# A Notion of Complexity for Theory of Mind via Discrete World Models

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#### Abstract

001 Theory of Mind (ToM) can be used to assess the capabilities of Large Language Models (LLMs) in complex scenarios where social reasoning is required. While the research community has proposed many ToM benchmarks, their hardness varies greatly, and their complexity is not well defined. This work proposes a framework 007 to measure the complexity of ToM tasks. We quantify a problem's complexity as the number of states necessary to solve it correctly. Our 011 complexity measure also accounts for spurious states of a ToM problem designed to make it 012 apparently harder. We use our method to assess the complexity of five widely adopted ToM benchmarks. On top of this framework, we design a prompting technique that augments the information available to a model with a descrip-017 tion of how the environment changes with the agents' interactions. We name this technique 019 Discrete World Models (DWM) and show how it elicits superior performance on ToM tasks.<sup>1</sup>

#### 1 Introduction

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Theory of Mind (ToM) studies how agents form and use beliefs to reason in dynamic environments (Premack and Woodruff, 1978). Originally developed to describe human interactions (Preston and De Waal, 2002; Tomasello, 2009) as well as toddlers' psychological development (Wimmer and Perner, 1983; Baron-Cohen et al., 1985), ToM has been quickly adopted by other fields, including artificial intelligence (McCarthy, 1979; Scassellati, 2002) and machine learning (Rabinowitz et al., 2018). In machine learning, ToM has both descriptive and prescriptive usage: on the one hand, ToM benchmarks assess the capabilities of a model in complex environments; on the other, ToM's frameworks such as theory-theory (Gopnik and Wellman, 1994) and simulation theory (Churchland, 2013)



Question: Where does **Bob** think the **apple** is?

**COT Answer: Bob** thinks the **apple** is on the **floor**. **X DWM Answer: Bob** thinks the **apple** is on the **table**. **V** 

Figure 1: Example of the DWM prompting technique on a classical *Sally-Anne* QA task (Baron-Cohen et al., 1985). Inspired by our complexity framework (Section 3.1), DWM takes the original task and splits it into sequences, the *state events* (see Def. 3.1), and prompts the LLMs to describe the states. We show that, in most cases, this aids the LLM in providing correct answers.

have been widely adopted to test the proficiency of Large Language Models (LLMs) in social tasks where humans excel (Strachan et al., 2024).

In this work, we propose a framework to characterise a ToM benchmark's difficulty, i.e., its **complexity**, as the number of *state events* that are sufficient to track the state of an object, including  $k^{\text{th}}$ -order beliefs.

We characterise the complexity of five standard ToM benchmarks, from false belief to commonsense and social reasoning, and compute their complexity as a proxy of their inherent difficulty. Inspired by prompting techniques that split a task into elementary sub-problems that are solved sequentially, like Tree of Thoughts (Yao et al., 2023) and least-to-most prompting (Zhou et al., 2023a), we introduce a technique that stimulates a model's reasoning capabilities via Discrete World Models (DWM). DWM leverages the notion of state-

<sup>&</sup>lt;sup>1</sup>Code and data for **full reproducibility** are available in the Code Material.

fulness via a succinct and coherent representa-058 tion of each state events, as illustrated in Fig-059 ure 1. We test DWM on ToMi (Le et al., 2019), 060 MindGames (Sileo and Lernould, 2023), Adv-CSFB (Shapira et al., 2023), SocialIQA (Sap et al., 2019), and FANToM (Kim et al., 2023), elicit-063 ing superior performance than Chain of Thoughts 064 (CoT) (Wei et al., 2022) and Tree of Thoughts (ToT) (Yao et al., 2023) on those problems whose state spaces are informative. We further as-067 sess whether memorisation affects a model's performance, and we discover that while this phenomenon happens for standard benchmarks such as ToMi (Le et al., 2019), with input-output pairs that can be retrieved word for word via prompting, it does not correlate with a drop of performance. We conduct our experiments on a variety of open- and closed-source LLMs, including GPT-3.5-Turbo, GPT-4 (OpenAI, 2023), LLaMA3-70B (AI@Meta, 2024) and Mixtral 8x7B (Jiang et al., 2024). In summary, in this paper:

- We introduce the concept of **complexity** of a ToM task to quantify the hardness of keeping track of the elements (e.g., agents' beliefs or objects' states) that are sufficient to produce the correct answer to different problems.
  - We propose DWM, a simple yet effective prompting technique that improves a model's capability by making **implicit** information explicit while not necessitating *exogenous information* (i.e., it does not require RAG or fine-tuning).

We consider our work a step towards a framework that formalizes the hardness of a ToM problem univocally inspired by the theory of World Models (Wong et al., 2023).

