v.s. Prompt	53.8% $(+7.6%)$	46.2%
ReTA v.s. CoT-SC	$63.2\% (+26.4\%)$	36.8%
ReTA v.s. ToT	72.1% (+44.2%)	27.9%
ReTA v.s. ReAct	78.0% (+56.0%)	22.0%

Table 6: Evaluations of ReTA in Texas Hold'em Poker.

Table 7: Evaluation of ReTA in Connect-4.

Majority Vote. For a given question x, we sim- 403 ply sample k_{mv} generations from LLMs and select 404 the high-frequency option or the mean value (if it **405** is a numerical situation) as the next move. **406**

Perturbation-based Uncertainty Quantification. **407**

We first prompt LLMs to perturb the original ques- 408 tion x for k_{pert} times while keeping the semantics 409 unchanged, then we sample generations based on **410** both original question x and perturbed questions \tilde{x} 411 and apply a majority vote over these generations. **412**

5.2 Experimental Settings and Evaluations **413**

We utilize the same settings as in Section [3.](#page-2-1) For **414** Tic-Tac-Toe, we execute 100 matches with each **415** agent going first for 50 matches. For Connect-4 **416** and Texas Hold'em Poker, we execute 20 matches. **417**

In Table [5,](#page-7-0) we conduct comprehensive ablation **418** studies and evaluations of ReTA over Tic-Tac-Toe. **419** We take ToT as the opponent of ReTA because ToT **420** achieves the best performance among all reasoning **421** agents in Section [3.](#page-2-1) It is shown that the proposed **422** ReTA agent significantly boosts the strategic rea- **423** soning of LLMs. Further experiments carried out **424** on the open-source Llama-2-13b-chat also show **425** distinct advantages for ReTA, suggesting the strong **426** transferability regarding different LLM backbones. **427**

In Tables [6](#page-7-1) and [7,](#page-7-2) the empirical results obtained **428** over Texas Hold'em Poker and Connect-4 present **429** that ReTA could be generalized to other scenarios. **430**

6 Conclusion **⁴³¹**

In this paper, we propose *MARSBench*, a compre- **432** hensive benchmark for multi-turn strategic reason- **433** ing of LLMs. *MARSBench* provides online agent **434** racing and offline reasoning probing, offering an **435** in-depth examination of strategic behaviors. Our **436** work introduces a new dimension to LLMs evalu- **437** ation, and we hope it will inspire further research **438** into the multi-turn strategic reasoning of LLMs. **439**

⁴⁴⁰ 7 Ethical Considerations

 Prompting and Evaluating LLMs to be strategic reasoning agents increases real-world autonomy for LLMs and brings a lot of potential applications in the real world. As a result, AI-driven decision- making may potentially reduce the role of human skill and creativity. It also raises the question of who should be responsible for the decisions of LLMs. Besides, ensuring fairness and avoiding biases in the model's strategy is essential, as biases can influence game outcomes and player experi- ences. It is also important to consider the impact of advanced strategic reasoning on the integrity of games, particularly in competitive settings, to maintain a level playing field for all players.

⁴⁵⁵ 8 Limitations

 Although *MARSBench* considers both complete- and incomplete-gaming tasks, there are still other game forms not covered. We will take expanding more strategic games as the future work. Also, even though the proposed ReTA outperforms exist- ing reasoning agents, it is still significantly worse than optimization-based solvers, such as MinMax agents. Strategic reasoning requires strong instruc- tion following capabilities. Currently, only com- mercial LLMs (e.g., ChatGPT and GPT-4) are capa- ble of following complex instructions, while other open-source LLMs (e.g., Llama-2-chat) are still un- desirable to be the backbone of strategic reasoning **469** agents.

