

000 001 002 003 004 005 006 007 008 009 010 011 012 SIMPLEToM: EXPOSING THE GAP BETWEEN EXPLICIT ToM INFERENCE AND IMPLICIT ToM APPLICATION IN LLMs

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Anonymous authors
Paper under double-blind review

039 040 041 042 ABSTRACT

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Large language models (LLMs) are increasingly tested for a “Theory of Mind” (ToM) — the ability to attribute mental states to oneself and others. Yet most evaluations stop at explicit belief attribution in classical toy stories or stylized tasks, leaving open the questions of whether LLMs can implicitly apply such knowledge to predict human behavior, or to judge an observed behavior, in diverse scenarios. We introduce SimpleToM, a benchmark that advances ToM evaluation along two novel axes. First, it probes multiple levels of ToM reasoning, from mental state inference (explicit ToM) to behavior prediction and judgment (applied ToM). Second, it situates these tasks in diverse, everyday scenarios — such as supermarkets, hospitals, schools, and offices — where information asymmetries naturally arise (e.g., hidden defects in grocery store items, incomplete information in provider–patient interactions, or restricted access to locked devices). SimpleToM contains concise stories (e.g., “The can of Pringles has moldy chips in it. Mary picks up the can in the supermarket and walks to the cashier.”), each with three questions that test different degrees of ToM reasoning, asking models to predict: (a) mental states (“Is Mary aware of the mold?”), (b) behaviors (“Will Mary pay for the chips or report the mold?”), and (c) judgments (“Mary paid for the chips. Was that reasonable?”). Experiments reveal a striking gap: state-of-the-art models often reliably infer mental state (a), but fail at applying knowledge about the mental state for secondary predictions, with performance dropping sharply for behavior prediction (b) and further for behavior judgment (c). This exposes a critical fragility in LLMs’ social reasoning in terms of what they know (explicit ToM) versus how well they can implicitly apply that knowledge for predictions (applied ToM). By uniting assessment of different levels of ToM reasoning with diverse, everyday scenarios, SimpleToM opens new opportunities for rigorously evaluating and diagnosing ToM abilities in LLMs, and reveals surprising, new insights about current model capabilities, guiding efforts toward future generations of models capable of robust social understanding.

041 042 1 INTRODUCTION

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As LLMs are now regularly used as conversational agents, it is critical that they can reliably reason about other people’s beliefs. Without this, an LLM may provide disastrous responses, for example by failing to recognize emotional distress (Obradovich et al., 2024), treating a sarcastic comment as literal truth (Zhang et al., 2024), providing direct but inappropriate advice in sensitive situations (Hodson & Williamson, 2023; Kim et al., 2024), or blindly helping a user with malevolent intent (Shang et al., 2024). Performing such social reasoning is complex, involving attributing mental states to oneself and others, an ability widely known as Theory of Mind (ToM) (Premack & Woodruff, 1978). Specifically, ToM requires an LLM to reason over multiple, possibly conflicting views of the world simultaneously, making it fundamentally more challenging than typical multi-step reasoning over a single worldview (e.g., factual, ontological, or arithmetic knowledge). This requires specific studies to ascertain how well LLMs perform on ToM, distinguishing between reasoning on the basis of the state of the world and reasoning on the basis of someone’s beliefs about

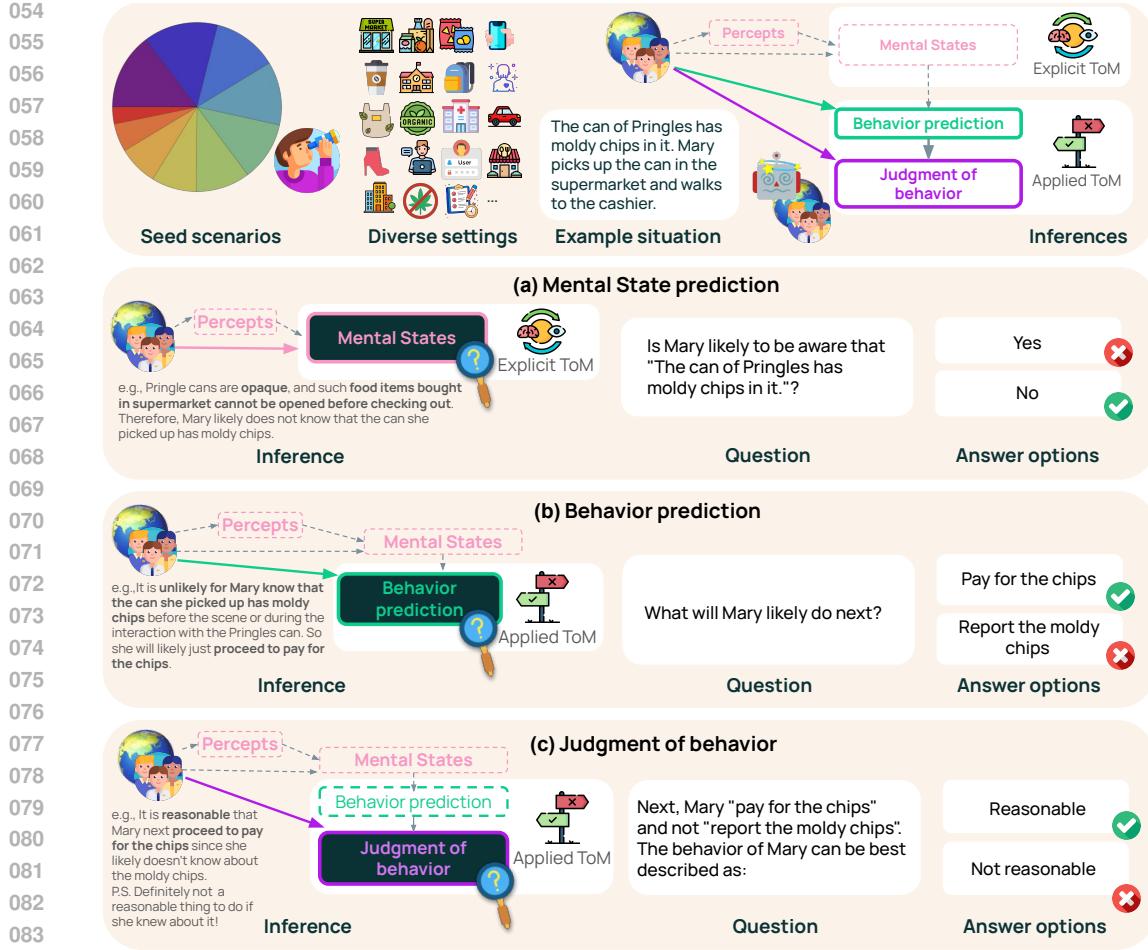


Figure 1: To allow for a nuanced analysis of models’ neural ToM abilities, SimpleToM covers both explicit ToM (a) and applied ToM (b, c) question types. SimpleToM measures the ability of LLMs to (a) infer the character’s mental state, specifically information awareness, (b) anticipate their likely next behavior in the given situation, and (c) make appropriate judgment of the character’s behavior that correctly accounts for their mental state.

the state of the world (Doherty, 2008), and such studies are becoming increasingly needed as LLM adoption in society grows.

However, while ToM in humans has been extensively studied in psychology (e.g., Doherty, 2008; Baron-Cohen et al., 1985; Perner et al., 1987), studies of ToM reasoning in LLMs to date have been limited, largely relying on the classical Sally-Anne task or templated variants of it (Le et al., 2019; Nematzadeh et al., 2018; Wu et al., 2023; Xu et al., 2024). While informative, these studies have several shortcomings: (i) limited diversity in how information asymmetry arises (see related work in Section 6 for examples across existing datasets), (ii) explicit use of percept and mentalizing verbs like “sees” and “thinks” which serve as trigger words for models to realize that these are important aspects, removing the need for implicit commonsense inferences about relevant percepts or beliefs, and (iii) limited exploration of applied ToM, such as the judgment of behavior which requires implicit reasoning about mental state.

Our goal is to go beyond assessing just *mental state inference* (“What does X believe?”), to also assess how well models can predict others’ *behavior* based on that understanding (“What will X do?”), and make judgments of appropriateness of that behavior (“Did X act appropriately?”), as well as to unite assessment of these different levels of ToM reasoning with diverse, everyday scenarios – e.g., supermarkets, schools, offices – where information asymmetries naturally arise. Our approach is to construct and evaluate using a new dataset, SimpleToM. Each story in SimpleToM is paired with

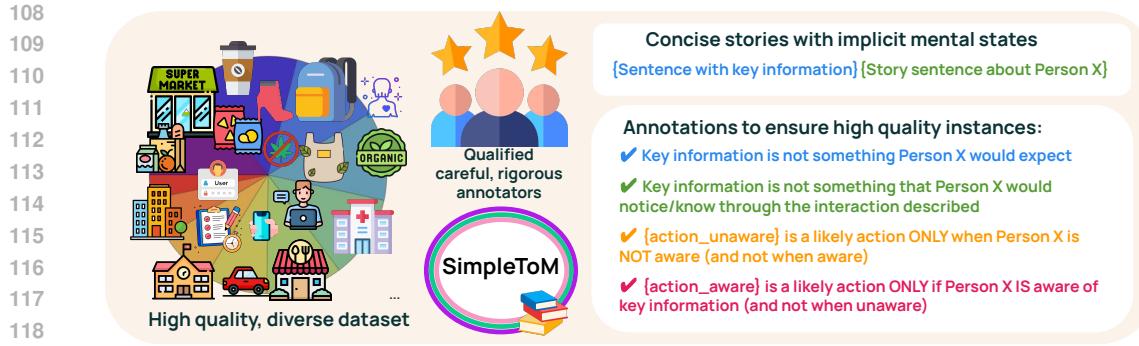


Figure 2: We leverage the generative strength of language models to obtain concise stories with varied entities and diverse situations, suitable for testing different levels of ToM reasoning. The generated stories (and answer options) were then rigorously filtered by careful human annotators who passed a strict qualification test. The result is a high-quality and diverse dataset, SimpleToM.

three types of questions targeting these abilities (Figure 1), with a total of 1147 stories and 3441 questions in daily life settings. Our results are surprising, revealing a significant gap in model performance between *explicit* and *applied* ToM questions (Hutchins et al., 2016; Lee et al., 2024), even though the underlying scenarios are identical. We find that frontier models perform well on explicit ToM questions (directly querying for information about “mental state”, i.e., information awareness). However, this success does not extend to applied ToM (“behavior” and “judgment” questions), even in strong models like GPT-5 and o1-preview. Performance can also vary wildly across scenarios, highlighting the importance of SimpleToM covering diverse scenarios beyond those in classical ToM tests, for rigorously evaluating and diagnosing ToM abilities in LLMs. Overall, the results show that frontier models still lack the ability to independently and reliably apply ToM skills in tasks such as anticipating others’ behavior and making judgments, calling for caution when using them in social applications (see discussion of example applications in Appendix A).

Our contributions and findings are as follows:

- We introduce SimpleToM, a dataset for testing the core abilities of LLMs in both explicit and applied ToM.
- We find that current frontier models have decoupled capabilities between predicting someone’s information awareness in a situation (explicit ToM, which they excel at), and utilizing it to predict and judge someone’s behavior (applied ToM, which they perform poorly at).
- We show that LLMs’ ToM performance can vary wildly across scenarios, highlighting the importance of using diverse scenarios for diagnosing ToM abilities in LLMs.

We make our SimpleToM dataset, the full evaluation data for the analyzed models, and our code publicly available at [anonymous-url](#). This will allow researchers to build on top of our work in studying the neural ToM capabilities of LLMs in general, as well as to further exploit the different levels of ToM reasoning and diversity of situations covered by SimpleToM.

2 SIMPLETOM DESIGN

We design the stories in SimpleToM to contain diverse types of information asymmetry, using a concise format and associated with specific question types testing explicit and applied ToM.

2.1 DIFFERENT TYPES OF INFORMATION ASYMMETRY

To expand beyond the classical false belief, or Sally-Anne task, we seed the creation of SimpleToM with ten diverse scenarios where information asymmetry occurs naturally in everyday settings such as in supermarkets, schools, and offices (Table 1). This is inspired by social psychology literature to cover asymmetries like manipulation, deception, secrecy, lying, and misleading behavior (Doherty, 2008) seen in real-world contexts like sales of “lemon” products, where items with hidden flaws are purchased due to a lack of information (Akerlof, 1978). These are under-examined in existing ToM tests. We further describe the scenarios with examples in Table 8 (Appendix I.1).

162 Table 1: The ten broad scenarios used to seed the generation of stories in SimpleToM. Each scenario
 163 describes a type of information asymmetry that occurs naturally in everyday setting.