# 2 Related Work

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Over 40 years of research on ToM in psychology (Premack and Woodruff, 1978; Baron-Cohen et al., 1985; Dennett, 1988; Wellman, 2017) on human development has created a fertile ground for the development of these ideas in adjacent fields. In the last decade, many works studied ToM in artificial intelligence and machine learning (Baker et al., 2011; Rabinowitz et al., 2018), with applications to multi-agent systems and reinforcement learning (Gronauer and Diepold, 2022). More recently, the rise in popularity of LLMs shifted the interest towards understanding and benchmarking large models' capacity to solve increasingly complex 107 ToM tasks (Aru et al., 2023; Zhou et al., 2023b; 108 Mahowald et al., 2024). While some researchers 109 believe LLMs have already become proficient in 110 solving ToM tasks (Bubeck et al., 2023; Kosinski, 111 2023; Strachan et al., 2024), others show scepti-112 cism and illustrate cases where they fail on trivial 113 variations of well-known problems (Ullman, 2023; 114 Shapira et al., 2023; Sap et al., 2023). In a joint 115 effort between computer scientists and psycholo-116 gists, many ToM benchmarks have been developed 117 and used to test neural-network models, includ-118 ing LLMs (Gandhi et al., 2022; Chen et al., 2024; 119 Strachan et al., 2024). Recently, concepts such as 120 World Models (Ha and Schmidhuber, 2018) have 121 found applicability and mostly as discrete prompt-122 ing techniques in conjunction with optimisation 123 procedures (Hao et al., 2023; Moghaddam and 124 Honey, 2023). Researchers have found evidence 125 of an emergent internal representation (e.g., World 126 Model's surrogates) of the state games (Li et al., 127 2022; Toshniwal et al., 2021) and state-tracking 128 abilities (Li et al., 2021; Kim and Schuster, 2023; 129 Kim et al., 2024), necessary for correct belief track-130 ing in ToM problems. The works more similar to 131 our complexity framework are only tangentially re-132 lated to ToM. Inspired by the work in (Zhou et al., 133 2023a) and the results in (Zhou et al., 2023b). Our 134 prompting technique is inspired by (Park et al., 135 2023) and (Nye et al., 2021): the former devel-136 ops an architecture to record the agent's experi-137 ences. The latter proposes a prompting technique 138 that forces a model to express the intermediate com-139 putational steps to solve a problem. 140

# 3 Methodology

In this section, we introduce a notion of complexity for ToM problems: such notion quantifies the hardness of a problem as the number of *computational steps* humans take to solve them. We then present the DWM prompting technique within the complexity framework and show how it differs from standard methods like CoT and ToT. We further characterise its efficiency with the number of input/output tokens and queries to a model as the control variables. 141

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# 3.1 On the Complexity of ToM

Providing a consistent representation of the envi-<br/>ronment, including each agent's beliefs, inspired us<br/>to characterise the complexity of a ToM problem153154155



$$Complexity(obj_2) = T_{obj2} + \tau (T_{obj1} + T_{obj3})$$
  
stateful stateless

Figure 2: How statefulness and statelessness (Def. 3.2) are computed for the motivating example in Fig. 1. For  $obj_1$ , an optimal split to track the **apple** merges the first two states and chunks of the input prompt. For  $obj_2$ , which involves the 1<sup>st</sup>-order belief of **Bob**, the statefulness is higher, with  $e_2$  that cannot be merged with  $e_3$  as it introduces partial observability. The complexity of the task (bottom) is computed as per Eq. 2, with the complexity of stateless objects that is discounted as not directly relevant to the question/answer.

in terms of **sufficient elements to track** to output the correct result. Consider a problem prompt p, expressed in natural language, that describes how multiple agents interact with an environment object **obj**, as illustrated in Figure 2 (top). In our framework, an object can be the state of the apple as well as the  $k^{\text{th}}$ -order belief of an agent about the apple position. Our framework naturally extends to multiple objects by considering their union.

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Suppose that in p, the state of **obj** is modified T > 0 times, thus identifying T unique configurations, namely  $E_{obj} = \{e_1, ..., e_T\}$ . To correctly solve a ToM task where p is complemented by a query about **obj**, a model should distinguish between the interactions that modify the configuration of **obj**, i.e., the **stateful** states, from those that modify any other **stateless** object  $Obj \setminus obj$ , i.e., those one does not need to track.

We first show how to define the cost of tracking a task's stateful states, which we complement with that of the stateless. Both definitions concur in defining the **complexity** of a ToM task.

#### 3.1.1 Stateful and Stateless Complexity

For a ToM task, expressed as p, that describes the evolution of an environment where an unknown number of atomic iterations T modifies **obj** or its perception, each environment state  $e_t \in E_{obj}$  can be coupled with the prompt prefix  $p_{\leq t}$  s.t.  $p_{\leq t} \oplus$   $p_{>t} = p$ , that describes such configuration. We denote  $(e_t, p_{\leq t})$  as a generic *state description*, as illustrated in Figure 2 (top).

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**Definition 3.1** (State event). A *state event* for an object **obj** is an event that links adjacent *state descriptions* that involve, for both the environment state  $e_t$  and the sub-prompt  $p_{\leq t}$ , a state change of **obj**. Formally, we define a relation,  $F_{obj}$ , to specify which pairs of state descriptions form a state event:  $F_{obj}((e_t, p_{\leq t}), (e_{t+1}, p_{\leq t+1})) \equiv e_t \neq e_{t+1} \land p_{\leq t+1} = p_{\leq t} \oplus p_{t+1}$  where  $1 \leq t \leq |p|$ . (|p| denotes the number of atomic prompts.)

Thus a state event  $F_{obj}$  identifies those state descriptions  $(e_t, p_{\leq t})$  which have a successor  $(e_{t+1}, p_{\leq t+1})$  where obj has changed its configuration.

In the context of ToM tasks, a *state event* could be a person who moves an object, exits (thus introducing partial observability) or witnesses a change in the environment (as now the description of the environment will take that change into account), as illustrated Figure 2 (middle). Our prompting technique, namely DWM (Section 3.2.1), aims at making implicit observations about objects explicit.

We finally introduce the notion of *partition function* to connect the **maximum number** of nonempty *state events* relative to a prompt. Such a notion will serve as the building block to compute the complexity of a ToM problem.

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**Definition 3.2** (Partitions). A partition  $part_{obj}$ w.r.t. **obj** identifies those *state events* which partition a ToM prompt p into sequential segments where **obj** changes its value. Formally:

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Let 
$$part_{\mathbf{obj}} = \{(e_t, p_{\leq t}) :$$
  
 $F_{\mathbf{obj}}((e_t, p_{\leq t}), (e_{t+1}, p_{\leq t+1}))$  (1)  
 $\land e_t \in E_{\mathbf{obj}}\}$ 

Def. 3.2 describes an optimal partition,  $part_{obj}$ of *state descriptions* that covers all the relevant changes to obj. The partition is represented by the set of event descriptions where obj changes its description immediately after. Note that this set of event descriptions is unique for any obj.