⁴⁷⁰ References

- **471** Ning Bian, Peilin Liu, Xianpei Han, Hongyu Lin, Yaojie **472** Lu, Ben He, and Le Sun. 2023. [A drop of ink makes](http://arxiv.org/abs/2305.04812) **473** [a million think: The spread of false information in](http://arxiv.org/abs/2305.04812) **474** [large language models.](http://arxiv.org/abs/2305.04812)
- **475** Karl Cobbe, Vineet Kosaraju, Mohammad Bavarian, **476** Mark Chen, Heewoo Jun, Lukasz Kaiser, Matthias **477** Plappert, Jerry Tworek, Jacob Hilton, Reiichiro **478** Nakano, Christopher Hesse, and John Schulman. **479** 2021. [Training verifiers to solve math word prob-](https://api.semanticscholar.org/CorpusID:239998651)**480** [lems.](https://api.semanticscholar.org/CorpusID:239998651) *ArXiv*, abs/2110.14168.
- **481** Marc-Alexandre Côté, Ákos Kádár, Xingdi Yuan, **482** Ben A. Kybartas, Tavian Barnes, Emery Fine, James **483** Moore, Matthew J. Hausknecht, Layla El Asri, Mah-**484** moud Adada, Wendy Tay, and Adam Trischler. 2018. **485** [Textworld: A learning environment for text-based](https://api.semanticscholar.org/CorpusID:49552345) **486** [games.](https://api.semanticscholar.org/CorpusID:49552345) *ArXiv*, abs/1806.11532.
- **487** Xiang Deng, Yu Gu, Boyuan Zheng, Shijie Chen, **488** Samuel Stevens, Boshi Wang, Huan Sun, and Yu Su.

2023. [Mind2web: Towards a generalist agent for the](https://api.semanticscholar.org/CorpusID:259129428) **489** [web.](https://api.semanticscholar.org/CorpusID:259129428) $ArXiv$, abs/2306.06070. **490**

- [A](https://api.semanticscholar.org/CorpusID:106854475)vinash Dixit and Barry Nalebuff. 2010. [The art of](https://api.semanticscholar.org/CorpusID:106854475) **491** [strategy: A game theorist's guide to success in busi-](https://api.semanticscholar.org/CorpusID:106854475) **492** [ness and life.](https://api.semanticscholar.org/CorpusID:106854475) 493
- Danny Driess, Fei Xia, Mehdi SM Sajjadi, Corey Lynch, **494** Aakanksha Chowdhery, Brian Ichter, Ayzaan Wahid, **495** Jonathan Tompson, Quan Vuong, Tianhe Yu, et al. **496** 2023. Palm-e: An embodied multimodal language **497** model. *arXiv preprint arXiv:2303.03378*. **498**
- Jinhao Duan, Hao Cheng, Shiqi Wang, Chenan Wang, **499** Alex Zavalny, Renjing Xu, Bhavya Kailkhura, and **500** Kaidi Xu. 2023. Shifting attention to relevance: To- **501** wards the uncertainty estimation of large language **502** models. *arXiv preprint arXiv:2307.01379*. **503**
- Zorik Gekhman, Jonathan Herzig, Roee Aharoni, Chen **504** Elkind, and Idan Szpektor. 2023. [Trueteacher: Learn-](http://arxiv.org/abs/2305.11171) **505** [ing factual consistency evaluation with large lan-](http://arxiv.org/abs/2305.11171) **506** [guage models.](http://arxiv.org/abs/2305.11171) **507**
- Wenlong Huang, Pieter Abbeel, Deepak Pathak, and **508** Igor Mordatch. 2022a. Language models as zero- **509** shot planners: Extracting actionable knowledge for 510 embodied agents. In *International Conference on* **511** *Machine Learning*, pages 9118–9147. PMLR. **512**
- Wenlong Huang, Fei Xia, Ted Xiao, Harris Chan, **513** Jacky Liang, Pete Florence, Andy Zeng, Jonathan **514** Tompson, Igor Mordatch, Yevgen Chebotar, et al. **515** 2022b. Inner monologue: Embodied reasoning **516** through planning with language models. *arXiv* **517** *preprint arXiv:2207.05608*. **518**
- Ziwei Ji, Nayeon Lee, Rita Frieske, Tiezheng Yu, Dan **519** Su, Yan Xu, Etsuko Ishii, Ye Jin Bang, Andrea **520** Madotto, and Pascale Fung. 2023. Survey of halluci- **521** nation in natural language generation. *ACM Comput-* **522** *ing Surveys*, 55(12):1–38. **523**
- Albert Q Jiang, Alexandre Sablayrolles, Arthur Men- **524** sch, Chris Bamford, Devendra Singh Chaplot, Diego **525** de las Casas, Florian Bressand, Gianna Lengyel, Guil- **526** laume Lample, Lucile Saulnier, et al. 2023. Mistral **527** 7b. *arXiv preprint arXiv:2310.06825*. **528**
- [M](http://arxiv.org/abs/2304.03245)arzena Karpinska and Mohit Iyyer. 2023. [Large lan-](http://arxiv.org/abs/2304.03245) **529** [guage models effectively leverage document-level](http://arxiv.org/abs/2304.03245) **530** [context for literary translation, but critical errors per](http://arxiv.org/abs/2304.03245) [sist.](http://arxiv.org/abs/2304.03245) **532**
- Bo Liu, Yuqian Jiang, Xiaohan Zhang, Qiang Liu, **533** Shiqi Zhang, Joydeep Biswas, and Peter Stone. **534** 2023a. Llm+ p: Empowering large language models **535** with optimal planning proficiency. *arXiv preprint* 536
arXiv:2304.11477. 537 *arXiv:2304.11477*. **537**
- Ruibo Liu, Ruixin Yang, Chenyan Jia, Ge Zhang, Denny **538** Zhou, Andrew M Dai, Diyi Yang, and Soroush **539** Vosoughi. 2023b. Training socially aligned language **540** models in simulated human society. *arXiv preprint* **541** *arXiv:2305.16960*. **542**