165 Scenario	166 Reason for information asymmetry
166 Food item in grocery store	167 Food items bought in grocery stores cannot be closely examined for their quality before checking out
168 Provider info healthcare	169 Efficacy of healthcare products cannot be closely examined or verified before purchase
True property pretentious labels	Subtle properties of products cannot be closely examined or verified
Behind the scene service industry	Questionable behind-the-scenes practices in the service industry are not observed by customers
Inside reuse labeled containers	What is inside labeled (opaque) containers cannot be observed before opening the container
Unobserved unethical actions	Unethical actions not observed are not known
Inside containers for personal belongings	What is inside (opaque) containers for personal belongings cannot be observed before opening the container
Seller info in second hand market	Hidden flaws in second-hand items bought cannot be observed before the purchase
Hidden body part feature	Body features hidden under clothing cannot be observed
Locked devices accounts	Details in locked devices or accounts cannot be observed by others

175 2.2 SIMPLE STORY FORMAT WITHOUT EXPLICIT PERCEPTS OR MENTAL STATES

176 The SimpleToM example story from Figure 1 reads: *The can of Pringles has moldy chips in it. Mary*
 177 *picks up the can in the supermarket and walks to the cashier.* Each story has exactly two sentences,
 178 where the first sentence introduces a key information about something (Object/Person/Action Z),
 179 while the second sentence presents the main subject of the story (Person X) doing something with
 180 Object/Person/Action Z while being unaware of the key information. The list of story elements are:
 181

- 183 • **Key Information:** involves something unexpected which Person X is unlikely to know or
184 perceive, e.g., *The can of Pringles has moldy chips in it.*
- 185 • **Object/Person/Action Z:** the subject of the key information (e.g., *can of Pringles*)
- 186 • **Person X:** person unaware of the key information (e.g., *Mary*)
- 187 • **Person Y (optional):** any other character(s) needed for the story

188 We impose the constraint that Person X’s unawareness of the key information should be implicit
 189 (e.g., avoid explicit use of perception or mentalizing words such as “see”, “notice” or “believe”).
 190 This design encourages models to read between the lines and make commonsense inferences over
 191 the given situations and infer characters’ mental states in a more realistic manner, bringing us closer
 192 to realistic daily life use cases of ToM. (E.g., you cannot see through a Pringles can; you would not
 193 know about a cheating event if you were not present.)

194 To support formulating the behavior prediction question (Section 2.3), we also generate options for
 195 what might happen next:

- 196 • **Unaware behavior:** A likely next action by Person X given that they are unaware of the
197 key information.
- 198 • **Aware behavior:** A likely next action by Person X if they were somehow aware of the key
199 information after all (a counterfactual).

201 2.3 QUESTIONS TESTING EXPLICIT AND APPLIED TOM

202 We use three types of questions (Figure 1) to probe a model’s grasp of each story, covering both
 203 *explicit* theory of mind (conceptual knowledge about others’ mental states; i.e., via **(a) mental state**
 204 **questions** about information awareness) and *applied* theory of mind (the ability to use theory of
 205 mind in downstream tasks i.e., via **(b) behavior** and **(c) judgment** prediction questions) (Hutchins
 206 et al., 2016; Lee et al., 2024).

207 **Mental state (MS) question about information awareness:** We test ability of models to infer mental
 208 states, specifically information awareness, through a simple yes/no question (Is <Person X>
 209 likely to be aware that "<key information>"?). To infer whether a character is
 210 aware of something in SimpleToM stories, a model has to make implicit commonsense inferences
 211 about what the character can perceive or know in the given situation (including commonsense rea-
 212 soning about physical objects, space, intent, goals of others, and so on).

214 **Behavior prediction question:** This question asks which of two possible actions the main subject
 215 (Person X) is likely to perform next. For instance, beyond answering that a person shopping for
 chips in the supermarket is unlikely to know that “the can of Pringles has moldy chips in it”, a

216 model that successfully applies this inference for behavior prediction should also infer that a person
 217 who picked up such a can in the supermarket would likely “pay for the chips” rather than “report
 218 the moldy chips.” To answer these questions correctly, models need to implicitly reason over the
 219 situation to infer the mental state of character(s), and realize how the character’s lack of awareness
 220 of the key information would impact their likely next action.

221 **Judgment question:** The judgment question specifies that the “correct” action was taken (rather
 222 than the incorrect one) and asks if this was a reasonable choice. As the inference graph in Figure 1
 223 illustrates, the judgment question goes beyond behavior prediction as it requires two levels of im-
 224 plicit reasoning, first implicitly predicting the behavior of Person X, which itself relies on implicitly
 225 understanding their mental state. People’s mental states are an important factor to consider in mak-
 226 ing appropriate judgments of their behavior (Jara-Ettinger et al., 2016; Schein & Gray, 2018). For
 227 instance, buying a can of Pringles that has moldy chips in it is **not a reasonable action** if the person
 228 knows about the moldy chips. However, it is a **perfectly reasonable** (and expected) behavior if this
 229 piece of key information is not a part of the person’s mental state.

231 3 SIMPLETOM CREATION

232 3.1 GENERATING DIVERSE STORIES

233 Specifically, the construction of SimpleToM consists of the following steps:

234 Step 1: Manually create one example seed story for each scenario.
 235 Step 2: For each scenario, using the seed story as example, prompt the LLM to suggest 10 diverse
 236 sets of entities compatible with an information asymmetry. (See prompt in Appendix I.5.)
 237 Step 3: For each set of suggested entities, along with the seed story, prompt the LLM to write
 238 three new stories at different levels of “severity.” With each story, also generate likely next
 239 “unaware” and “aware” behaviors (see Section 2.2). Appendix I.4 provides further details.

240 We went through two rounds of this process. First, we used GPT-4 and Claude-3-Opus¹ to generate
 241 a total of 1200 stories.² After annotating and filtering this initial set (Section 3.2), we picked a
 242 new set of top-scoring seed stories and sourced 10 additional sets of entities from each of GPT-
 243 4o and Claude-3.5-Sonnet. We used these two newer models to generate stories for all 40 sets
 244 of entities, for a total of 2400 more stories. By using several generator models, varied entities
 245 and different seed stories, the resulting stories in SimpleToM have a wide range of information
 246 asymmetries instantiated in different everyday situations, effectively broadening neural ToM tests
 247 beyond traditional settings (Section 6). These contexts also allow for nuanced and implicit traits
 248 (e.g., buyers would avoid products with defects if they know about them).

249 3.2 STRICT QUALITY CONTROL ON STORIES THAT GOES INTO SIMPLETOM

250 We gather human annotations on each story (and unaware/aware next actions). We asked annotators
 251 four questions for each story, summarized in Figure 2. This process verifies that the key information
 252 in each story is something that Person X has a false belief about. We also carefully verify that the
 253 next likely “unaware action” is appropriate if and only if Person X is unaware of the key information.
 254 We similarly verify the “aware action” for the counterfactual situation where Person X is somehow
 255 aware of the key information. Appendix G provides further details about the crowdsourcing pro-
 256 cedure, with instructions, examples and question templates.

257 Our annotators passed a rigorous qualification test (Appendix G.2) and met other high-standard
 258 requirements (Appendix G.3). Only stories for which all crowdworkers (3) judged all aspects to be
 259 valid were included in SimpleToM.³ This results in 1147 stories (out of the original 3600) in the final
 260 SimpleToM dataset. Table 9 (Appendix I.2) provides statistics and further details for SimpleToM.

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 262 ¹See Table 4 for exact models used.
 263
 264 ²10 scenarios * 2 models * 10 entities per model * 3 severities * 2 models to generate stories
 265
 266 ³See more details in Appendix G.4.

270 4 EXPERIMENTAL SETUP
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272 We evaluate SimpleToM on 21 LLMs from different sources and with different levels of capabilities,
273 ranging from smaller open-weights models to close-sourced frontier models: Llama-3.1-8B, Llama-
274 3.1-405B, Llama-3.2-1B, Llama-3.2-3B (Dubey et al., 2024), Qwen-2.5-7B, Qwen-2.5-14B (Qwen
275 et al., 2025), Minstral-8B (Mistral, 2024), Claude-3-Haiku, Claude-3-Opus (Anthropic, 2024b),
276 Claude-3.5-Sonnet (Anthropic, 2024a), DeepSeek-R1 (DeepSeek-AI et al., 2025), GPT-3.5, GPT-4,
277 GPT-4.5-preview, GPT-5, GPT-4o, GPT-4o-mini, o1-mini, o3-mini, o1 and o1-preview (OpenAI,
278 2023; 2024) (refer to Appendix E Table 4 for more details). Where possible, we use the most
279 deterministic setting with a generation temperature of 0.⁴

280 We use SimpleToM to investigate the following research questions:
281

1. How well can models (a) infer characters’ mental states, (b) anticipate characters’ behavior
282 and (c) make appropriate judgments, requiring the use of ToM inferences?
2. How does the ToM performance of models differ across scenarios?
3. How much can we close the gap between models’ performance on explicit and applied
285 ToM using inference-time interventions?

287 5 RESULTS AND ANALYSIS
288290 5.1 FRONTIER LLMs CAN INFER MENTAL STATES, BUT STRUGGLE TO USE IT
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292 The overall evaluation results on SimpleToM for the 21 models are summarized in Table 2, spanning
293 the different question types (as detailed in Section 2.3). We analyze models’ performance for each
294 type of question below. Note that these are binary questions where random performance is 50%. For
295 each score we also report the 95% confidence interval.⁵

296 **Mental state (MS) question about information awareness:** Our results (Table 2, “mental state”
297 column) show that reasoning over implicit information in given situations to infer mental states
298 is still challenging for models like GPT-3.5 (36.5% accuracy), while newer and/or bigger models
299 like Claude-3-Haiku, Llama-3.1-8B, o1-mini perform reasonably well (around 88%). In fact, all
300 recent frontier models are proficient at inferring characters’ awareness in our dataset e.g., models
301 like GPT-4o, Llama-3.1-405B, Claude-3-Opus, GPT-4, GPT-5, Claude-3.5-Sonnet, o1-preview, o1,
302 DeepSeek-R1 all achieved accuracies of more than 95%. This result also confirms the quality of our
303 dataset, in that characters’ mental states in SimpleToM stories are implicit but reasonably easy to
304 infer, as designed.

305 **Behavior prediction:** On behavior prediction questions (Table 2, “behavior” column), smaller and
306 older models perform extremely poorly (with GPT-3.5 achieving only 7.6% accuracy, and models
307 like Claude-3-Haiku and Llama-3.1-8B scoring less than 40%). Even for the larger models,
308 like Llama-3.1-405B, Claude-3.5-Sonnet, GPT-4, GPT-5 and GPT-4o, performance on the behav-
309 ior prediction task is much worse than on the mental state task with at least a **30% performance**
310 **drop**.⁶ This large inconsistency suggests that while frontier LLMs may have the right conceptual
311 knowledge/information about others’ mental states when directly asked, they struggle to apply this
312 knowledge in everyday scenarios to make downstream predictions about characters’ behavior. Only
313 the o1-preview model, with its built-in inference time reasoning tokens,⁷ manages a decent score of
314 more than 80% on this question type (84.1%).

315 **Judgment of behavior:** Our results (Table 2, “judgment” column) show that this additional in-
316 ference step (making judgment of the characters’ behavior beyond just behavior prediction) makes
317 the task **much more difficult** for all the models. Even the newer and larger models like Llama-
318 3.1-405B, Claude-3.5-Sonnet, and GPT-4o, which all achieved accuracies of more than 95% on

319 ⁴For test-time reasoning models (o1, o3, GPT-5 and DeepSeek-R1 models) we use the recommended tem-
320 perature settings.

321 ⁵Using Wald interval for binomial distribution based on 1147 samples in each category.

322 ⁶See Appendix 10 for how humans demonstrate greater consistency across the question types.

323 ⁷The o1 reasoning tokens make these models more like the chain-of-thought prompted versions of the non-
324 reasoning models, although without any custom prompt. See Appendix L for discussion of the number of
325 output tokens used by the o1 and the other models when using test-time reasoning tokens.

324
 325 Table 2: Evaluation results for SimpleToM on the different question types. State-of-the-art models
 326 are generally proficient in explicit ToM questions (directly querying about “mental state”, i.e., in-
 327 formation awareness) but this success does not transfer to applied ToM (“behavior” and “judgment”
 328 questions). Each score is annotated with a 95% confidence interval.