#### 3.1.2 The Complexity of a ToM Task

We can now define the notion of **statefulness** of a ToM task specified as a prompt p as the size of Eq. 3.2, namely  $T_{obj} = |E_{obj}|$ . The process of computing the statefulness of an object or its belief is illustrated in Fig. 2.

For a ToM task where the question to solve relates to an object obj, one must ensure that changes to any other object, namely  $Obj \setminus obj$ , do not affect obj. While tracking the evolution of what is irrelevant to answer the question is unnecessary, a computation model must assess whether a particular environmental change affected obj. We thus introduce the notion of statelessness, i.e., the cost of discerning whether a change in the environment affects obj. The computation is similar to that of Def. 3.2, with obj that is replaced by any object in  $Obj \setminus obj$ ; yet, for stateless objects, we introduce a discount factor  $\tau$  to penalise the complexity of *state* events that do not affect obj. Mathematically, we formalise the statelessness of a ToM task involving an object obj as  $\tau \sum_{obj \in Obj \setminus obj} T_{obj}$ .

Finally, we formalise the complexity of a ToM task w.r.t. an object **obj** as the complexity of the stateful states plus the (discounted) sum of the others (i.e., stateless). Namely:

$$T_{\mathbf{obj}} + \tau \sum_{obj \in Obj \setminus \mathbf{obj}} T_{obj}$$
(2)

The process of computing the complexity of a ToM task is illustrated in Figure 2.

#### 3.2 Discrete World Models

We first introduce the background notation for prompting LLMs and assessing their accuracy on a standard classification task. We then propose our technique, namely DWM, which we eventually connect with the notion of statefulness of a ToM task.

Background notation. A (Large) Language Model is a function that predicts the next token (out of a finite vocabulary) conditioned on the sequence of previously fed/generated tokens, namely  $\psi: \mathbf{v} \in V^* \to v \in V$ . Such a mechanism can be used to sample multiple token outputs until an 'end-of-text' token is predicted by invoking  $\psi$ in an auto-regressive fashion, i.e.,  $\psi(v|\mathbf{v})$ . In our setting, a problem is specified as a tuple (p, Q), where p is a ToM problem and Q is a query function that modifies p according to a prompting technique, namely  $Q: p \to p'$ . The LLMs output y for an input Q(p) is then compared for correctness against an oracle  $\Omega$ , i.e.,  $\Omega: \psi(Q(p)) \to \{0,1\}$ , where 1 means correct classification (0, otherwise). On a sample of N > 0 ToM problems, the accuracy of a model  $\psi$  is then measured as  $\frac{1}{N} \sum_{i=1}^{N} \Omega(\psi(Q(p_i)))$ , i.e., the average number of times a model is correct in its prediction.

#### 3.2.1 Discrete World Models via Prompting

Given a ToM problem p and a constant  $T \leq |p|$ , we can rewrite p as  $p_1 \oplus p_2 \oplus \cdots \oplus p_T$ . Our *query* function adds a standard preamble x similar to that of CoT. DWM inserts, after each "split"  $p_t$ , an additional prompt w like 'Now, provide a succinct description of the state of the environment and each agent's belief.' and query an LLM to provide a representation of the current *state description* of the environment. An LLM is initially queried with  $x \oplus p_1 \oplus w$ , and the answer  $a_1$  is concatenated to the next query, i.e.,  $\psi(x \oplus p_1 \oplus w \oplus a_1 \oplus p_2 \oplus w)$  to retrieve  $a_2$ . The process is carried on for each of the T chunks, and, at the end, y is concatenated to eventually prompt the model for the correct answer to p.

Let  $z_1 = \psi(x \oplus p_1), z_t = \psi(x \oplus p_1 \oplus z_1 \oplus p_2 \oplus \cdots \oplus z_{t-1} \oplus p_t) = \psi(x \oplus \left(\bigoplus_{i=1}^{t-1} p_i \oplus z_i\right) \oplus p_t),$ then, the final query is

$$\psi(x \oplus \left(\bigoplus_{t=1}^{T} p_t \oplus z_t\right) \oplus y)$$
(3)

In this sense, our **partition function** (Def. 3.2) 299 consists of splitting a prompt into sequential chunks 300 of the prompt, while the LLM is prompted to 301 provide each *state event* at time  $1 \le t < T$  as  $e_t = \psi(x \oplus (\bigoplus_{t'=1}^t p_{t'} \oplus z_{t'}) \oplus \omega)$ . The process 303



Figure 3: Left: illustration of DWM prompting as per the example in Figure 1. We interactively prompt an LLM with a ToM problem, asking to provide a succinct representation of each agent's beliefs. Right: schematic presentation of the DWM method. We first break the input string into T state descriptions. Then, for each part, we ask the LLM to provide the **state event** of the environment and how it changes. In the last step, every part of the input and description is fed to the LLM with another prompt to get the answer for the task.

of prompting a model with DWM is illustrated in Figure 3.

#### 3.2.2 On the Complexity of DWM

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DWM progressively calls an LLM T > 0 times to generate informative states. For a ToM problem of length n (i.e., the number of input tokens), which we assume, w.l.o.g., that can be split into k chunks of approximately the same length  $|x \oplus p_i \oplus w| = \frac{n}{T}$ , the number of tokens generated by an LLM is in the order of  $\mathcal{O}(\sum_{t=1}^{T} |x \oplus p_t \oplus w \oplus a_t|^2)$ , where  $p_t(a_t)$ is the portion of the problem (answer) prompted (retrieved) at iteration t. With the further assumption that each answer retrieved at split t < T has the same length o, the complexity is further simplified to be asymptotic to  $\mathcal{O}((\frac{n}{T}+o)^2)$ . Compared to CoT, whose complexity is  $\mathcal{O}(n+o)$ , DWM requires an additional linear number of calls to the model. On the other hand, ToT with the same number of splits  $\frac{n}{T}$  and m > 1 experts results in even higher complexity, i.e., asymptotic to  $\mathcal{O}(m(\frac{n}{T}+o)^2)$ .