- **543** Xiao Liu, Hao Yu, Hanchen Zhang, Yifan Xu, Xu-**544** anyu Lei, Hanyu Lai, Yu Gu, Yuxian Gu, Hangliang **545** Ding, Kai Men, Kejuan Yang, Shudan Zhang, Xiang **546** Deng, Aohan Zeng, Zhengxiao Du, Chenhui Zhang, **547** Shengqi Shen, Tianjun Zhang, Yu Su, Huan Sun, **548** Minlie Huang, Yuxiao Dong, and Jie Tang. 2023c. **549** [Agentbench: Evaluating llms as agents.](https://api.semanticscholar.org/CorpusID:260682249) *ArXiv*, **550** abs/2308.03688.
- **551** Potsawee Manakul, Adian Liusie, and Mark John Fran-**552** cis Gales. 2023. Selfcheckgpt: Zero-resource black-**553** box hallucination detection for generative large lan-**554** guage models. *ArXiv*, abs/2303.08896.
- **555** Xavier Puig, Kevin Ra, Marko Boben, Jiaman Li, **556** Tingwu Wang, Sanja Fidler, and Antonio Torralba. **557** 2018. Virtualhome: Simulating household activities **558** via programs. In *Proceedings of the IEEE Confer-***559** *ence on Computer Vision and Pattern Recognition*, **560** pages 8494–8502.
- **561** Noah Shinn, Federico Cassano, Beck Labash, Ashwin **562** Gopinath, Karthik Narasimhan, and Shunyu Yao. **563** 2023. [Reflexion: Language agents with verbal rein-](https://api.semanticscholar.org/CorpusID:258833055)**564** [forcement learning.](https://api.semanticscholar.org/CorpusID:258833055)
- **565** Mohit Shridhar, Xingdi Yuan, Marc-Alexandre Côté, **566** Yonatan Bisk, Adam Trischler, and Matthew **567** Hausknecht. 2020. Alfworld: Aligning text and em-**568** bodied environments for interactive learning. *arXiv* **569** *preprint arXiv:2010.03768*.
- **570** David Silver, Aja Huang, Chris J. Maddison, Arthur **571** Guez, L. Sifre, George van den Driessche, Julian **572** Schrittwieser, Ioannis Antonoglou, Vedavyas Pan-**573** neershelvam, Marc Lanctot, Sander Dieleman, Do-**574** minik Grewe, John Nham, Nal Kalchbrenner, Ilya **575** Sutskever, Timothy P. Lillicrap, Madeleine Leach, **576** Koray Kavukcuoglu, Thore Graepel, and Demis Has-**577** sabis. 2016. [Mastering the game of go with deep](https://api.semanticscholar.org/CorpusID:515925) **578** [neural networks and tree search.](https://api.semanticscholar.org/CorpusID:515925) *Nature*, 529:484– **579** 489.
- **580** David Silver, Thomas Hubert, Julian Schrittwieser, Ioan-**581** nis Antonoglou, Matthew Lai, Arthur Guez, Marc **582** Lanctot, L. Sifre, Dharshan Kumaran, Thore Graepel, **583** Timothy P. Lillicrap, Karen Simonyan, and Demis **584** Hassabis. 2017. [Mastering chess and shogi by self-](https://api.semanticscholar.org/CorpusID:33081038)**585** [play with a general reinforcement learning algorithm.](https://api.semanticscholar.org/CorpusID:33081038) **586** *ArXiv*, abs/1712.01815.
- **587** Simon Stepputtis, Joseph Campbell, Yaqi Xie, **588** Zhengyang Qi, Wenxin Sharon Zhang, Ruiyi Wang, **589** Sanketh Rangreji, Michael Lewis, and Katia Sycara. **590** 2023. [Long-horizon dialogue understanding for role](https://api.semanticscholar.org/CorpusID:265128935) **591** [identification in the game of avalon with large lan-](https://api.semanticscholar.org/CorpusID:265128935)**592** [guage models.](https://api.semanticscholar.org/CorpusID:265128935) In *Conference on Empirical Methods* **593** *in Natural Language Processing*.
- **594** Hugo Touvron, Louis Martin, Kevin Stone, Peter Al-**595** bert, Amjad Almahairi, Yasmine Babaei, Nikolay **596** Bashlykov, Soumya Batra, Prajjwal Bhargava, Shruti **597** Bhosale, et al. 2023. Llama 2: Open founda-**598** tion and fine-tuned chat models. *arXiv preprint* **599** *arXiv:2307.09288*.
- Xingyao Wang, Zihan Wang, Jiateng Liu, Yangyi Chen, **600** Lifan Yuan, Hao Peng, and Heng Ji. 2023. [Mint:](https://api.semanticscholar.org/CorpusID:262053695) **601** [Evaluating llms in multi-turn interaction with tools](https://api.semanticscholar.org/CorpusID:262053695) **602** [and language feedback.](https://api.semanticscholar.org/CorpusID:262053695) *ArXiv*, abs/2309.10691. **603**
- Xuezhi Wang, Jason Wei, Dale Schuurmans, Quoc **604** Le, Ed Chi, Sharan Narang, Aakanksha Chowdhery, **605** and Denny Zhou. 2022a. Self-consistency improves **606** chain of thought reasoning in language models. *arXiv* **607** *preprint arXiv:2203.11171*. **608**