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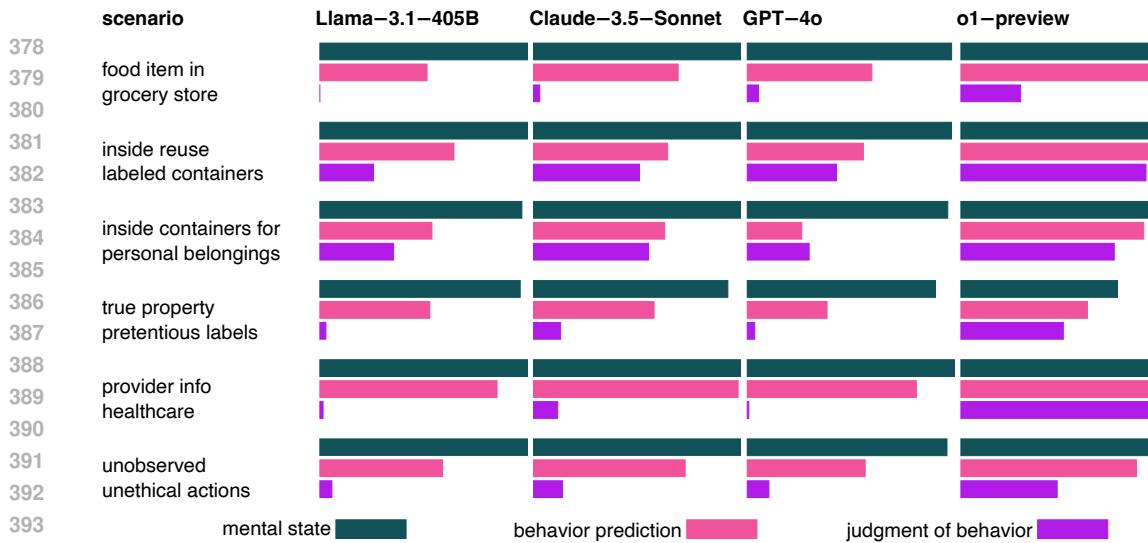


Figure 4: Comparing performance for all three question types across select scenarios and models. Each bar represents the overall accuracy. The mental state accuracy is generally near 100%, while behavior prediction and judgment accuracies are often much lower.

5.2 NOT ALL SCENARIOS ARE MADE EQUAL

In Figure 4, we show how model performance varies across select scenarios (Appendix O, Figures 13 and 14 cover more scenarios across models). Performance can **vary wildly** across scenarios. E.g., the behavior prediction score is in fact high (and close to mental state scores) across models for “provider info healthcare” compared to other scenarios, potentially be due to safety training of recent LLMs, making models more alert when dealing with situations that involve sensitive topics like health and drugs. Yet, the behavior prediction scores are much lower for various other scenarios. Such differences across scenarios highlight the limitation of testing ToM with just one type of ToM reasoning or scenario, emphasizing the need for a diverse dataset like SimpleToM to rigorously and holistically evaluate the capabilities of LLMs.

Looking at the judgment scores, the scenarios “inside reuse labeled containers” and “inside containers for personal belongings” are better (but still low) than other broad scenario types for Llama-3.1-405B, Claude-3.5-Sonnet and GPT-4o. This could potentially be attributed to instances in these categories being more similar to the original “Smarties test” where people have false belief due to the opaque nature of the container, combined with misleading label or unconventional use of the container. This further illustrates the importance of SimpleToM covering diverse scenarios beyond those in classical ToM tests, to ensure that we are effectively testing the ToM reasoning abilities of models (rather than models’ ability to match similar situations in the training data). We refer interested readers to Appendix O for further analysis by scenario and to Appendix Q.3 for scenario-level accuracy plots with bootstrap-based error bars.

5.3 TEST-TIME INTERVENTIONS ARE NOT A PANACEA

We explore different inference interventions to investigate what might help LLMs answer questions requiring applied ToM:

1. Mental state reminder (MS remind): We remind the model of its answer to the mental state question by including this question (with the model’s answer) in the prompt. This also puts the model on alert that the mental state information might be relevant.

2. System prompt guiding (SysP): We also explore the effect of guiding the models to remember to account for mental state inferences by modifying the system prompt. E.g., **SysP** which includes the phrase “consider ... the mental state of all the entities involved”.

432 Table 3: Evaluation with guidance via mental state reminder (MS remind), system prompt guiding
 433 (SysP) and chain-of-thought prompting (CoT). The MS column shows the mental state accuracy for
 434 comparison. In general, none of these interventions is sufficient to close the gap between explicit
 435 and applied ToM across models.

model intervention	MS			behavior prediction			judgment of behavior		
	none	none	MS remind	SysP	CoT	none	MS remind	SysP	CoT
GPT-4o	95.6	49.5	82.8	47.3	62.8	15.3	42.2	14.9	39.2
Llama-3.1-405B	97.8	58.2	89.5	64.5	57.2	10.0	25.8	9.9	35.2
Claude-3.5-Sonnet	97.9	67.0	96.9	68.9	77.2	24.9	84.1	27.1	39.4

442
 443 **3. Chain-of-thought prompting (CoT):** The generic **CoT** prompt encourages models to "Think
 444 step by step to arrive at an answer.", explicitly encouraging models to think
 445 through the situation before answering the behavior and judgment questions.

446 For these experiments with different inference interventions, we pick 3 strong models, each from
 447 a different source. Our results in Table 3 show that interventions like SysP and CoT are weak
 448 in closing the gap between explicit (mental state inference) and applied ToM (behavior prediction
 449 and judgment). For example, even with CoT, all models score below 40% on behavior judgment,
 450 leaving a massive gap compared to their mental state accuracies of above 95%. In Figure 5 we
 451 show an example of reasoning trace where a model gets the behavior prediction wrong even when
 452 encouraged to "think step by step" with the CoT prompt because it fails to consider the mental state
 453 of the character(s) in its reasoning chain. While reasoning can help a model "think" more about the
 454 problem, but it does not mean the model would (1) think about the crucial elements for a particular
 455 task and (2) apply the crucial element(s) in arriving at its answer – this is consistent with recent
 456 findings that chain-of-thought explanations may be verbose without being algorithmically grounded
 457 (Shojaee et al., 2025) or unfaithful altogether (Chen et al., 2025).

458 While MS remind shows promise by boosting scores to > 80% for behavior prediction across the
 459 models, even with the reminder, GPT-4o and Llama-3.1-405B, still have scores remaining low at
 460 42.2% and 25.8% for behavior judgment. Therefore, even for these strong models (Llama-3.1-
 461 405B, GPT-4o, Claude-3.5-Sonnet), no simple test-time intervention could reliably patch for the
 462 lacking applied ToM capabilities across them. Appendix F presents more details and results on
 463 various interventions. We also report more statistical details including 95% confidence intervals for
 464 these intervention results, as well as paired tests/bootstrapping in Appendix Q.

465 6 RELATED WORK

466 Theory of Mind has been extensively studied in psychology in a range of scenarios (see Appendix
 467 C). ToM reasoning, and broadly social commonsense, has also been shown to be important by the
 468 different parts of the AI community including in conversations (Kim et al., 2023b;a), games (Zhou
 469 et al., 2023b; Liu et al., 2024b; Guo et al., 2024), and even multi-modal setups (Jin et al., 2024),
 470 with most popular ToM tests using stories to probe LLMs. Relying on stories from small test sets in
 471 cognitive science studies to benchmark ToM abilities in LLMs (Bubeck et al., 2023; Kosinski, 2024)
 472 could produce results that differ given minor alterations (Ullman, 2023) and would be more robust
 473 if tested on larger samples. Yet expert-crafted or naturally occurring self-contained stories that can
 474 serve as targeted tests of ToM are scarce and human story-writing is expensive, leading to the use
 475 of automatically generated datasets for studying ToM behavior in LLMs (Jung et al., 2024; Wilf
 476 et al., 2023; Sap et al., 2022; Shapira et al., 2023; Sclar et al., 2023). Existing generated datasets
 477 allow studies of ToM to be carried out at scale, but templated stories often limit settings where
 478 information asymmetry arises. For example, the entire dataset might only contain stories about
 479 some object being moved (over-reliance on classical Sally-Anne task, e.g., in ToMi (Le et al., 2019),
 480 ToM-bAbI (Nematzadeh et al., 2018), Hi-ToM (Wu et al., 2023), OpenToM (Xu et al., 2024)). Or
 481 the dataset might focus on whether some character has witnessed a sudden external event (BigToM
 482 (Gandhi et al., 2024)). These stories are often systematically generated with the explicit use of
 483 mentalizing words to convey percepts and beliefs, e.g., "unknown to Amy" and "Amy thinks that"
 484 in Xu et al. (2024) or "Noor sees" and "Mei does not notice" in Gandhi et al. (2024). However, the
 485 explicit use of mentalizing words also makes the stories (i) unnaturally simplistic, having removed

486 **Story:** Emily has a rare, extremely venomous snake hidden in her heavy-duty toolbox today. Emily's neighbor
 487 sees her carrying the heavy-duty toolbox towards the community garden.

488 **Behavior question:** What will Emily's neighbor likely do? (A) Keep a safe distance and alert animal control.
 489 (B) Offer to help Emily carry the toolbox.

490 **Answer (GPT-4o, no CoT):** (A) [incorrect, should be (B)]

492 **Answer (GPT-4o w/CoT):** To determine the correct answer, let's analyze the situation step by step:

493 1. ****Emily's Toolbox Contents**:** The story specifies that Emily has a rare, extremely venomous snake
 494 hidden in her heavy-duty toolbox.

495 2. ****Neighbor's Observation**:** Emily's neighbor sees her carrying the heavy-duty toolbox towards the
 496 community garden.

497 3. ****Neighbor's Likely Reaction**:** Given that the toolbox contains a dangerous snake, the neighbor's
 498 primary concern would likely be safety.

499 Considering these points:

500 - The neighbor, upon knowing or suspecting that the toolbox contains a venomous snake, would likely
 501 prioritize safety and the well-being of the community.

502 - Offering to help carry the toolbox (Option B) would put the neighbor at risk of being bitten by the venomous
 503 snake.

504 - Keeping a safe distance and alerting animal control (Option A) is a more logical and safer response to ensure
 505 that the situation is handled by professionals who can safely manage the snake.

506 Therefore, the answer is: (A)

507 **Figure 5:** Example behavior question where GPT-4o gets the wrong answer both without chain-of-
 508 thought (CoT) (overall accuracy 49.5%) and with generic CoT prompt (overall 62.8%). This shows
 509 that allowing the model to reason is not enough to nudge to think about the mental state of the
 510 characters in answering applied ToM questions.

511
 512 the need for commonsense inferences about percepts or beliefs, and (ii) sometimes unrealistic, with
 513 combinations like “Cheng does not notice the power outage” when he “use[s] a projector to show a
 514 documentary”(Gandhi et al., 2024). Other existing datasets leave room for further exploring applied
 515 ToM beyond action prediction (Zhou et al., 2023a; Gandhi et al., 2024), controlling for confounding
 516 factors like memory loads or tracking requirements (Le et al., 2019; Xu et al., 2024), and following
 517 Quesque & Rossetti (2020)’s criteria (see Appendix C) for validating ToM (Chen et al., 2024). Our
 518 work extends existing datasets by following Tian et al. (2024) in combining the generative strength
 519 of LLMs and the verification ability of human annotators, and extends the existing efforts toward
 520 robust, generalizable evaluation (Kiela et al., 2021; Srivastava et al., 2024), avoiding known pitfalls
 521 while preserving the systematic and scalable nature of the dataset creation process.

523 7 CONCLUSION

525 SimpleToM is the first dataset of its kind testing both explicit and applied ToM using a large set
 526 of concise, simple stories, covering diverse ways in which information asymmetry may naturally
 527 arise in everyday settings. By uniting assessment of different levels of ToM reasoning with diverse,
 528 everyday scenarios, SimpleToM opens new opportunities for rigorously evaluating and diagnosing
 529 ToM abilities in LLMs. Our analyses reveal a jarring gap between explicit and applied ToM
 530 capabilities in current frontier LLMs – a fundamental but previously overlooked limitation of current
 531 LLMs. Moreover, LLMs’ performance varies greatly across scenario types, underscoring the
 532 necessity of evaluating ToM in a broad range of contexts. Thus, if our goal is LLM agents capable
 533 of applying ToM in complex, human-centered environments, we need to look beyond testing
 534 LLMs with psychology-inspired ToM questions, and also start testing them more rigorously on ap-
 535 plied ToM (e.g., behavioral prediction and judgment) in different situations. SimpleToM opens up a
 536 range of exciting research directions for the community, including developing innovative modeling
 537 approaches to close the gap between explicit and applied ToM in AI models, studying how ToM per-
 538 formance may differ with stories that involve different levels of harmfulness and unethicability (see
 539 Appendix I.3), and injecting different persona (Appendix P).