#### 4 Experimental Evaluation

The experiments are organised as follows. We first test the performance of DWM on ToMi (Le et al., 2019), MindGames (Sileo and Lernould, 2023), Adv-CSFB (Shapira et al., 2023), SocialIQA (Sap et al., 2019), and FANToM (Kim et al., 2023), comparing it with CoT (Wei et al., 2022), ToT (Yao et al., 2023) and prompting with structured data (struct), i.e., the model is queried to first represent the problem in a structured format such as JSON or Yaml. We further show that ToMi has been memorised *word for word* by GPT models, with CoT (and any technique that leaves the input unchanged) being the best-performing method. We then quantify the complexity of the benchmarks introduced above and highlight the correlation with the models' performances. Our framework shows complexity ranges between easy and hard problems, even within a benchmark. We conduct our experiments on GPT-3.5-Turbo, GPT-4 (OpenAI, 2023), LLaMA3-70B (AI@Meta, 2024) and Mixtral 8x7B (Jiang et al., 2024).

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#### 4.1 DWM on ToM Benchmarks

We report results for GPT-3.5-Turbo and Mixtral 8x7B on the five ToM benchmarks: for reasons of space, results for LLaMA3-8B, LLaMA3-70B and GPT-4 are reported in the Appendix, Section B.1. As illustrated in Figure 4 (top), DWM improves the performance of GPT-3.5-Turbo on Mindgames, FANToM and Adv-CSFB by a solid margin. On SocialIQa, which has very short inputs, DWM performs slightly worse than CoT but better than ToT. On the other hand, on ToMi, the best prompting techniques are CoT and ToT. As analysed in the next section, we believe this not be caused by memorisation, which we prove happening, but by the inherent complexity of the task. With Mixtral 8x7B (Fig. 4 (bottom)), DWM improves the performance on ADVcsfb, FANToM, ToMi and Mindgames, and pairs that of CoT on SocialIOa.

**DWM elicits more informed** *state spaces.* We qualitatively analysed the information elicited by an LLM when prompted with DWM and discovered that it forces a model to output information **not explicitly** available in the prompt. Consider the ToMi example in Figure 5 where GPT-4 is prompted with a situation where agents interact



Figure 4: Benchmarks of GPT-3.5-Turbo (top) and Mixtral 8x7B (bottom) models on different ToM tasks for DWM (one to five splits), CoT, ToT and structured prompts (JSON and Yaml).

	ToMi	FANToM	Mindgames	Adv-CSFB	SocialIQa
Memorisation - perfect match	52%	35%	2%	0%	0%
Memorisation - fuzzy	$89\pm15\%$	$74\pm24\%$	$64\pm18\%$	$51\pm11\%$	$40\pm12\%$
DWM	0.625	0.579	0.618	0.8364	0.691
СоТ	0.629	0.403	0.552	0.7091	0.736

Table 1: Summary of the memorisation test on five ToM benchmarks. We prompted GPT-3.5-Instruct to predict the continuation of 100 randomly sampled test points. We computed the exact and fuzzy memorisation rate (second row, similarity score computed via the Levenshtein distance, see the thefuzz package), which we complement with the best performance across models of CoT and DWM.

	ToMi	FANToM	Mindgames	Adv-CSFB	SocialIQa
Statefulness	$2.62 \pm 1.68$	$2.44\pm0.96$	$1.22\pm0.90$	$3.24 \pm 1.35$	$1.\pm 0.$
Statelessness	$4.27\pm2.1$	$59.42 \pm 18.91$	$5.24 \pm 2.71$	$2.86 \pm 1.34$	$1.14\pm0.447$
DWM - Best Split	3	3	1	4	1

Table 2: Summary of the statefulness and statelessness of different ToM benchmarks. At the bottom, the value of the split that guarantees max performance of GPT-3.5-Turbo with DWM, which we notice is strongly correlated with the statefulness of each benchmark.



Figure 5: Example of a real ToMi example where GPT-4 fails when prompted with CoT, yet succeeds with DWM. CoT elicits an untruthful reasoning process (in **red**), while DWM correctly informs the model with the implicit information about Benjamin's first-order belief (in **green**). More examples are reported in the Appendix, Section B.2.



Figure 6: Each boxplot summarizes the complexity analysis of the five ToM benchmarks in ascending order. We report the average **error rate** (i.e., 1-accuracy) of GPT-3.5-Turbo, GPT-4, Mixtral 8x7B and LLaMA3-70B on the task when prompted with CoT.

and are then queried with the first-order belief of Benjamin. With CoT, the model makes an erroneous assumption about the presence of Benjamin and Isabella in the room. On the other hand, when prompted with DWM, GPT-4 provides an informative description of each *state space*, particularly the knowledge and the uncertainty of each agent's beliefs, and eventually answers correctly. One example per benchmark is available in the Appendix, Section B.2, while many more are available for inspection in the Code Supplementary Material. Such phenomenon is ubiquitous to all the ToM tasks we tested, a hint that DWM elicits the ToM capabilities of LLMs without requiring external information or solvers.