- Xuezhi Wang, Jason Wei, Dale Schuurmans, Quoc Le, **609** Ed Huai hsin Chi, and Denny Zhou. 2022b. [Self-](https://api.semanticscholar.org/CorpusID:247595263) **610** [consistency improves chain of thought reasoning in](https://api.semanticscholar.org/CorpusID:247595263) **611** [language models.](https://api.semanticscholar.org/CorpusID:247595263) *ArXiv*, abs/2203.11171. **612**
- Jason Wei, Yi Tay, Rishi Bommasani, Colin Raffel, **613** Barret Zoph, Sebastian Borgeaud, Dani Yogatama, **614** Maarten Bosma, Denny Zhou, Donald Metzler, et al. **615** 2022a. Emergent abilities of large language models. **616** *arXiv preprint arXiv:2206.07682*. **617**
- Jason Wei, Xuezhi Wang, Dale Schuurmans, Maarten **618** Bosma, Fei Xia, Ed Chi, Quoc V Le, Denny Zhou, **619** et al. 2022b. Chain-of-thought prompting elicits rea- **620** soning in large language models. *Advances in Neural* **621** *Information Processing Systems*, 35:24824–24837. **622**
- Wikipedia. 2023a. Algebraic notation (chess) **623** — Wikipedia, the free encyclopedia. [http:](http://en.wikipedia.org/w/index.php?title=Algebraic%20notation%20(chess)&oldid=1184027217) **624** [//en.wikipedia.org/w/index.php?title=](http://en.wikipedia.org/w/index.php?title=Algebraic%20notation%20(chess)&oldid=1184027217) **625** [Algebraic%20notation%20\(chess\)&oldid=](http://en.wikipedia.org/w/index.php?title=Algebraic%20notation%20(chess)&oldid=1184027217) **626** [1184027217](http://en.wikipedia.org/w/index.php?title=Algebraic%20notation%20(chess)&oldid=1184027217). [Online; accessed 15-December- **627** 2023]. **628**
- Wikipedia. 2023b. Forsyth–Edwards Nota- **629** tion — Wikipedia, the free encyclopedia. **630** [http://en.wikipedia.org/w/index.php?](http://en.wikipedia.org/w/index.php?title=Forsyth%E2%80%93Edwards%20Notation&oldid=1176345997) **631** [title=Forsyth%E2%80%93Edwards%20Notation&](http://en.wikipedia.org/w/index.php?title=Forsyth%E2%80%93Edwards%20Notation&oldid=1176345997) **632** [oldid=1176345997](http://en.wikipedia.org/w/index.php?title=Forsyth%E2%80%93Edwards%20Notation&oldid=1176345997). [Online; accessed 15- **633** December-2023]. **634**
- Zhenyu Wu, Ziwei Wang, Xiuwei Xu, Jiwen Lu, **635** and Haibin Yan. 2023. Embodied task plan- **636** ning with large language models. *arXiv preprint* **637** *arXiv:2307.01848*. **638**
- Zhiheng Xi, Wenxiang Chen, Xin Guo, Wei He, Yiwen **639** Ding, Boyang Hong, Ming Zhang, Junzhe Wang, **640** Senjie Jin, Enyu Zhou, et al. 2023. The rise and **641** potential of large language model based agents: A **642** survey. *arXiv preprint arXiv:2309.07864*. **643**
- Jiannan Xiang, Tianhua Tao, Yi Gu, Tianmin Shu, Zirui **644** Wang, Zichao Yang, and Zhiting Hu. 2023. Lan- **645** guage models meet world models: Embodied expe- **646** riences enhance language models. *arXiv preprint* **647** *arXiv:2305.10626*. **648**
- Zhilin Yang, Peng Qi, Saizheng Zhang, Yoshua Ben- **649** gio, William W Cohen, Ruslan Salakhutdinov, and **650** Christopher D Manning. 2018. Hotpotqa: A dataset **651** for diverse, explainable multi-hop question answer- **652** ing. *arXiv preprint arXiv:1809.09600*. **653**
- Shunyu Yao, Howard Chen, John Yang, and Karthik Narasimhan. 2022a. [Webshop: Towards scalable](https://api.semanticscholar.org/CorpusID:250264533) [real-world web interaction with grounded language](https://api.semanticscholar.org/CorpusID:250264533) [agents.](https://api.semanticscholar.org/CorpusID:250264533) *ArXiv*, abs/2207.01206.
- Shunyu Yao, Dian Yu, Jeffrey Zhao, Izhak Shafran, Thomas L Griffiths, Yuan Cao, and Karthik Narasimhan. 2023. Tree of thoughts: Deliberate problem solving with large language models. *arXiv preprint arXiv:2305.10601*.
- Shunyu Yao, Jeffrey Zhao, Dian Yu, Nan Du, Izhak Shafran, Karthik Narasimhan, and Yuan Cao. 2022b. **665 React: Synergizing reasoning and acting in language**
666 **models** *arXiv preprint arXiv*: 2210.03629. models. *arXiv preprint arXiv:2210.03629*.
- Shuyan Zhou, Frank F Xu, Hao Zhu, Xuhui Zhou, Robert Lo, Abishek Sridhar, Xianyi Cheng, Yonatan Bisk, Daniel Fried, Uri Alon, et al. 2023. Webarena: A realistic web environment for building autonomous agents. *arXiv preprint arXiv:2307.13854*.