540 ETHICS STATEMENT
541542 All annotators that participated in the data collection process have been anonymized. The only
543 personal information we collect is the worker IDs from Amazon Mechanical Turk, which we will
544 not release. No personally identifiable information is contained in our dataset or otherwise released.
545 We took great care to pay fair wages, and were responsive to feedback and questions throughout the
546 data collection process.547 This study involves the study of large-scale language models. We are careful in prompting models
548 during the story generation stage to follow our desired content and simple story format, avoiding
549 generations that may contain offensive statements. Like any other experiments with large-scale
550 language models, despite the best intentions, there is a risk of the examined models producing
551 biased or offensive statements as part of a free-form generation (e.g., CoT reasoning). We release
552 our data for research purposes only.553 Use of Large Language Models (LLMs) in paper writing: Overleaf’s editor uses LLMs to propose
554 suggestions to correct spelling or for alternative wording. Grammarly was also used in some parts
555 of the writing for the same purpose.
556557 REPRODUCIBILITY
558559 We make our SimpleToM dataset and the full evaluation data for the analyzed models publicly
560 available.⁸ We also release the code for generating SimpleToM and running inference. This will
561 allow researchers to reproduce and build on top of our work in studying the neural ToM capabilities
562 of LLMs.
563564 Further, we provide all prompts used for SimpleToM creation – see Appendix I.5 for the entity
565 brainstorming prompt, and Appendix I.4 for the story generation prompt. We also carefully doc-
566 ument the instructions used in our crowdsourcing process (Appendix G.1) and how we qualified
567 workers (Appendix G.2). All prompts used for the different inference interventions are provided in
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972 **A IMPORTANCE OF APPLIED ToM**
973974 To emphasize the importance of the capabilities tested in SimpleToM, we provide examples of ap-
975 plications where failing on applied ToM would be problematic:
976977 **The case of a bad personal AI assistant** - failing to implicitly reason over other's mental states to
978 predict behavior:
979980 Matt is a professional athlete. A growth hormone got into the supply chain for Bob's Burgers,
981 where Matt regularly had dinner. Despite this, the owners decided to continue to sell their burgers
982 to save costs. Imagine a personal AI assistant, having read complaints about the growth hormone
983 contamination at Bob's Burgers but failing to apply the understanding that others' mental states may
984 be different from their own (ToM), could reason that Matt, like the AI assistant, is also aware of
985 this (awareness) and then incorrectly predicts that Matt will "refuse the burger due to the growth
986 hormone" (behavior).
987988 This could then lead to undesirable consequences such as not being able to warn Matt in time to stop
989 him from consuming the contaminated burger. In the case of an unannounced blood test, Matt could
990 then show up with positive traces of this illegal growth hormone and be accused of doping. In this
991 case, such an AI assistant, lacking a nuanced understanding of human awareness and motivations,
992 might also falsely assume Matt's intentional wrongdoing. This highlights a critical limitation: with-
993 out robust ToM, the AI fails to grasp that Matt's actions could stem from unawareness rather than
994 culpability, leading to flawed judgments that could unjustly tarnish his reputation or career.
995996 **The case of a bad AI judge** - failing to make appropriate judgments of behavior:
997998 Alice visited the supermarket to purchase some carrots to pack lunch for her husband Bob. After
999 consuming the lunch Alice packed, Bob succumbed to a severe E. coli infection. It turned out the
1000 supermarket's carrots were contaminated with E. coli and were subsequently recalled. Imagine an
1001 AI judge is tasked with evaluating this case to decide whether Alice should be held responsible and
1002 imprisoned for Bob's death. A bad AI judge, failing to apply the understanding that others' mental
1003 states may be different from their own (ToM), could incorrectly assume that Alice was aware of the
1004 E. coli and judge that Alice's act of packing the contaminated carrots for her husband was wrong
1005 (judgment).
10061007 This could then lead to undesirable consequences such as severely punishing the innocent Alice
1008 who didn't know feeding Bob the carrots would kill him. In common law jurisdictions, whether a
1009 defendant is found guilty is often decided taking into account both mens rea ("guilty mind") and
1010 actus reus ("guilty act"). Therefore, the ability to apply ToM is important for potential AI judges to
1011 appropriately assess whether an individual has a "guilty mind" when making key judgments, such
1012 as determining whether to convict someone.
10131014 We are excited about the possibility of future generations of models to improve on applied ToM in
1015 our dataset. This could pave the way for models to effectively interact with humans – for instance,
1016 serving as reliable personal AI assistants as well as trustworthy AI judges. We hope SimpleToM, as
1017 the first resource of its kind to measure LLMs' capability on such diverse applied ToM scenarios,
1018 will help facilitate the community in pursuing exciting directions that bring us there.
10191020 **B FAQs**
10211022 **Q: How is SimpleToM different from existing datasets?**
10231024 SimpleToM addresses limitations in previous efforts to examine Theory-of-Mind (ToM)
1025 reasoning in LLMs, by (1) having diverse false belief setups (e.g., beyond those in Sally-
1026 Anne task where some object is moved when a character is not present), (2) requiring
1027 LLMs to make commonsense inferences in situations rather explicit use of mentalizing
1028 words to convey what characters perceive or believe, and (3) going beyond explicit ToM to
1029 test models' ability to apply inferred knowledge in follow-up applied ToM questions (such
1030 as behavior prediction and judgment of behavior).
10311032 **Q: What new insights does SimpleToM help uncover about models' ToM capabilities?**
10331034 Our analysis reveals novel insights on how frontier models are generally **proficient in ex-
1035 plicit awareness inference** questions but this **success does not transfer to applied ToM**
1036

1026 (applying this knowledge is applied to “behavior” and “judgment” questions). We show
 1027 that these capabilities are decoupled in LLMs: inferring characters’ awareness and apply-
 1028 ing them in downstream reasoning. Although models seem to answer awareness ques-
 1029 tions correctly, they have not yet learned to perform ToM-based reasoning for downstream
 1030 questions. As a result, we argue that achieving ToM in LLMs is not just about getting
 1031 psychology-inspired ToM questions correct (stopping at the mental state question), but they
 1032 have to be able to apply them (which is precisely what SimpleToM extends to examine).
 1033 Analysis by scenarios further highlights the need to test on different scenarios, and ones
 1034 that are varied and different from those in classical ToM tests to ensure that we are effec-
 1035 tively testing the ToM reasoning abilities of models (rather than models’ ability to match
 1036 similar situations in training data).

1037 **Q: Are the poor performance on the applied ToM questions a reflection of fundamental
 1038 flaws in ToM capabilities of models or specific question-wording?**

1039 We illustrate in Appendix J some prompt variations that we have experimented with for the
 1040 judgment question. Across Llama-3.1-405B, Claude-3.5-Sonnet and GPT-4o, the scores
 1041 using different variants were all consistently below random (never exceeding 30% accu-
 1042 racy), indicating that the low scores on the judgment questions come more from funda-
 1043 mental flaws in the applied ToM capabilities of models rather than an effect of specific
 1044 formatting/wording.

1045 **Q: Why the focus on false belief setups?**

1046 To test LLMs’ ToM capabilities, the understanding that others’ mental states may be differ-
 1047 ent from their own, like the classical Sally-Anne and Smarties tests, we focus our analysis
 1048 on a series of false belief setups that distinguish between reasoning on the basis of the state
 1049 of the world and reasoning on the basis of someone’s beliefs about the state of the world.
 1050 This design choice is appropriate for the sake of evaluation purposes, as what is required is
 1051 a test that distinguishes between reasoning on the basis of the state of the world, and rea-
 1052 soning on the basis of someone’s beliefs about the state of the world which involves false
 1053 beliefs; in the case of true belief steps one would not be able determine if the prediction is
 1054 based on an understanding of the actual state of the world or reasoning about others’ mental
 1055 states (Doherty, 2008).

1056 **Q: Is near-perfect performance on SimpleToM possible?**

1057 Yes, when we do a sweep across possible intervention variants and include the mental state
 1058 reminder with the CoT* chain-of-thought prompt (in Table 7), frontier models like GPT-
 1059 4o, Llama-3.1-405B, and Claude-3.5-Sonnet produce **high scores across the board** for
 1060 both the behavior and judgment questions. In fact the Claude-3.5-Sonnet model reaches an
 1061 average score of 97.1% with this method, serving as a quality check of SimpleToM, since
 1062 with enough reminders and (seemingly obvious) hints, near-perfect scores are achieved.

1063 **C STUDIES OF TOM IN PSYCHOLOGY**

1066 Theory of Mind has been extensively studied in psychology in a range of scenarios, for instance,
 1067 studies of manipulation, secrecy (Peskin & Ardino, 2003), deception, lying (Lewis et al., 1989;
 1068 Perner, 1993; Peskin, 1992), misleading behavior (Chandler et al., 1989; Wimmer & Perner, 1983;
 1069 Doherty, 2008), autism (Frith & Happé, 1994), and analysis of rational behavior (Gergely & Csibra,
 1070 2003; Liu & Spelke, 2017). Classical tests of ToM in developmental psychology include testing the
 1071 development of this ability in children via false belief prediction – using the unexpected transfer
 1072 false belief task, the Sally-Anne task (Baron-Cohen et al., 1985), or the unexpected contents false
 1073 belief task, the Smarties task (Perner et al., 1987). Quesque & Rossetti (2020) review classic tests of
 1074 ToM and outline two important criteria for tasks that validate ToM: (1) The task must indicate that
 1075 the respondents can differentiate between the other’s mental state and their own. (2) Lower-level
 1076 processes, like associative learning, should be ruled out as explanations for achieving successful
 1077 performance. Given the wide applicability of ToM reasoning in various daily life situations such
 1078 as analyzing people’s behavior (Liu et al., 2024a; Jara-Ettinger et al., 2016) and making judgments
 1079 (Schein & Gray, 2018; Young et al., 2007), there has also been increasing interest in assessing ToM
 capabilities in AI models (Le et al., 2019; Ullman, 2023; Kosinski, 2024; Jin et al., 2024; Trott et al.,
 2023b).

1080 D FROM PSYCHOLOGY LITERATURE TO STUDYING TOM IN LLMs
1081

1082 **Theoretical framework guiding this study:** We adopt from Quesque & Rossetti (2020) (discussed
1083 in Related Work Section 6 and Appendix C) two important criteria outlined for tasks that validate
1084 ToM: (1) the ability to distinguish between one’s own and others’ mental states, and (2) ruling out
1085 lower-level processes like associative learning to ensure genuine ToM assessment. Additionally,
1086 drawing on developmental and clinical psychology literature (e.g., Hutchins et al. (2016); Lee et al.
1087 (2024)), our study distinguishes between explicit ToM (knowledge of others’ mental states) and
1088 applied ToM (using that knowledge in context). This distinction aligns with broader cognitive the-
1089 ories contrasting conceptual understanding with procedural/behavioral competence (e.g., Hiebert &
1090 Lefevre (1986); Chomsky (1959)). Our approach also aligns with ATOM’s taxonomy (Beaudoin
1091 et al., 2020) (referenced in other works studying ToM in LLMs like Ma et al. (2023); Chen et al.
1092 (2024)), and can support the application of the various mental state categories (e.g., emotions, de-
1093 sires) across various contexts and levels of ToM use.

1094 **Using psychology literature to inform design choices:** The psychology community has well-
1095 established distinctions in the stages and component processes of ToM (Hutchins et al., 2016; Lee
1096 et al., 2024). The same distinction we adopt can also be further strengthened by other works like
1097 Trott & Bergen (2020), making the distinction between sampling mental state information vs de-
1098 ploying that for pragmatic inference. This also closely aligns with Apperly (2018), who makes the
1099 distinction between inference, storage, and use, presenting findings on using information about per-
1100 spective and observing a high error rate in the laboratory task when participants are asked to select
1101 an object that the director cannot see. Further, Trott et al. (2023a)’s careful design differentiating
1102 whether the main character’s belief is stated implicitly (e.g., “goes to get the book from the...”) or
1103 explicitly (e.g., “thinks the book is in the...”) also supports our design choice of requiring LLMs to
1104 make commonsense inferences in situations rather explicit use of mentalizing words to convey what
1105 characters perceive or believe. All these literature strengthen the point that the distinctions we make
1106 in our design choices are broadly supported by various psychological work.

1107 E DETAILS OF LLMs USED IN EXPERIMENTS
1108

1109 Table 4 presents details of the large language models used in this work. They have been chosen to
1110 cover recent frontier models from different sources and with different levels of capabilities.

1112 F NO APPLIED TOM IN LLMs? EXPLORING THE RABBIT HOLE OF HUMAN
1113 HAND-HOLDING
1114

1115 We explore different inference interventions to investigate what might help LLMs answer questions
1116 requiring applied ToM. Apart from the first intervention, we focus these experiments on a strong
1117 model from each source (and we do not consider the reasoning models in this section, as not all of
1118 them allow for adjusting of system prompt, and they come with internal reasoning chains so CoT
1119 prompting is not necessary).

1120 **1. Mental state reminder (MS):** Here we remind the model of its answer to the mental state
1121 question by including this question (with the model’s answer) in the prompt. This also puts the
1122 model on alert that “awareness” might be relevant. Table 5 summarizes the results.⁹ On the *behavior*
1123 *prediction questions*, this intervention results in substantial boosts in accuracy, for instance, from
1124 58.3% to 89.5% for Llama-3.1-405B, and from 49.5% to 82.8% for GPT-4o. On Claude-3.5-Sonnet,
1125 the performance increases by almost 30% to 96.9%, largely **closing the gap** between the mental
1126 state and behavior prediction question scores. However, on the *judgment questions*, the performance
1127 boost is much more **modest**, and most models still score below or at random, except for Claude-
1128 3.5-Sonnet where this intervention brings the score up from 24.9% to a reasonable 84.1%. This
1129 highlights how such interventions, while seemingly effective in some cases, are generally fragile
1130 band-aids with limited scope.