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387 Memorisation in Theory of Mind. Recent
388 works expressed concern about ToM benchmarks'

efficacy in memorisation (Jacovi et al., 2023; La Malfa et al., 2024). This motivated us to quantify and then analyse the impact of memorisation of ToM benchmarks on performance. We computed the percentage of memorised prompts to understand whether that affects the performance of techniques, such as DWM, that split the prompt into chunks and introduce additional information instead of CoT, which leaves the input prompt unchanged. As illustrated in Table 1, ToMi and FAN-ToM have been heavily memorised, with entire portions of the benchmarks that can be retrieved word for word from GPT-3.5-Instruct (the autocomplete model by OpenAI). Despite that, no clear evidence of a performance drop in DWM induced by memorisation exists. For GPT-3.5, despite CoT having higher performance on ToMi, DWM is better on FANToM (Figure 4). We hypothesise that as long as a memorised problem is prompted, either in its exact form (as for CoT) or split as in DWM, the most potent models can recover it alongside the ground truth label, thus invalidating the test for both. We conclude with a note of caution. While we discovered that ToMi and FANToM are memorised by GPT-3.5-Instruct, that doesn't imply any LLM, including GPT-3.5-Turbo and GPT-4, whose training details are not released publicly, has been trained on that data.

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#### 4.2 Statefulness of ToM Benchmarks

We used the complexity framework introduced in418Section 3.1 to characterise the statefulness and419statelessness of the five ToM benchmarks used for420the experimental evaluation. We randomly sampled42150 problems from each dataset, identified the objects, and manually labelled stateful and stateless422



Figure 7: Each boxplot summarizes the statefulness (left), statelessness (middle, y-axis in log-scale) and complexity analysis (right) of the five ToM benchmarks. We report mean, standard deviation and outliers alongside the best DWM method (by the number of prompt splits) and observe a strong correlation between the number of splits and the statefulness.

424 state events. We release the split samples alongside a web application that facilitates manual labelling. 425 As illustrated in Figure 7 (left), the statefulness 426 of each problem, i.e., that of the object a model 427 must track to answer correctly, strongly correlates 428 with the best-performing DWM split. The stateless-429 ness complexity, reported in Figure 7 (middle), i.e., 430 that of objects that a model does not need to track, 431 grows larger for problems such as FANToM, only 432 partially influencing the models' performance. We 433 hypothesise that the most potent models developed 434 435 some competency in discerning the relevant part of a prompt (the stateful events) from the confound-436 ing ones. We finally report, in Figure 7 (right), the 437 complexity of each problem computed as per Eq. 2, 438 with  $\tau$  set in a range between 0.05 and 0.2 (i.e., 439 the relative weight of stateless compared to stateful 440 events). Results suggest that FANToM is the most 441 difficult ToM task for humans and LLMs (see Fig-442 443 ure 4), followed by ToMi (the second most difficult for LLMs as well) and Adv-CSFB (which seems 444 easier than the others); in contrast, Mindgames and 445 SocialIQa tend to be easier. Finally, in Figure 6, we 446 compare the accuracy of GPT-3.5-Turbo, GPT-4, 447 Mixtral 8x7B and LLaMA3-70B when prompted 448 with CoT (i.e., without split) on the five ToM bench-449 marks with the complexity of the task as per Def. 2. 450 We observe a strong correlation between the error-451 rate and the complexity of a task, i.e., our frame-452 work correctly identifies the tasks that are harder 453 both for humans and current state-of-the-art LLMs. 454

#### 5 Conclusions

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This paper introduces a complexity framework to measure the difficulty of Theory of Mind (ToM) problems. It quantifies the difficulty by tracking necessary states (stateful) and unnecessary states (stateless), with the latter discounted in the complexity computation. The framework evidences a strong correlation between complexity and model performance. Inspired by this framework, we propose DWM, a prompting technique that splits a prompt into parts to query a model for a consistent representation of the environment and agents' beliefs. DWM outperforms CoT and ToT by extracting implicit but relevant information. 459

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#### Limitations

**Higher order belief tracking.** Our theoretical framework reduces the problem of solving a belief ToM problem to finding the correct descriptions that need to be tracked. It extends seamlessly to tasks with much higher complexity, however, we have not had the opportunity to test this theory in those settings. We noticed that most theory of mind tasks available in the community only require one to five states to be correctly answered. A possible extension would be testing the theory upon tasks with higher state complexity, e.g.  $k^{\text{th}}$ -order belief tracking tasks. However, it is unclear whether this could be useful in real applications as most human belief tracking is limited to 5 or 6 orders (Cargile, 1970; Dennett, 1988).

**On task splitting methods.** It is not straightforward to automatically find the correct task splits in a manner that correctly describes the state. An LLM could find a way to split it by itself correctly and use those splits to answer the question. We attempted this approach, yet with a simple prompting method, the model splits every sentence, making the descriptions much noisier and less accurate. Future work could try to find the best splits auto494 matically.

495 **Memorization analysis.** Training and evaluating on the same dataset produce positively biased data 496 on the model's performance. While running our 497 benchmarks on ToMi, we discovered that the GPT-498 3.5 model had completely memorized parts of the 499 dataset. This motivated us to extend the memorization test to the other tasks. We urge the research community to include a memorization section on every benchmark study with public datasets used in their works. This data is crucial to conduct fair 504 and unbiased research on evaluating LLMs' abilities (Jacovi et al., 2023). Future works will include 506 an analysis of the memorisation rate of other ToM tasks alongside tests to quantify their impact on different models. 509

# 510 Ethical Statement

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The datasets and pre-trained LLMs that we use are all publicly available. This paper focuses on ToM problems' hardness and prompting methods. We highlight that LLMs do not guarantee the production of factual data or correct reasoning steps, and the prompting methods developed here should not be regarded as the source of truth in making decisions.