⁶⁷² A Prompt Templates

 In this section, we provide all the prompt templates used in this work. In *MARSBench*, there are three types of prompts for each <game, agent> pair: sys- tem prompt, head prompt, observation prompt, and step prompt.

 System Prompt. A system prompt in Large Lan- guage Models (LLMs) is a predefined instruction or command embedded within the model's inter- face, guiding its responses or actions according to specific user needs or operational protocols.

683 We utilize the following sentence as the system **684** prompt for all the environments:

> System Prompt: You are a helpful assistant who strictly follows the users instructions.

685 Head Prompt. Head Prompts provide high-level **686** descriptions of games, including game rules and **687** symbol representation formats.

 Observation Prompt. An observation prompt provides necessary information and observations to the reasoning agent, such as currently available actions, opponent moves, etc.

 Step Prompt. Step prompts define how agents reason given prompts. Different agents may con- tain more than 1 step prompt. All the variables are **denoted as <variable name>.**

696 A.1 Environment Prompt Templates for **697** Tic-Tac-Toe

Head Prompt: Tic Tac Toe is a two-player game played on a grid. Players take turns marking a space with their respective symbols. The goal is to get multiple of ones own symbols in a row, either horizontally, vertically, or diagonally, before the opponent does. If all nine squares are filled and no player has three in a row, the game is a draw. The Tic Tac Toe game is played on a 3 by 3 grid, with the winning length as 3. Each move is represented by a string consisting of two parts: the column (C) and the row (R) , in that order. For instance, C1R2 means the movement at the position of the first column and the second row of the grid. You are playing this game with the user (opponent).