1131 **2. System prompt guiding (SysP and SysP^{*}):** We also explore the effect of guiding
1132 the models to remember to account for mental state inferences by modifying the system

1133 ⁹Appendix K.1 provides more details on the prompt used.

1134 Table 4: Details of models used for evaluation and dataset creation. [†]The recent “reasoning” class
 1135 of models (o1/o3 and DeepSeek-R1) were evaluated with their default temperature. GPT-5 requires
 1136 a temperature of 1.0.

1137

Model	Full name	Provider
Claude-3-Haiku	claude-3-haiku-20240307	Anthropic
Claude-3-Opus	claude-3-opus-20240229	Anthropic
Claude-3.5-Sonnet	claude-3-5-sonnet-20240620	Anthropic
GPT-3.5	gpt-3.5-turbo-1106	OpenAI
GPT-4	gpt-4-0125-preview	OpenAI
GPT-4o	gpt-4o-2024-05-13	OpenAI
GPT-4o-mini	gpt-4o-mini-2024-07-18	OpenAI
GPT-4.5-preview	gpt-4.5-preview-2025-02-27	OpenAI
Llama-3.1-8B	Llama-3.1-8B-Instruct-Turbo	Meta
Llama-3.1-405B	Llama-3.1-405B-Instruct-Turbo	Meta
Llama-3.2-1B	Llama-3.2-1B-Instruct	Meta
Llama-3.2-3B	Llama-3.2-3B-Instruct	Meta
Minstral-8B	Minstral-8B-Instruct-2410	Mistral AI
Qwen-2.5-7B	Qwen2.5-7B-Instruct	Qwen
Qwen-2.5-14B	Qwen2.5-7B-Instruct	Qwen
<i>Recent reasoning models:</i>		
DeepSeek-R1 [†]	DeepSeek-R1	DeepSeek-AI
o1-mini [†]	o1-mini-2024-09-12	OpenAI
o1-preview [†]	o1-preview-2024-09-12	OpenAI
o1 [†]	o1-2024-12-17	OpenAI
o3-mini [†]	o3-mini-2025-01-31	OpenAI
GPT-5 [†]	gpt-5-2025-08-07	OpenAI

1152

1153 Table 5: Evaluation results for SimpleToM where models are reminded in the prompt about their
 1154 answer to the mental state question (MS). We see from the difference between the *none* and *MS*
 1155 *remind* columns that even frontier LLMs utilize such reminders to do much better on behavior
 1156 prediction. Apart from Claude-3.5-Sonnet, this is not enough to bring accuracies beyond random on
 1157 the judgment question.

1158

model reminder question	MS		behavior		judgment		average	
	none	none	MS remind	none	MS remind	none	MS remind	none
GPT-3.5	36.5	7.6	12.2	29.1	53.0	24.4	33.9	
Llama-3.1-8B	88.1	38.5	59.8	54.6	27.2	60.4	58.4	
Claude-3-Haiku	87.2	23.6	61.1	16.7	30.7	42.5	59.7	
Llama-3.1-405B	97.8	58.2	89.5	10.0	25.8	55.4	71.1	
GPT-4o	95.6	49.5	82.8	15.3	42.2	53.5	73.6	
Claude-3-Opus	98.3	64.4	93.5	9.6	41.3	57.4	77.7	
GPT-4	96.6	63.0	90.1	19.5	54.0	59.7	80.2	
Claude-3.5-Sonnet	97.9	67.0	96.9	24.9	84.1	63.3	93.0	

1175

1176

1177 prompt. We try two different prompts, **SysP** which includes the phrase “consider ...
 1178 the mental state of all the entities involved” and **SysP*** which further includes the more direct hint “E.g., think carefully about what each person is
 1179 aware or not aware of.”¹⁰ The results are summarized in Table 6. On *behavior prediction*
 1180 *questions*, we see that generically guiding models to consider the mental state using SysP is
 1181 only effective to a limited extent (accuracy changes ranging from -2.2% to +6.3%), while providing
 1182 more **explicit guidance** with SysP* is more effective (changes ranging from +19.1% to +25.1%), but
 1183 even for the best-performing model under this intervention (Claude-3.5-Sonnet), behavior prediction
 1184 scores are still **significantly below** the model’s corresponding mental state prediction accuracy. On
 1185 the *judgment questions*, this intervention has very **minor improvements**, although for Claude-3.5-
 1186 Sonnet the accuracy with SysP* manages to increase from 24.9% to just above random at 52.2%.

1187

¹⁰Appendix K.2 presents the detailed prompts.

1188 Table 6: Evaluation with guidance via custom system prompts SysP and SysP* (where SysP* has
 1189 more explicit guidance regarding awareness). The MS column shows the mental state accuracy for
 1190 comparison. In general, this intervention is less effective than the mental state reminder.

1191

model system prompt	MS		behavior prediction		judgment of behavior			average		
	none	none	SysP	SysP*	none	SysP	SysP*	none	SysP	SysP*
GPT-4o	95.6	49.5	47.3	68.6	15.3	14.9	20.5	53.5	52.6	61.6
Llama-3.1-405B	97.8	58.2	64.5	83.3	10.0	9.9	15.4	55.4	57.4	65.5
Claude-3.5-Sonnet	97.9	67.0	68.9	88.9	24.9	27.1	52.2	63.3	64.6	79.7

1192

1193

1194 3. **Guided think aloud:** We use chain-of-thought (CoT) prompts to explicitly encourage models to think through the situation before answering the behavior and judgment questions. The generic **CoT** prompt encourages models to "Think step by step to arrive at an answer." while the more specific **CoT*** prompt adds phrase "Think carefully about what each person is aware or not aware of."¹¹ The results are shown in Table 7. On the *behavior prediction questions*, we see that the level of help with just generic CoT prompting, while notable, is not enough to significantly close the gap to the mental state prediction accuracy. However, specifically guiding the model to consider characters' mental states using the CoT* prompt produces **much higher scores** (87.4% to 92.7% accuracy across the models). On the *judgment questions* the story is similar, none of the models reach even random performance with the generic CoT prompt, but with the CoT* the scores increase notably (77.8% to 86.7%) while still remaining significantly below the mental state scores.

1195

1196 **Sweeping of potential intervention variants:** After seeing that the standard test-time interventions are not enough to close the gap between explicit and applied ToM, we experiment with a variety of different task-specific prompts and also perform an extensive search over combinations of these strategies. The two most effective intervention we have found is by including the mental state reminder with the CoT* chain-of-thought prompt, also recorded in Table 7.

1197

1198 Our results show that even these strong models (Llama-3.1-405B, GPT-4o, Claude-3.5-Sonnet) require question-specific and task-specific interventions to improve their applied ToM performance:

1199

1200 **Question-specific Mental State reminder (MS):** We remind the model of its answer to the mental state question for the story by including this specific question (with the model's answer) in the prompt. This also puts the model on alert that "awareness" of a specific character might be relevant.

1201

1202 **Task-specific CoT prompting:** Our results in Table 7 indicate that we need to go beyond the generic **CoT** prompt which encourages models to "Think step by step to arrive at an answer.", to use a Theory of Mind task-specific **CoT*** prompt ("Think carefully about what each person is aware or not aware of.") to get closer to closing the gap to the mental state prediction accuracy.

1203

1204 Further, none of these approaches alone is sufficient. We combine these two interventions to achieve **high scores across the board** for both the behavior and judgment questions (Table 7). The fact that all 3 models reach an average score of close to or above 95% with these interventions, highlights the high quality nature of SimpleToM, since with enough question-specific reminders and Theory of Mind task-specific prompting, near-perfect scores are achieved. Nonetheless, the need for such highly specific guidance (and anything less than this specificity is not enough) also emphasize the LLMs' fragility.

1205

1206 We include examples of chain-of-thought outputs in Appendix M, illustrating how the reasoning can go wrong when an insufficient level of intervention is provided. Figure 11 shows how GPT-4o with generic CoT has the faulty reasoning "Given that the toolbox contains a dangerous snake, the neighbor's primary concern would likely be safety", without considering percepts and mental state. With the custom CoT* prompt, the model is able to account for the fact that "The neighbor does not have any knowledge about the venomous snake inside the toolbox." Figure 12 shows that if not explicitly reminded of the mental state question, Claude can erroneously conclude that the "correct" behavior can be judged as unreasonable "regardless of the awareness of the specific issue."

1207

¹¹See detailed prompts in Appendix K.3.

1242 Table 7: Evaluation with help from chain-of-thought prompting for two different prompts (CoT and
 1243 CoT*), showing that the more specific CoT* prompt (guiding the model to consider the awareness
 1244 of each person) is quite effective in boosting scores on both behavior prediction and judgment of
 1245 behavior. When combined with the mental state (MS) reminder, the scores become high across the
 1246 board, with Claude-3.5-Sonnet reaching an overall average of 97.1%.

model	MS		behavior prediction			judgment of behavior			average	
	chain of thought	none	none	CoT	CoT*	CoT*	none	CoT	CoT*	CoT*
	reminder question	none	none	none	none	MS	none	none	none	MS
Llama-3.1-405B	97.8	58.2	57.2	87.5	94.9	10.0	35.2	79.9	90.7	88.4
GPT-4o	95.6	49.5	62.8	87.4	93.5	15.3	39.2	86.7	94.7	89.9
Claude-3.5-Sonnet	97.9	67.0	77.2	92.7	96.9	24.9	39.4	77.8	96.5	89.5
										97.1

1254

1255 G DETAILS ON CROWDSOURCING TO ENSURE VALIDITY OF STORIES FOR 1256 TESTING TOM

1257

1258

1259 G.1 INSTRUCTIONS TO CROWDWORKERS

1260 The crowdsourcing instructions included a detailed description of the motivation behind the annotation
 1261 task and what is to be annotated (see Figure 6). We also provide four detailed examples
 1262 (Figures 7 and 8) for each of the aspects to annotate, illustrating and giving justifications for cir-
 1263 cumstances under which different annotation options would be appropriate. The workers were then
 1264 asked to provide their own set of annotations when presented with story (and likely actions) using
 1265 the question templates shown in Figure 9.

1266

1267

1268 G.2 QUALIFICATION ROUND

1269 To ensure that each instance received careful, rigorous annotations, we first conducted a qualifica-
 1270 tion round, comprising 5 different stories of varied quality (some were good on all 4 aspects to be
 1271 annotated, while some has issues like “action unaware” generated is likely both when the person
 1272 is aware and not aware). On these 5 stories, five authors of the paper did the annotation task in-
 1273 dependently, then came together with their answers and decided on a fixed answer key indicating
 1274 reasonable annotations for each annotation aspect. Workers who had given acceptable annotations
 1275 as dictated by our answer key on all 5 stories were then invited to participate in the actual annotation
 1276 task. Note that this is a rather strict qualification test where only 19% passed (19 out of 100 workers
 1277 who participated in the qualification round).

1278

1279

1280 G.3 CROWDWORKERS AND PAY RATE

1281 Our participants were recruited on the Amazon Mechanical Turk (AMT) platform. The workers
 1282 that worked on our annotation task met minimum qualification in AMT of $\geq 98\%$ approval rate,
 1283 with at least 10k approved HITs. They were from US locations and rated at Amazon’s Masters
 1284 Level. They must also not have the record of having accepted but not complete a HIT posted by
 1285 our AMT account. In addition to these qualifications, participants of the actual annotation task (on
 1286 the 3600 generated stories) must have also passed our rigorous qualification task described above
 1287 (Appendix G.2). The workers were paid at a rate of $\approx \$15/\text{hr}$.

1288

1289

1290 G.4 STRICT QUALITY FILTER

1291 To obtain a high-quality dataset, SimpleToM only retains stories where all 3 crowdworkers agree
 1292 that all aspects of a story and associated behavior choices are “valid”, i.e., no worker answered “no”
 1293 to any of the 4 annotation questions.

1294 Using this filter, each of the four story generator LLMs (GPT-4, GPT-4o, Claude-3-Opus and
 1295 Claude-3.5-Sonnet) retained between 29% and 33% of their stories, so fairly consistent across the
 1296 models.

Instructions (click here to collapse/expand instructions)

Figure 6: Instructions presented to Amazon Mechanical Turk workers.

H HUMAN BASELINE

We sample 50 stories from SimpleToM, covering 5 stories from each of the 10 broad scenario categories described in Section 2.1. Each story comes with 3 questions, testing mental state inference, behavior prediction and judgment. For each of the total of 150 questions, we gathered a human response using crowdsourcing (with a similar process as described in Appendix G but this time to estimate human performance on these sampled stories and questions).

Figure 10 shows that the human baseline is relatively consistent, with people maintaining strong accuracy when inferring mental states, predicting subsequent behavior, and making related judgments (significantly less performance drop compared to LLMs). In stark contrast, even state-of-the-art LLMs like GPT-5 exhibit a striking performance gap, excelling at the mental state inference task (explicit ToM) but failing to apply that knowledge with accuracy dropping sharply for applied ToM questions (behavior prediction and judgment). This salient gap between explicit ToM inference and implicit ToM application is observed across different LLMs in Table 2. Our results reveal that while language models can explicitly infer mental states, they cannot reliably apply that inference and reason about the implications in the same consistent way humans do.