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# A Experimental Setup

# A.1 Experimental Details

Most of the language models used in this work follow the Language Models as a Service (LMaaS) paradigm (La Malfa et al., 2023). This model of service does not allow transparency and hinders reproducibility. Reproducibility is difficult to achieve as common software development frameworks, such as CI/CD pipeline, ease the update of the public service, but change the underlying entity. From this follows that the model tested by the researcher could change at any time. This is not solvable from the outside. Researchers have no control over the software engineering practices inside a LMaaS, but could set some parameters to offer the highest possible grade of reproducibility. We set the temperature to zero or enable greedy decoding by default (this does not imply determinism even if model weights are not changed).<sup>2</sup> In prompting methods where the creativity of the response is exploited for better performance, e.g., Tree of Thoughts (Yao et al., 2023), we set the temperature to 0.7, the value proposed in the reference papers.

**LMaaS providers.** We use Huggingface for Mixtral 8x7B. Groq Cloud for LLama-3-7B and LLama-3-70B. Microsoft sponsorship for GPT-3.5 and GPT-4 access.

# A.2 Prompting Templates

We present the different prompting techniques, taking as an example the following prompt from ToMi and GPT-3.5-Turbo as the reference model:

Benjamin entered the workshop.
 Isabella entered the workshop.
 Hannah entered the workshop.
 Isabella hates the onion
 Hannah hates the t-shirt
 The pajamas is in the bottle.
 Isabella moved the pajamas to the drawer.
 Benjamin exited the workshop.
 Isabella exited the workshop.
 Benjamin entered the workshop.
 And the following question:

Where does Benjamin think that Isabella searches for the pajamas?

# **Chain of Thought**

	772			
Consider the following dialogue where multiple	773			
agents interact. At the end, I will ask you	774			
a question to answer.	775			
Here's the dialogue:	776			
	777			
1. Benjamin entered the workshop.	778			
<ol><li>Isabella entered the workshop.</li></ol>	779			
3. Hannah entered the workshop.	780			
4. Isabella hates the onion	781			
5. Hannah hates the t-shirt	782			
6. The pajamas is in the bottle.	783			
7. Isabella moved the pajamas to the drawer.	784			
8. Benjamin exited the workshop.	785			
9. Isabella exited the workshop.	786			
10. Benjamin entered the workshop.	787			
	788			
This is the end of the dialogue. Now, this is a	789			
question for you to answer.	790			
	791			
Question: Where does Benjamin think that	792			
Isabella searches for the pajamas?	793			
	794			
Think step by step, answer the question with	795			
one word and provide the answer between	796			
<answer></answer> tags.	797			
For example, reply with <answer>vase</answer> .	798			
	799			
Tree of Thought	800			
We first prompt an LLM to propose different solu-				
tion paths to solve a task.				

We then pick the best idea via a majority vote over three agents simulated by the LLM itself:

4. Isabella hates the onion

<sup>&</sup>lt;sup>2</sup>The main explanation are the https://github.com/ pytorch/pytorch/issues/75240"non deterministic cuda cores" another could "be batched inference in sparse MoE models", see https://152334h.github.io/blog/ non-determinism-in-gpt-4/here

##	Here we insert the output of the previous prompt.
W	e eventually ask the model for a final answer.
Gi 1. 2. 3. 4. 5. 6. 7. 8. 9. 10	<pre>ven this dialogue and possible observations, answer the question with one word and provide the answer between <answer></answer> tags. Benjamin entered the workshop. Isabella entered the workshop. Hannah entered the workshop. Isabella hates the onion Hannah hates the t-shirt The pajamas is in the bottle. Isabella moved the pajamas to the drawer. Benjamin exited the workshop. Isabella exited the workshop. . Benjamin entered the workshop.</pre>
Qu	estion: Where does Benjamin think that Isabella searches for the pajamas?
##	Here we insert the observations generated by the LLM with the previous prompts.
Fo	r example, reply with <answer>vase</answer> .
Di	screte World Models - 1 Split
=o #	<pre>give you a phrase of a dialogue between agents. I will reveal more parts of it later. At the end, I will give you a question you must answer. r each phrase, you must: 1. Write down a succinct description of what each agent knows about the environment and about the other agents. Keep the description short and do not produce redundant information. 2. Each considerations you make must be preceded by the symbol #GPT#. re's the dialogue:</pre>
1. 2. 3. 4. 5. 6.	Benjamin entered the workshop. Isabella entered the workshop. Hannah entered the workshop. Isabella hates the onion Hannah hates the t-shirt The pajamas is in the bottle.

5. Hannah hates the t-shirt

6. The pajamas is in the bottle.

8. Benjamin exited the workshop.

9. Isabella exited the workshop.

10. Benjamin entered the workshop.

Here are some possible observations:

7. Isabella moved the pajamas to the drawer.

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- 9. Isabella exited the workshop.
- 10. Benjamin entered the workshop.
- This is the end of the dialogue. Now, this is a question for you to answer.
- Question: Where does Benjamin think that Isabella searches for the pajamas?

Think step by step, answer the question with					
one word and provide the answer between					
<answer></answer> tags.					
For example, reply with <answer>vase</answer> .					