698 Observation Prompt: Now, your opponent

has finished moves: <opponent_moves>. You have finished moves: $\langle \text{agent}\rangle$ moves. The legal positions are <legal_moves>.

A.2 Environment Prompt Templates for Texas **700** Hold'em Poker **701**

Head Prompt: You are playing Texas Holdem Poker with other <num_players> players. The aim of each player in Texas Hold'em poker is to win chips or money from other players by either having the best hand at showdown or by convincing other players to fold their hands. The small blind bet of this game is 1 and the big blind bet of this game is 2.

Observation Prompt: Here are the situations you are facing: You are in the \langle stage \rangle round at present. <round_prior_player_actions>. The current round pot is \langle sound pot and the community pot is <community_pot>. Your card is <card>. Your remaining stack is <remaining_stack>. round prior player actions: In this round, after the small blind and big blind actions, the prior players have made the following actions: Player at <player_info> takes action <action>.

A.3 Environment Prompt Templates for **702** Connect-4 **703**

Head Prompt: Connect 4 is a two-player connection board game, where the players choose a color and then take turns dropping colored discs into a vertically suspended grid. The pieces fall straight down, occupying the next available space within the column. The objective of the game is to be the first to form a horizontal, vertical, or diagonal line of four of one's own discs. You are a gaming agent that aims to beat me in Connect 4 games. Each move is represented by a string consisting of two parts: the column (C) and the row (R) , in that order. For instance, C1R2 means the movement at the position of the first column and the second row of the grid.

Observation Prompt: Now, your opponent has finished moves: \leq opponent moves $>$. You have finished moves: <agent_moves>. The legal positions are <legal moves>.

C Reasoning Agent Adaptions **⁷³²**

ns to the ReAct agent *Particular 737*

rompts from their official codebase first-think-then-action procedures. for challenges is that we need to paces for our tasks. For example, $\frac{741}{ }$ [2022b\)](#page-10-2), the action space defined QA dataset is SEARCH[entity], y], and FINISH. To do that, we de- $\frac{744}{ }$ ng actions for strategic reasoning: $\frac{745}{ }$

ction, which means to block winning of your opponent (e.g., below from forming sequences

ction, which means to win the create forks, control the center,

LLMs to select which type of ac tion is more defensive or offensive. Then, $\frac{747}{ }$ based action, we prompt LLMs to move. The overall step prompt for ReAct is as follows:

704 A.4 Step Prompt Templates for the **Prompt**

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751 C.2 Adaptions to the **ToT** agent

 For the ToT agent, we follow the implementation of the text generation task as in the official codebase [5](#page-13-1)4 of ToT⁵. Specifically, follow the 2-step ToT man- ner, i.e., 1) generate plans; 2) vote for the plan; 3) generate action according to the selected plan; 4) vote for action. The prompts used in this process are shown as follows:

> Step Prompt: First think about your current situation, then choose one move from legal positions to set up advantages.

> Your output should be of the following format: Thought:

Your thought. Move:

Your move.

759 After executing step prompts in a breath-first search **760** manner, we utilize the following voting prompt to **761** select the plan and move:

> Vote Prompt: Conclude in the last line "The best choice is s", where s is the integer id of the choice.

⁷⁶² D Generative Hyperparameters

 For all the model queries and generations, we set the max token number as 1024 and the tempera- ture as 0.2. For other parameters, we follow the default settings as in OpenAI API and Langchain interfaces.

⁷⁶⁸ E Recursively Thinking Ahead (**ReTA**)

769 As we mentioned in Section [5.1,](#page-7-3) to make LLMs **770** think ahead, we incorporate an imaginary enemy **771** before the LLMs makes the final decision.

772 E.1 Implementation

773 To simulate this process, we formulate ReTA as the **774** ensemble of modules, utilizing multiple individual **775** actors:

- **776** Main Actor *M*: interacting with the envi-**777** ronment, gathering feedback from other ac-*778* tors, and generating the next action, i.e., $a_t \sim$ $P_M(a_t|s_t, x)$ where s_t is the current state and 780 x is the external instructions/feedback.
- **781 Reward Actor** M_R : working as a signal func-**782** tion to evaluate the reward signals of different 783 **actions, i.e.,** $r \sim P_R(r|s_t, x)$.