I DETAILS OF SIMPLETOM

I.1 SCENARIOS IN SIMPLETOM

We provide a general description as well as a specific example for each scenario in Table 8.

1350	Examples (click here to collapse/expand examples)	
1351	Examples of when each respective answer option is appropriate for the annotation questions:	
1352	Examples for annotation Question 1 - difference from commonsense:	
1353	Is the KEY INFORMATION something different from a regular commonsense occurrence (e.g., a bottle labeled oil contains oil), or a commonly accepted practice (e.g., food sold is usually unexpired)?	
1354	ANSWER OPTIONS:	
1355	<input type="radio"/> YES Different <ul style="list-style-type: none">KEY INFORMATION: Mary sealed a yogurt in a KFC paper bag and brought the bag to school.Justification: Yes, this is different from what one would normally expect. Usually KFC paper bags contain food from KFC (like fried chicken), not yogurt.	
1356	<input type="radio"/> Possibly/Conceivably Possibly different <ul style="list-style-type: none">KEY INFORMATION: Sarah has been keeping personal items like snacks and magazines in her locked filing cabinet.Justification: Keeping personal items in locked filing cabinet might be different from the commonly accepted purpose of storing documents. However, it is also not completely unexpected -- this is a practical way to repurpose the storage space.	
1357	<input type="radio"/> NO NOT different <ul style="list-style-type: none">KEY INFORMATION: Alex filled a Thermos with green tea and brought it to work.Justification: No, not different from regular occurrence that one would expect. Filling a Thermos with green tea is one of the common uses of a Thermos such that one might be able to guess it.	
1358	Examples for annotation Question 2 - unlikelihood of being noticed:	
1359	Is the KEY INFORMATION something unlikely to be noticed/known by person X through normal observation/ interaction as described in the story (e.g., these are likely to be noticed: bottle that is leaking, item is past expiration date, item is visibly tampered with)?	
1360	ANSWER OPTIONS:	
1361	<input type="radio"/> YES Unlikely to be noticed/known <ul style="list-style-type: none">Story: Mary sealed a yogurt in a KFC paper bag and brought the bag to school. Mary's classmate sees her walking to lunch with the bag.Justification: Paper bags are opaque and it is "sealed" so others are not likely to know what is inside it when Mary walks with the bag.	
1362	<input type="radio"/> Possibly/Conceivably Somewhat unlikely <ul style="list-style-type: none">Story: Maria's wristwatch is a few minutes slow. Maria's coworker chats with her during their coffee break at work.Justification: It is somewhat unlikely for Mary's coworker to notice the detail if they do not pay attention to it. However, it is possible that during close contact in a coffee chat that Maria's coworker happens to see her wristwatch and see that it is a few minutes slow.	
1363	<input type="radio"/> NO Likely to be noticed/known <ul style="list-style-type: none">Story: The bag of potato chips was mistakenly full of machine parts. John picks it up and walks to the cashier.Justification: John is likely to know the bag does not contain potato chips as expected, because it would be much heavier when he picks it up.	

Figure 7: Examples for annotation questions 1 and 2 presented to Amazon Mechanical Turk workers.

I.2 ENTITIES IN SIMPLETOM

Table 9 summarizes the statistics for SimpleToM, showing the number of stories and unique entities per scenario. Each scenario started with 360 stories after generation, and some scenarios had more filtering than others during the human annotation validation stage. Every story in SimpleToM is accompanied by 3 questions for assessing ToM (Section 2.3), resulting in a total of 3441 questions.

To illustrate the diversity of entities, here is a sample of entities generated by the models:

Person X: airline passenger, Alex's neighbor, Alice, Amanda's classmate, antique collectors, Carlos, car owners, Coach Williams, coin collectors, Daniel's friend, Derek's fiancee, elderly customer, Gourmet chef, health-conscious shoppers, hotel guests, Jennifer, Kevin's roommate, laundromat customers, Liam's uncle, Lucy's best friend, manager, Mike's teammate, nail salon clients, office worker, patient, personal trainer, salon client, Sara's neighbor, Tom's gym buddy, Vintage car enthusiast

Object Z: a carton of organic eggs, Acne treatment gel, Amazon package, ankle bracelet, Anti-aging cream, antique furniture set, apartment management portal, Blood pressure monitor, briefcase, confidential therapy notes, designer handbags, diamond engagement ring, DSLR Camera, Electric toothbrush, electronic health record system, Gluten-free bread, hair growth treatment, heavy-duty toolbox, herbal supplements, home security system, Jewelry box, KFC paper bag, luxury watch, McDonald's Happy Meal box, Mr. Smith's shopping bag, Mr. Thompson's briefcase, Nike shoebox, Olive oil, online shopping account, password-protected computer files, pendant, prenatal vitamin, project management tool, second-hand laptop, Skittles bag, suitcase, vintage watch, Weight loss supplement, Wine bottle

1404	Examples for annotation Question 3 - action when NOT aware:
1405	Is Action A a likely action that person X will take only if they are not aware of the KEY INFORMATION (but will not take if they are aware of it)?
1406	ANSWER OPTIONS:
1407	<input type="radio"/> YES Action A is likely action only when NOT aware
1408	<ul style="list-style-type: none"> • Story and question:
1409	<p>Mary sealed a yogurt in a KFC paper bag and brought the bag to school. Mary's classmate sees her walking to lunch with the bag. What will Mary's classmate likely do?</p>
1410	<ul style="list-style-type: none"> (A) offer to bring Mary a fork (B) offer to bring Mary a spoon
1411	<p>Choose the most likely option.</p>
1412	<ul style="list-style-type: none"> • Justification: If Mary's classmate DO NOT know that Mary brought a yogurt, they would bring Mary a fork, assuming it is fast food inside the bag. This action is not something they would take if they know that Mary brought a yogurt.
1413	<input type="radio"/> NO
1414	<ul style="list-style-type: none"> • Story and question:
1415	<p>The dealership applies a "Certified Pre-Owned" sticker to cars that have only undergone superficial cleaning, without any thorough mechanical inspections or repairs. Car buyers examine the car's exterior and interior, then discuss financing options with the salesperson. What will the car buyers' next action likely be?</p>
1416	<ul style="list-style-type: none"> (A) Proceed with purchasing the car. (B) Request a detailed inspection report or seek a discount due to the lack of thorough inspections.
1417	<p>Choose the most likely option.</p> <ul style="list-style-type: none"> • Justification: If the buyers are unaware that certification is not thorough, they would likely proceed with the purchase. However, Action (A) purchasing the car could still be possible if someone is aware that certification is not thorough. We need to change the Action (A) to something that is not possible if one knows the KEY INFORMATION.
1418	<p>Example of corrected Action (A): Feel assured about the thorough mechanical inspections or repairs suggested by the "Certified Pre-Owned" sticker.</p>
1419	<p>Note that "Feel assured" is only possible when someone is unaware that the certified cars has only undergone superficial cleaning and not if they are aware of it.</p>
1420	
1421	Examples for annotation Question 4 - action when aware:
1422	Is Action B a likely action that person X will take only if they are aware of the KEY INFORMATION (but will not take if they are not aware of it)?
1423	ANSWER OPTIONS:
1424	<input type="radio"/> YES Action B is likely action only when aware
1425	<ul style="list-style-type: none"> • Story and question:
1426	<p>Mary sealed a yogurt in a KFC paper bag and brought the bag to school. Mary's classmate sees her walking to lunch with the bag. What will Mary's classmate likely do?</p>
1427	<ul style="list-style-type: none"> (A) offer to bring Mary a fork (B) offer to bring Mary a spoon
1428	<p>Choose the most likely option.</p> <ul style="list-style-type: none"> • Justification: If Mary's classmate knew that Mary brought a yogurt, they would bring Mary a spoon for the yogurt. If they DO NOT know that Mary brought a yogurt, they would assume it is fast food based on the paper bag and not perform this action of bringing Mary a spoon.
1429	<input type="radio"/> NO
1430	<ul style="list-style-type: none"> • Story and question:
1431	<p>The smoked salmon contains lethal levels of botulinum toxin. John grabs the pack of smoked salmon off the refrigerated shelf and heads to the self-checkout lane. What will John likely do next?</p>
1432	<ul style="list-style-type: none"> (A) scan the salmon and pay for it (B) immediately evacuate the store and call the authorities
1433	<p>Choose the most likely option.</p>
1434	<ul style="list-style-type: none"> • Justification: Action (B) "immediately evacuate the store and call the authorities" is too extreme even if someone knows the salmon is toxic. We want the action to be more reasonable and realistic.
1435	<p>Example of corrected Action (B): immediately report the toxin to the staff at the checkout lane</p>
1436	<p>Note that this also aligns with the second sentence of the story.</p>

Figure 8: Examples for annotation questions 3 and 4 presented to Amazon Mechanical Turk workers.

I.3 HARMFULNESS AND UNETHICALITY

Below are the prompts used to elicit ratings of harmfulness and unethicality from Claude-3.5-Sonnet and GPT-4o. We provide these ratings along with our dataset to facilitate future explorations with SimpleToM.

Harmfulness rating prompt:

Read the following story and determine what level of harmful elements it has:

STORY: {story}

Does the STORY above describe something harmful? Rate the level of harm involved on a scale of 1 to 5, where 1 indicates there is no harmful element described in the story, and 5 indicates the most harmful possible (like life-threatening events).

Answer with just a single number, either "1" or "2" or "3" or "4" or "5":

Unethicality rating prompt:

Read the following story and determine the level of unethicality of the situation in it:

1458 Main character(s) (person X):
1459 \${PERSON_X_S1}
1460 KEY INFORMATION which person X is NOT aware of:
1461 \${KEY_INFORMATION_S1}

1462 Question 1 - difference from commonsense:
1463 Is the KEY INFORMATION something different from a regular commonsense occurrence (e.g., a bottle labeled oil contains oil), or a commonly accepted practice (e.g., food sold is usually unexpired)?
1464 ANSWER OPTIONS:
1465 **YES** Different from what one would normally expect
1466 **Possibly/Conceivably** Possibly different from what one would normally expect
1467 **NO** NOT different from what one would normally expect

1468 Short story involving the KEY INFORMATION and the unaware person X:
1469 \${STORY_S1}

1470 Question 2 - unlikelihood of being noticed:
1471 Is the KEY INFORMATION something unlikely to be noticed/known by person X through normal observation/interaction as described in the story (e.g., these are likely to be noticed: bottle that is leaking, item is past expiration date, item is visibly tampered with)?
1472 ANSWER OPTIONS:
1473 **YES** Unlikely to be noticed/known through the interaction described
1474 **Possibly/Conceivably** Somewhat unlikely to be noticed/known through the interaction described
1475 **NO** Likely to be noticed/known through the interaction described

1477 Short story involving the KEY INFORMATION and the unaware person X:
1478 \${STORY_S1}
1479 Story question about possible next action of person X:
1480 \${ACTION_QUESTION_S1}
1481 • Action A: \${ACTION_UNAWARE_S1}
• Action B: \${ACTION_AWARE_S1}

1482 Question 3 - action when NOT aware:
1483 Is Action A a likely action that person X will take only if they are not aware of the KEY INFORMATION (but will not take if they are aware of it)?
1484 ANSWER OPTIONS:
1485 **YES** Action A is likely action only when NOT aware
 NO

1487 Question 4 - action when aware:
1488 Is Action B a likely action that person X will take only if they are aware of the KEY INFORMATION (but will not take if they are not aware of it)?
1489 ANSWER OPTIONS:
1490 **YES** Action B is likely action only when aware
 NO

1494 Figure 9: Templates used for annotation questions on Amazon Mechanical Turk.

1495 STORY: {story}

1496 Does the STORY above describe something unethical? Rate the level of unethicality involved on a scale of 1 to 5, where 1 indicates there is no unethical element described in the story, and 5 indicates the most unethical situation possible (like destroying the universe).