#### **Discrete World Model - 3 Split**

T sins was a shares of a dislams between	915
I give you a phrase of a dialogue between	910
later At the end I will give you a	018
question you must answer	010
For each phrase you must:	920
# 1 Write down a succinct description of what	921
each agent knows about the environment and	922
about the other agents. Keep the	923
description short and do not produce	924
redundant information.	925
# 2. Each considerations you make must be	926
preceded by the symbol #GPT#.	927
Here's the dialogue:	928
	929
1. Benjamin entered the workshop.	930
2. Isabella entered the workshop.	931
3. Hannah entered the workshop.	932
## Here the LLM provides a description of the	933
environment so tar described by the dialogue.	934
	936
4. Isabella hates the onion	937
5. Hannah hates the t-shirt	938
6. The pajamas is in the bottle.	939
## Here the LLM provides a description of the	940
environment so far described by the	941
dialogue.	942
7. Isabella moved the pajamas to the drawer.	944
8. Benjamin exited the workshop.	945
9. Isabella exited the workshop.	946
10. Benjamin entered the workshop.	947
	948
This is the end of the dialogue. Now, this is a	949
question for you to answer.	950
	951
Question: Where does Benjamin think that	952
Isabella searches for the pajamas?	953
Think stop by stop proven the substice with	954
inink step by step, answer the question with	955
one word and provide the answer between	930
Sanswer//answer/ Lags. For example reply with canswer/vases/answer/	050
- or champte, repty with fallower/vabes/allower/.	959
Yaml/JSON	960
	961
Consider the following dialogue where multiple	962
agents interact.	963
1 Ponjamin ontored the workshap	964
1. Denjamin entered the workshop. 2. Isabella entered the workshop	905
2. Isobella entered the workshop	900 067
4 Isabella hates the onion	907
5. Hannah hates the t-shirt	960
6. The pajamas is in the bottle	970
7. Isabella moved the pajamas to the drawer	971
8. Benjamin exited the workshop	972
9. Isabella exited the workshop.	973
10. Benjamin entered the workshop.	974
	975
Here is the YAML representation of the text.	976
## Here we substitute the JSON/Yaml	977
representation of the dialogue (see next	978

#### prompt).

Question: Question: Where does Benjamin think that Isabella searches for the pajamas?
Answer between the tags with a single word that is the answer of the above question For example <answer>vase</answer> .
The JSON/YAML representation is required with the following prompt:
<ul> <li>Consider the following dialogue where multiple agents interact.</li> <li>1. Benjamin entered the workshop.</li> <li>2. Isabella entered the workshop.</li> <li>3. Hannah entered the workshop.</li> <li>4. Isabella hates the onion</li> <li>5. Hannah hates the t-shirt</li> <li>6. The pajamas is in the bottle.</li> <li>7. Isabella moved the pajamas to the drawer.</li> <li>8. Benjamin exited the workshop.</li> <li>9. Isabella exited the workshop.</li> <li>10. Benjamin entered the workshop.</li> </ul>
Now give a structured representation of the dialogue in YAML format. Keep track of the

information that each agent has access to at each point in the dialogue. It is important to have a relative representation of the information that each agent has access to at each point in the dialogue.

#### **B** Additional Results

#### B.1 DWM Prompting

In this section, and, in particular in Figure 8, we report results for LLaMA3-7B, LLaMA3-70B and GPT-4 on the five ToM benchmarks and for different prompting techniques, namely DWM (one to five splits), JSON, Yaml, CoT and ToT.

B.2 DWM Elicits More Informed Mental States in LLMs

In this section, we report and discuss an example of a real prompt and the answers provided by GPT-4 for each ToM task we evaluated in this paper. For FANToM (Figure 10), we just reported the portion of the prompt that induces an unfaithful reasoning process in GPT-4, due to the prohibitive length of the input prompts. Results for ToMi, FANToM, ADV-csfb, Mindgames and SocialIQa are reported respectively in Figures 9, 10, 11, 12 and 13.



Figure 8: Benchmarks of LLaMA3-7B (top), LLaMA3-70B (middle) and GPT-4 (bottom) models on different ToM tasks for DWM (one to five splits), CoT, ToT and structured prompts (JSON and Yaml). For GPT-4 and ToT, we tested 50 samples (instead of 1000).

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Input Prompt	Chain of Thoughts
Benjamin entered the workshop. Isabella entered the workshop. Hannah entered the workshop. Isabella hates the onion Hannah hates the t-shirt The pajamas is in the bottle.	"The pajamas are initially in the bottle. [] <b>Benjamin's Presence: Benjamin is</b> <b>not present in the workshop when Isabella moves the pajamas.</b> He exits before this action and re-enters after Isabella has already left. Based on this sequence of events, <b>Benjamin was not present to witness Isabella moving the</b> <b>pajamas to the drawer.</b> Therefore, in Benjamin's understanding, the last known location of the pajamas would still be where they were originally placed before he left, which is the bottle <answer>bottle</answer> "V
Benjamin exited the workshop. Isabella exited the workshop. Benjamin entered the workshop.	"Benjamin knows that he entered the workshop, that Isabella and Hannah also entered, that Isabella hates onion and Hannah hates t-shirts, that the pajamas
Where does Benjamin think that Isabella searches for the pajamas?	were in the bottle but Isabella moved them to the drawer, and that he exited and re-entered the workshop. He doesn't know that Isabella exited the workshop. [] <answer>drawer</answer> "
Question	Discrete World Models

Figure 9: Example of a real ToMi example where GPT-4 fails when prompted with CoT, yet succeeds with DWM. CoT elicits an untruthful reasoning process (in **red**), while DWM correctly informs the model with the correct information about Benjamin's first-order belief (in **green**).

#### Input Prompt

[...]

**Conor:** Raegan, you were saying about being a vegetarian. Has it had a big impact on your personal life?

**Raegan:** Absolutely, Conor. It's definitely been a transformation. Initially, it was challenging to find vegetarian alternatives to my favorite meals, but over time, it's made me be more aware of what I'm eating. It's also made me try out a lot of new and interesting foods, vegan ones included! **Conor:** That's really insightful. I've been considering it, mainly for health reasons, but haven't taken

the leap yet. Maybe trying out that vegan restaurant is a good place to start.

**Raegan:** Definitely! Exploring vegan or vegetarian food can be a great first step. The variety and flavors might surprise you! Conor: I'll keep that in mind. It's always exciting to discover something new!

**Brittney:** Hey guys, I'm back! I find our talks about food trends so interesting. [...]

# Ouestion

What does Brittney believe were Conor's primary motivations for considering a shift to vegetarianism?