• **Anticipation Actor** M_O : an imaginary oppo- 784 nent, predicting action $a_{o,t}$ to beat M at state 785 s_t , i.e., $\hat{a}_{o,t} \sim P_O(\hat{a}_{o,t}|s_t, x)$. 786

Here P_M , P_R and P_Q are the generative distributions of the backbone LLMs for M , M_R and M_Q , 788 respectively. **789**

Assume at the beginning of gaming step t, e.g., $\frac{790}{200}$ the t-th turn, we first sample *n* desired actions 791 $\mathcal{A}_t = \{\tilde{a}_t^1, \tilde{a}_t^2, \cdots, \tilde{a}_t^n\} \sim P_M(\tilde{a}_t|s_t, x) \text{ from } M$ 792 as the candidacy actions, given current state s_t . Then, the think-ahead process is formulated as the **794** *pseudo-gaming* between M and M*O*, as the follow- **⁷⁹⁵** ing sequence: **796**

 $(s_t, \tilde{a}_t, s_{t+1}, \hat{a}_{o,t+1}, s_{t+2}, \tilde{a}_{t+2}, \cdots, s_T),$ (1) 797

where $\tilde{a}_t \in A_t$ is a candidacy action at pseudo- 798 gaming step t, $\hat{a}_{o,t+1} \sim P_0(\hat{a}_{o,t}|s_{t+1}, x)$ is the 799 sampled action from imaginary opponent M_O , and 800 s*^T* is a terminal state, e.g. achieves win/draw/lose **⁸⁰¹** situation or achieves state s_{t+k} where k is the max- 802 imum allowed number of think-ahead steps. Once **803** the terminal state is achieved in pseudo-gaming, **804** the reward agent M_R will perform situation assess- 805 ment by answering an advantage score, r_T , to de- 806 scribe how many advantages the actor M has at 807 state s_{*T*}: $r_{s_T} \sim P_o(r_T | s_T, T, x)$, (0 ≤ r ≤ 1). 808 Theoretically, if we traverse all the possible com- **809** binations of candidacy actions and always take k **810** steps to achieve terminal states, there will be a 811 k-layer decision-making tree constructed with n^k leave nodes, which indicates there will be at most **813** n^k terminal states and advantage scores in total. 814

Once we finish traversing this decision tree and **815** obtain advance scores for each terminal state, we **816** will perform reward signal backtracking from state 817 s_T to s_t and select action a_t , in a minimax manner: 818

$$
\max_{a_t \in \mathcal{A}} \min_{\hat{a}_{t+1} \in \mathcal{A}} (r_{s_t} P_O(\hat{a}_{t+1}|s_{t+1}) P_M(a_t|s_t)). \quad (2) \tag{319}
$$

With this minimax reward backtracking, we assume 820 that the opponent will always choose the "worst **821** case" during the gaming, which makes our agent **822** more robust to the opponents. Once the traceback **823** happens to the root of the tree, there will be a re- **824** ward signal for each candidacy action in A_t . Then, 825 we select the action with the highest rewards as the **826** next move. The key design of recursively thinking **827** ahead is the imaginary opponent M_O that tries to 828 block the winning of M and the minimax reward **829** signal backtracking. **830**

⁵ [https://github.com/princeton-nlp/](https://github.com/princeton-nlp/tree-of-thought-llm/blob/master/src/tot/prompts/text.py)

[tree-of-thought-llm/blob/master/src/tot/prompts/](https://github.com/princeton-nlp/tree-of-thought-llm/blob/master/src/tot/prompts/text.py) [text.py](https://github.com/princeton-nlp/tree-of-thought-llm/blob/master/src/tot/prompts/text.py)

Figure 7: The tree representation of the proposed recursively think ahead in ReTA.

831 E.2 Step Prompt Templates for **ReTA**

Selection Prompts: First think about your situations, then choose \langle num k \rangle moves from legal positions to set up advantages. Your output should be in the following format: Thought: Your thought. Selection: 1. selected move 2. selected move

Evaluation Prompts: Assume you will take \le next move \ge as the next move. What is the advantage score for this move? Use a score on a scale of 0 - 100 to represent this score. Conclude in the last line "The advantage score for me is s", where s is the score.