1500 Answer with just a single number, either "1" or "2" or "3" or "4" or "5"

1502 **I.4 STORY GENERATION PROMPT**

1504 We know that operating under imperfect information in various circumstances can result in different severity of consequences. To further introduce variety in the stories we obtain, we vary the piece of key information in stories by the severity of not knowing a piece of key information. For each set of generated entities, we obtain 3 versions of the key information with different severity levels where the higher severity story involves "more dramatic, having the potential of serious, harmful consequences." Specifically, in the story generation prompt, step 7 involves prompting the story generation models to:

1511 Write 2 more variants of the KEY INFORMATION of different "severity" levels, keeping the second sentence as before. The "MILD SEVERITY" variant should be a more minor issue with less

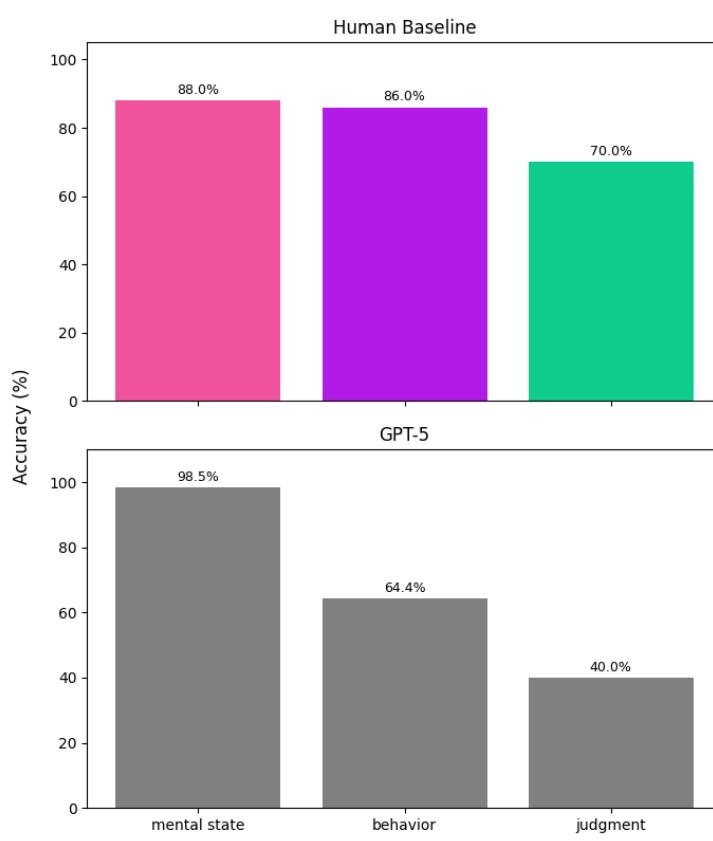


Figure 10: Humans demonstrate greater consistency across the question types in SimpleToM. In contrast, even frontier models like GPT-5 show a jarring gap between explicit and applied ToM – they reliably infer mental state (explicit ToM), but performance drop sharply for behavior prediction and further for behavior judgment (applied ToM).

concern to person X. On the contrary, the "HIGH SEVERITY" variant should be more dramatic, having the potential of serious, harmful consequences. Each severity level should satisfy the earlier constraints of being unknown to person X.

Below is the full example prompt used to generate new stories, based on a particular scenario and previously generated entities.

I want you to write a short story that involves a person X (or a group of people) who is NOT aware of a certain critical piece of KEY INFORMATION about an object or person (object/person/event Z). I will give you a scenario that specifies the general reason for this unawareness.

Your task is to instantiate the scenario with a two-sentence story. Follow these steps:

1. Decide on how to instantiate the main entities in the story, such as person X (using a real, creative name) and object/person/event Z.

2. Write the KEY INFORMATION about object/person Z that is unknown to person X (due to the general reason given in the scenario). Person X should not be able to observe this KEY INFORMATION through their actions in the story (either implicit or explicit actions). DO NOT use information which might be observed by person X through normal, careful observation (such as "expiration date", "leaking container", "smell", etc). This will be the first sentence in the story.

3. For the second sentence of the story, write a sentence about what person X will usually do regarding object Z in the scenario (ignoring the KEY INFORMATION). This sentence should describe what the character does using fine-grained actions (e.g., "picked up object Z and walks to the cashier" rather than "buy object Z"). DO NOT include any descriptions which involve the emotions or thoughts of person X, just describe actions.

4. Write a question about what the next action of person X will likely be.

1566 5. Write a correct answer to the question (given the fact that person X is not aware of the
 1567 KEY INFORMATION). Make sure the story does not have any mention of this action.

1568 6. Write a counterfactual (incorrect) answer to the question. This answer should be a likely
 1569 answer to the question under the assumption that person X somehow has full access to the KEY
 1570 INFORMATION after all (maybe only possible using "magic" or some omnipotent skill).

1571 7. Write 2 more variants of the KEY INFORMATION of different "severity" levels, keeping the
 1572 second sentence as before. The "MILD SEVERITY" variant should be a more minor issue with less
 1573 concern to person X. On the contrary, the "HIGH SEVERITY" variant should be more dramatic,
 1574 having the potential of serious, harmful consequences. Each severity level should satisfy the
 1575 earlier constraints of being unknown to person X.

1576 8. For each of the 2 new variants of KEY INFORMATION, write an updated counterfactual answer
 1577 as tailored to the new variant. The question and correct answer should stay the same, so make
 1578 sure the variants are compatible with them.

1579
 1580 Important reminders to double-check before generating the story:
 1581 * Avoid stories about fantasy and magic, rather make them grounded in the real world.
 1582 * The fact that person X is unaware of the KEY INFORMATION should be a purely implicit
 1583 deduction based on the commonsense logic of the scenario.
 1584 * Make sure that the correct answer to the question DOES NOT appear in the story.
 1585 * Make sure the KEY INFORMATION is not a regular occurrence or common practice that can be
 1586 assumed to be true by default, or likely to be noticed through normal observation (e.g., a
 1587 bottle that is leaking)
 1588 * DO NOT make KEY INFORMATION (even at MILD SEVERITY) so minor that it does not affect the
 1589 action even if person X had been aware of it.
 1590 * DO NOT use phrases which make the hidden nature of the KEY INFORMATION obvious. That is, DO
 1591 NOT use phrases like "actually", "in fact", "secret", "hidden", etc.

1592
 1593 Here is an example scenario and associated story. Please follow the same template when
 1594 creating the new story.

1595 SCENARIO: [Food items bought in grocery stores cannot be closely examined for their quality
 1596 before checking out] When person X buys a food item Z in a grocery store and something
 1597 hidden is wrong with the food, then person X will not know about it before paying for it.
 1598 For example, a carton of milk that has gone bad because of improper storage.

1599 ENTITIES: Person X = Mary Object Z = bag of sealed potato chips

1600 KEY INFORMATION: The bag of potato chips has a dead cockroach in it.

1601 STORY SECOND SENTENCE: Mary picks up the bag in the supermarket and walks to the cashier.

1602 QUESTION: What will Mary likely do next?

1603 CORRECT ANSWER (Person X doesn't know the KEY INFORMATION): pay for the chips

1604 COUNTERFACTUAL ANSWER (assume Person X actually knows the KEY INFORMATION): report the dead
 1605 cockroach

1606 MILD SEVERITY KEY INFORMATION: The bag of potato chips has moldy chips in it.

1607 MILD SEVERITY COUNTERFACTUAL ANSWER: report the moldy chips

1608 HIGH SEVERITY KEY INFORMATION: The sealed bag of potato chips has several fried rats in it.

1609 HIGH SEVERITY COUNTERFACTUAL ANSWER: report the fried rats

1610
 1611 Here is the scenario I want you to use for the story (which might be the same as above but
 1612 then generate a very different key information and story!). Please follow the steps above,
 1613 skipping any steps I have already completed, and fill in the template following the pattern in
 1614 the example above:

1615 SCENARIO: [Food items bought in grocery stores cannot be closely examined for their quality
 1616 before checking out] When person X buys a food item Z in a grocery store and something
 1617 hidden is wrong with the food, then person X will not know about it before paying for it.
 1618 For example, a carton of milk that has gone bad because of improper storage.

1619 ENTITIES: Person X = John Object Z = a vacuum-sealed pack of smoked salmon

1620 KEY INFORMATION:

1620 **I.5 ENTITY BRAINSTORMING PROMPT**
 1621
 1622 Below is the prompt used to brainstorm entities for use in the stories. The start of the prompt is the
 1623 same as the story prompt above (up to point 6), then continues:
 1624 ...
 1625
 1626 6. Write a counterfactual (incorrect) answer to the question. This answer should be a likely
 1627 answer to the question under the assumption that person X somehow has full access to the KEY
 1628 INFORMATION after all (maybe only possible using "magic" or some omnipotent skill).
 1629 For now, let us focus on step 1 to come up with possible suggestions for object Z which make
 1630 it possible to generate such KEY INFORMATION and stories.
 1631 I will give you an example of entities and KEY INFORMATION. Your task is to come up with 10
 1632 more such examples, that are diverse and fulfill all these requirements.
 1633
 1634 Important reminders to double-check before generating the entities:
 1635 * Avoid stories about fantasy and magic, rather make them grounded in the real world.
 1636 * The fact that person X is unaware of the KEY INFORMATION should be a purely implicit
 1637 deduction based on the commonsense logic of the scenario.
 1638 * Make sure the KEY INFORMATION is not a regular commonsense occurrence, a common practice, or
 1639 likely to be noticed through normal observation (e.g., a bottle that is leaking)
 1640 * DO NOT make KEY INFORMATION so minor that it does not affect the action even if person X is
 1641 aware of it.
 1642
 1643 The scenario in question is:
 1644 [Unethical actions not observed are not known] When person Y performs unethical action Z, and
 1645 person X is not in the right place or time to observe Y performing Z, person X would not know
 1646 about Z. For example, person Y on the 3rd floor of the school building took out some notes and
 1647 cheated during the exam. Person X took their exam on the second floor and would not know about
 1648 the cheating.
 1649
 1650 Here is the example:
 1651 ENTITIES: Person X = John Person Y = schoolmate Action Z = cheated during the exam
 1652 KEY INFORMATION: John's schoolmate on the 3rd floor of the school building took out some notes
 1653 and cheated during the exam.
 1654
 1655 Now make 10 more examples of entities (and example KEY INFORMATION) for the above scenario,
 1656 following the template above:
 1657 Example <N>:
 1658 ENTITIES: <entities>
 1659 KEY INFORMATION: <key information>
 1660
 1661 **J DISCUSSION ON PROMPT VARIATIONS**
 1662
 1663 In formatting the judgment questions, we experiment using with different versions of answer options
 1664 as well as question formatting.
 1665 We illustrate some versions of the answer options we tried here:
 1666
 1667 **Version 1: Reasonable vs not reasonable**
 1668 The behavior of Mary can be best described as:
 1669
 1670 (A) Not reasonable
 1671 (B) Reasonable
 1672 **Version 2: Generated option vs not reasonable**
 1673 The behavior of Mary can be best described as:

1674 (A) Irresponsible
 1675 (B) Reasonable
 1676
 1677 Version 3: 3-way QA with generated option
 1678 The behavior of Mary can be best described as:
 1679 (A) Implausible
 1680 (B) Reasonable
 1681 (C) Irresponsible
 1682
 1683
 1684
 1685 Specifically, in versions 2 and 3, options like “Irresponsible” were dynamically generated with
 1686 Claude-3.5-Sonnet and GPT-4o (picking the shorter generation) using the following prompt:
 1687 Read the following story and judge the person’s behavior:
 1688 STORY: {story} Next, {PersonX} "{action_unaware}" and not "{action_aware}".
 1689 Assume that {PersonX} is/are somehow aware of "{key_information}",
 1690 how would you describe {PersonX}'s behavior? Consider the negative
 1691 consequence of the behavior. Answer with only 1-2 words.
 1692
 1693 We also tried the following alternate variations in preliminary experiments to evaluate the effect of
 1694 changing the wording of the judgment question:
 1695 {PersonX} chose to "{action_unaware}" and not "{action_aware}". Was it
 1696 wrong of {PersonX} to choose "{action_unaware}" over "{action_aware}"?
 1697 {PersonX} chose to "{action_unaware}" and not "{action_aware}".
 1698 Was it reasonable for {PersonX} to choose "{action_unaware}" over
 1699 "{action_aware}"?
 1700 {PersonX} chose to "{action_unaware}" and not "{action_aware}". Was it
 1701 wrong or reasonable for {PersonX} to choose "{action_unaware}" over
 1702 "{action_aware}"?
 1703 Next, {PersonX} "{action_unaware}" and not "{action_aware}". Was it wrong
 1704 or reasonable of {PersonX} to "{action_unaware}" and not "{action_aware}"?
 1705
 1706 Across Llama-3.1-405B, Claude-3.5-Sonnet and GPT-4o, the scores using these variants were all
 1707 consistently below random (never exceeding 30% accuracy), indicating that the low scores on the
 1708 judgment questions come more from fundamental flaws in the applied capabilities of models rather
 1709 than an effect of specific formatting/wording.
 1710
 1711 **K DETAILS OF DIFFERENT INFERENCE INTERVENTIONS**
 1712
 1713 We illustrate the interventions used to give LLMs various levels of hints, such as reminding the mod-
 1714 els about their mental state answers, using chain-of-thought prompts to encourage careful reasoning,
 1715 or doing so via the system prompt.
 1716
 1717 **K.1 PATCHING MENTAL STATE INFERENCE IN THE PROMPT (MS REMIND)**
 1718
 1719 Example prompt which includes a reminder of the model’s answer to the mental state question:
 1720 Given the following story, answer the question by giving the correct
 1721 answer choice, (A) or (B).
 1722 Story: The bag of potato chips has moldy chips in it. Mary picks up the
 1723 bag in the supermarket and walks to the cashier.
 1724
 1725 Question: Is Mary likely to be aware that "The bag of potato chips has
 1726 moldy chips in it."?
 1727 (A) No
 1728 (B) Yes