# Chain of Thoughts

"Based on the dialogue, Brittney did not explicitly state what she believes Conor's primary motivations are for considering a shift to vegetarianism. However, **Conor himself mentions that he has been considering vegetarianism mainly for health reasons**. **Thus, if Brittney is aware of this part of the conversation**, she would likely think that health reasons are Conor's primary motivation for considering the change to a vegetarian diet. <answer>Health reasons</answer>"

# Discrete World Models

"Brittney knows that she was part of a conversation with Conor and Raegan. She had to leave temporarily due to her parking meter expiring. She also knows that the conversation was about food trends, specifically vegetarianism and veganism, and finds it interesting [...] She also knows that Conor is considering becoming a vegetarian and has suggested trying out vegan or vegetarian food as a first step. [...] <a href="https://www.answers.example.com">www.answers.example.com</a> a first step. [...] She also knows that conor is considering becoming a vegetarian and has suggested trying out vegan or vegetarian food as a first step. [...] <a href="https://www.answers.example.com">www.answers.example.com</a> shift to vegetarianism as she was not present during that part of the conversation.</a>

Figure 10: Example of a real FANToM example where GPT-4 fails when prompted with CoT, yet succeeds with DWM. CoT elicits an untruthful reasoning process (in **red**), while DWM correctly informs the model with the correct information about the partial observability Brittney has about Conor (in **green**).

#### Input Prompt

There is a closed glass box on the table of an empty meeting room, in which a seminar is about to take place.

#### Question

Fill in the blank with the best option. She loves writing with \_

- pens
- pencils

# Chain of Thoughts

"Based on the information provided, the attendee reads the label on the box marked "pencils" and feels delighted upon finding it. This suggests that she has a preference for what she believes the box contains, which according to the label are pencils, even though the box actually contains pens. Therefore, the best answer, given her reaction to the label, would be: <answer>pencils</answer>"

#### Discrete World Models

#### "Agent: James

James knows that the box on the table is filled with pens, not pencils, despite the label saying "pencils". He knows that he labeled the box himself. He is aware of his own actions and the contents of the box. He also knows that he is alone in the room and that a seminar is about to take place. <a href="mailto:<a href="mailto:saware?enswer?saware"><a href="mailto:saware?

Figure 11: Example of a real ADV-csfb example where GPT-4 fails when prompted with CoT, yet succeeds with DWM. CoT elicits an untruthful reasoning process (in **red**), while DWM correctly informs the model with the correct information about the content of the glass box (in **green**).

#### Input Prompt

There are three persons. Everyone is visible to others. Each person draws a card, face unrevealed (red or black). Leah's card is shown to Leah. Raymond's card is shown to Leah. Brittney's card is shown to Leah. Raymond. It is publicly announced that someone picked a red card.

#### Question

Leah can now know that Raymond can know whether or not nobody picked a red card. Is the above statement in entailment or contradiction with the previous situation?

#### Chain of Thoughts

"In the given situation, Leah sees Raymond's card and Brittney's card, but she does not see her own card. It is publicly announced that someone picked a red card, but Leah cannot determine whether it was Raymond or Brittney who picked the red card based on the information she has. <a href="mailto:<a href="mailto:see"><a href="mailto:</a> (answer> contradiction</a href="mailto://answer> tard"></a>

# Discrete World Models

"Leah: Knows the color of her own card. Does not know the color of the other two persons' cards. Knows that the other two persons can see her.

Other two persons: Do not know the color of their own cards or each other's cards. Knows that Leah knows the color of her card. Knows that Leah can see them.

Leah: Knows the color of her own card, Raymond's card, and Brittney's card. **Knows that Raymond knows the color of his card.** Knows that someone picked a red card. Raymond: Knows the color of his own card. Does not know the color of Leah's or Brittney's cards. Knows that Leah knows the color of his card and Brittney's card. Knows that someone picked a red card.

Brittney: Does not know the color of her own card or Raymond's card. Knows that Leah knows the color of her card and Raymond's card. Knows that Raymond knows the color of his card. Knows that someone picked a red card. <a href="mailto:<a href="mailto:</a> answer>entailment</a> answer>"

Figure 12: Example of a real Mindgames example where GPT-4 fails when prompted with CoT, yet succeeds with DWM. CoT elicits an untruthful reasoning process (in **red**), while DWM correctly informs the model with the correct information about the knowledge Leah has about Raymond (in **green**).

#### Input Prompt

Skylar was pushed by the bully in the lunch line, so Skylar poured milk over their head.

Question

Consider the following statement, you will need to infer the correct response. At the end, I will ask you a question to answer.

Here's the statement:

Skylar was pushed by the bully in the lunch line, so Skylar poured milk over their head.

This is the end of the dialogue. Now, this is a question for you to answer.

Question: What will Skylar want to do next?

- 1: Run away
- 2: Wait for a reaction
- 3: wanted to fight with the bully

#### Chain of Thoughts

"Based on the statement, Skylar's response to being pushed by the bully was to pour milk over their head. This suggests that Skylar wanted to retaliate or stand up to the bully, indicating a desire to fight back.

<answer>3: wanted to fight with the bully</answer> X

#### Discrete World Models

"Agent: Skylar Knowledge about the environment: Skylar knows they are in a lunch line and that there is a bully present. Skylar also knows they have access to milk. Knowledge about other agents: **Skylar knows the bully is aggressive and has pushed them.** 

Agent: The Bully Knowledge about the environment: The bully knows they are in a lunch line and that Skylar is present. Knowledge about other agents: The bully knows Skylar is someone they can push around, but may not anticipate Skylar's retaliatory action.

<answer>1: Run away</answer>"

Figure 13: Example of a real SocialIQa example where GPT-4 fails when prompted with CoT, yet succeeds with DWM. CoT elicits an untruthful reasoning process (in **red**), while DWM correctly informs the model with the correct next actionSkylar will take (in **green**).