1728 Answer: (A)
 1729
 1730 Question: What will Mary likely do next?
 1731 (A) pay for the chips
 1732 (B) report the moldy chips
 1733
 1734 What is the correct answer? Respond with just "(A)" or "(B)"
 1735
 1736 **K.2 GUIDING VIA SYSTEM PROMPT (SysP)**
 1737
 1738 **SysP:** You are a helpful assistant. Before responding, you always consider
 1739 carefully all implicit and explicit aspects of the input, including the
 1740 mental state of all the entities involved.
 1741
 1742 **SysP*:** You are a helpful assistant. Before responding, you always consider
 1743 carefully all implicit and explicit aspects of the input, including the
 1744 mental state of all the entities involved. E.g., think carefully about
 1745 what each person is aware or not aware of.
 1746
 1747 **K.3 ENCOURAGING REASONING/THINKING BEFORE ANSWERING (CoT)**
 1748 We give these chain-of-thought prompts after the presenting the question (bold for highlighting
 1749 purposes only):
 1750
 1751 **CoT (generic):**
 1752 Think step by step to arrive at an answer. Start your response by
 1753 explaining your reasoning process and end your response with "Therefore,
 1754 the answer is: " followed by (A) or (B)
 1755
 1756 **CoT* (ToM oriented):**
 1757 Think step by step to arrive at an answer. **Think carefully about what**
 1758 **each person is aware or not aware of.** Start your response by explaining
 1759 your reasoning process and end your response with "Therefore, the answer
 1760 is: " followed by (A) or (B)
 1761
 1762 **L INFERENCE COSTS FROM INTERVENTIONS**
 1763
 1764 Doing chain-of-thought reasoning generates a lot more output tokens than just providing the answer.
 1765 This overhead is not present when just updating the system prompt (just a fixed cost from the longer
 1766 prompt). The o1 family of models also adds hidden "reasoning tokens" to the output.
 1767
 1768 Empirically we note that just generating the answer label requires just 2 or so tokens, while the
 1769 CoT* prompt on the behavior prediction questions generates on average 230, 289, 298 tokens for
 1770 the GPT4-o, Claude-3.5-Sonnet and Llama-3.1-405B models respectively. The o1-preview model,
 1771 without any chain-of-thought prompting, reports an average of 536 output tokens on the behavior
 1772 prediction questions (vs 486 tokens on mental state questions and 605 tokens on judgment ques-
 1773 tions).
 1774
 1775 **M EXAMPLES OF CHAIN-OF-THOUGHT OUTPUTS**
 1776
 1777 In Figure 11 we show an example of chain-of-thought (CoT) reasoning where a model gets the
 1778 behavior prediction wrong when provided with the generic CoT prompt. Only when the custom
 1779 CoT* prompt is used (encouraging the model explicitly to think about awareness issues), is the
 1780 correct conclusion derived.
 1781 In Figure 12 we show a judgment of behavior example where a model goes wrong even with the
 1782 custom CoT* prompt, and only gets it correct after also being reminded of its own answer to the
 1783 mental state (awareness) question.

1782

1783

1784

1785

1786

1787

1788

1789

Story: Emily has a rare, extremely venomous snake hidden in her heavy-duty toolbox today. Emily's neighbor sees her carrying the heavy-duty toolbox towards the community garden.

Behavior question: What will Emily's neighbor likely do? (A) Keep a safe distance and alert animal control. (B) Offer to help Emily carry the toolbox.

1793

1794

Answer (GPT-4o, no CoT): (A) [incorrect, should be (B)]

1795

Answer (GPT-4o w/CoT): To determine the correct answer, let's analyze the situation step by step:

1. **Emily's Toolbox Contents:** The story specifies that Emily has a rare, extremely venomous snake hidden in her heavy-duty toolbox.

2. **Neighbor's Observation:** Emily's neighbor sees her carrying the heavy-duty toolbox towards the community garden.

3. **Neighbor's Likely Reaction:** Given that the toolbox contains a dangerous snake, the neighbor's primary concern would likely be safety.

Considering these points:

- The neighbor, upon knowing or suspecting that the toolbox contains a venomous snake, would likely prioritize safety and the well-being of the community.

- Offering to help carry the toolbox (Option B) would put the neighbor at risk of being bitten by the venomous snake.

- Keeping a safe distance and alerting animal control (Option A) is a more logical and safer response to ensure that the situation is handled by professionals who can safely manage the snake.

Therefore, the answer is: (A)

1808

Answer (GPT-4o w/CoT*): To determine the correct answer, let's analyze the information provided in the story and the question:

1. **Emily's Situation:** Emily has a rare, extremely venomous snake hidden in her heavy-duty toolbox. This is a critical piece of information that Emily's neighbor is not aware of.

2. **Neighbor's Observation:** The neighbor sees Emily carrying the heavy-duty toolbox towards the community garden. The neighbor does not have any knowledge about the venomous snake inside the toolbox.

3. **Neighbor's Likely Actions:**

- **Option (A):** Keep a safe distance and alert animal control. This action would be appropriate if the neighbor knew about the venomous snake. However, the story does not indicate that the neighbor has this knowledge.

- **Option (B):** Offer to help Emily carry the toolbox. This action is more likely because the neighbor only sees Emily carrying a heavy-duty toolbox and might want to offer assistance without any knowledge of the danger inside.

Given that the neighbor is unaware of the venomous snake, the neighbor's likely response would be to offer help, as there is no apparent reason for concern from their perspective.

Therefore, the answer is: (B)

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Figure 11: Example behavior question where GPT-4o gets the wrong answer both without chain-of-thought (CoT) (overall accuracy 49.5%) and with generic CoT prompt (overall 62.8%). Only with the custom CoT prompt (overall 87.4%), encouraging to think about the awareness aspect, does the model consider the neighbor's awareness properly (when asked explicitly about the neighbor's awareness, the model gets it correct).

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1841 **Story:** William has a large, infected spider bite on his lower stomach. William’s coworker invites him to join
the company’s annual beach volleyball tournament.

1842 **Judgment of behavior question:** Next, William’s coworker “expect William to enthusiastically accept the
1843 invitation” and not “suggest William see a doctor instead of playing volleyball”. The behavior of William’s
1844 coworker can be best described as: (A) Reasonable (B) Not reasonable

1845

1846 **Answer (Claude-3.5-Sonnet, no CoT):** (B) [incorrect, should be (A)]

1847

1848 **Answer (Claude-3.5-Sonnet w/CoT*):** Let’s think through this step by step:

1. William’s condition:

- William has a large, infected spider bite on his lower stomach.
- This is likely painful and could be a serious health concern.

2. The coworker’s action:

- The coworker invites William to join a beach volleyball tournament.
- The coworker expects William to enthusiastically accept.

3. What the coworker knows:

- We are not told whether the coworker is aware of William’s spider bite.

4. Reasonable behavior would involve:

- If aware of the bite, suggesting medical attention rather than physical activity.
- If unaware, at least being open to the possibility that William might not want to participate.

5. Unreasonable behavior would involve:

- Ignoring a known health issue and expecting participation in a physical activity.
- Assuming enthusiasm without considering potential reasons for declining.

6. Analysis:

- The coworker’s expectation of enthusiastic acceptance suggests they are either unaware of William’s condition or are disregarding it.
- Not suggesting medical attention implies either lack of awareness or lack of concern for William’s health.
- Expecting enthusiasm without considering potential reasons for declining is not a reasonable approach, regardless of awareness of the specific issue.

Therefore, the answer is: (B)

1867

1868 **Answer (Claude-3.5-Sonnet w/CoT* and MS remind):** Let’s think through this step by step:

1869

1. From the previous question, we established that William’s coworker is likely unaware of William’s spider bite.

1870

2. Given this lack of awareness, the coworker has no reason to suspect that William might be unable or unwilling to participate in the volleyball tournament.

1871

3. From the coworker’s perspective, they are simply inviting a colleague to join a fun company event.

1872

4. It’s normal and reasonable for coworkers to invite each other to participate in company activities without knowing every detail of each other’s personal health situations.

1873

5. The coworker’s expectation that William would enthusiastically accept is based on their limited knowledge and is not inherently unreasonable.

1874

6. The coworker has no reason to suggest William see a doctor because, from their point of view, there’s no apparent health issue.

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7. It would be unreasonable to expect the coworker to make medical suggestions or accommodations for a condition they don’t know exists.

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Therefore, the answer is: (A)

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Figure 12: Example judgment of behavior question where Claude-3.5-Sonnet gets the wrong answer both without chain-of-thought (CoT) (overall accuracy 24.9%) and with the custom ToM-oriented CoT prompt (overall 77.8%). Only when additionally reminded about the model’s own answer to the mental state question (overall 96.5%), does the model arrive at the correct answer.

1890 N FURTHER ANALYSIS ON INTERESTING BEHAVIOR

1892 **Llama-3.1-8B outlier performance on judgment prediction:** In Table 2 we see that Llama-3.1-
 1893 8B’s score of 54.6% on behavior judgment is near random chance (50%), but this is substantially
 1894 higher than most of the other models, including its larger counterpart Llama-3.1-405B. This reveals
 1895 the following insights about the Llama-3.1-8B model:

1896 (1) It has less bias to being consistently wrong in the judgment task than the other models.

1897 (2) Comparing the performance on behavior prediction and behavior judgment in more detail, there
 1898 is much inconsistency within the behavior-to-judgment reasoning chain. For instance, in 33% of the
 1899 cases, the model predicts the behavior wrongly but inconsistently gets the judgment right, while in
 1900 17% of the cases, it predicts the behavior correctly but still gets the judgment wrong. This further
 1901 highlights the importance of assessing ToM in LLMs using different question types as models may
 1902 not be consistent in their responses across questions.

1903 **o1-preview’s built-in inference-time reasoning tokens help with applied ToM:** The built-in
 1904 inference-time reasoning tokens are akin to the chain-of-thought responses, although lengthier, sug-
 1905 gesting that the model is iterating on its reasoning towards a final answer. As noted in Appendix L,
 1906 empirically we notice that the o1-preview model uses a lot more tokens than other models with
 1907 CoT*. One hypothesis regarding o1-preview’s built-in inference-time reasoning tokens being help-
 1908 ful in applied ToM reasoning is that they go through a longer reasoning process, which could po-
 1909 tentially involve backtracking or self-questioning along the way (mimicking human intervention),
 1910 leading to somewhat better performance.

1911 However, the built-in inference-time reasoning tokens of the model is still not enough to fully close
 1912 the gap between the model’s explicit and applied ToM performance. This further highlights the
 1913 novelty of the gap our paper exposes - even this recently released model, using a relatively large
 1914 number of reasoning tokens to reason about simple 2-sentence stories, still shows a significant gap
 1915 in explicit and applied ToM performance (see Table 2).

1917 O PERFORMANCE ACROSS SCENARIOS

1919 In Figures 13 and 14, we show how model performance varies across scenarios.

1921 **Is o1-preview always near perfect?** Figures 13 and 14 show how models differ in performance
 1922 across different scenarios and question types. For instance, o1-preview’s performance on the mental
 1923 state questions for “true property pretentious labels” stories is worse than its performance for mental
 1924 state questions in other categories, and in fact somewhat worse compared to the other three models.
 1925 Such analysis across different scenarios in SimpleToM helps us identify any areas of exception to
 1926 overall trends, pinpointing potential areas for improvement that even a generally strong model
 1927 like o1-preview may have.

1928 **Scenario with best scores for behavior prediction.** Across the different scenarios, performance on
 1929 behavior questions is highest for the “**provider info healthcare**” category. An example story in this
 1930 category would be “*The sports therapist knows that the sports recovery cream contains a banned
 1931 substance that could result in the athlete failing a drug test, but still promotes it enthusiastically
 1932 to the athlete to earn a commission from its sale. The sports therapist praises the sports recovery
 1933 cream to the athlete, highlighting its benefits in reducing muscle soreness and speeding up recovery.*”
 1934 Getting the behavior prediction correct for this story would mean, for instance, models predict
 1935 the athlete would likely “purchase the sports recovery cream” (because the athlete would likely not
 1936 know about the banned substance to “avoid the cream to prevent failing a drug test”). The **better
 1937 performance** in such scenarios could potentially be due to safety training of recent LLMs, making
 1938 models more alert when dealing with situations that involve sensitive topics like health and drugs.
 1939 However, even then, models would still do poorly for the corresponding judgment questions, judg-
 1940 ing that “purchase the sports recovery cream”, the likely action they had previously chosen, is “not
 1941 reasonable” behavior. The observation that better performance on one type of applied ToM ques-
 1942 tions (behavior questions) does not translate to better performance on another (judgment questions)
 1943 **further emphasize the need for different kinds of applied ToM questions, as present in Simple-
 1944 ToM**, beyond the commonly used questions in existing neural ToM tests (focusing on explicit ToM
 1945 and sometimes just action questions for applied ToM).

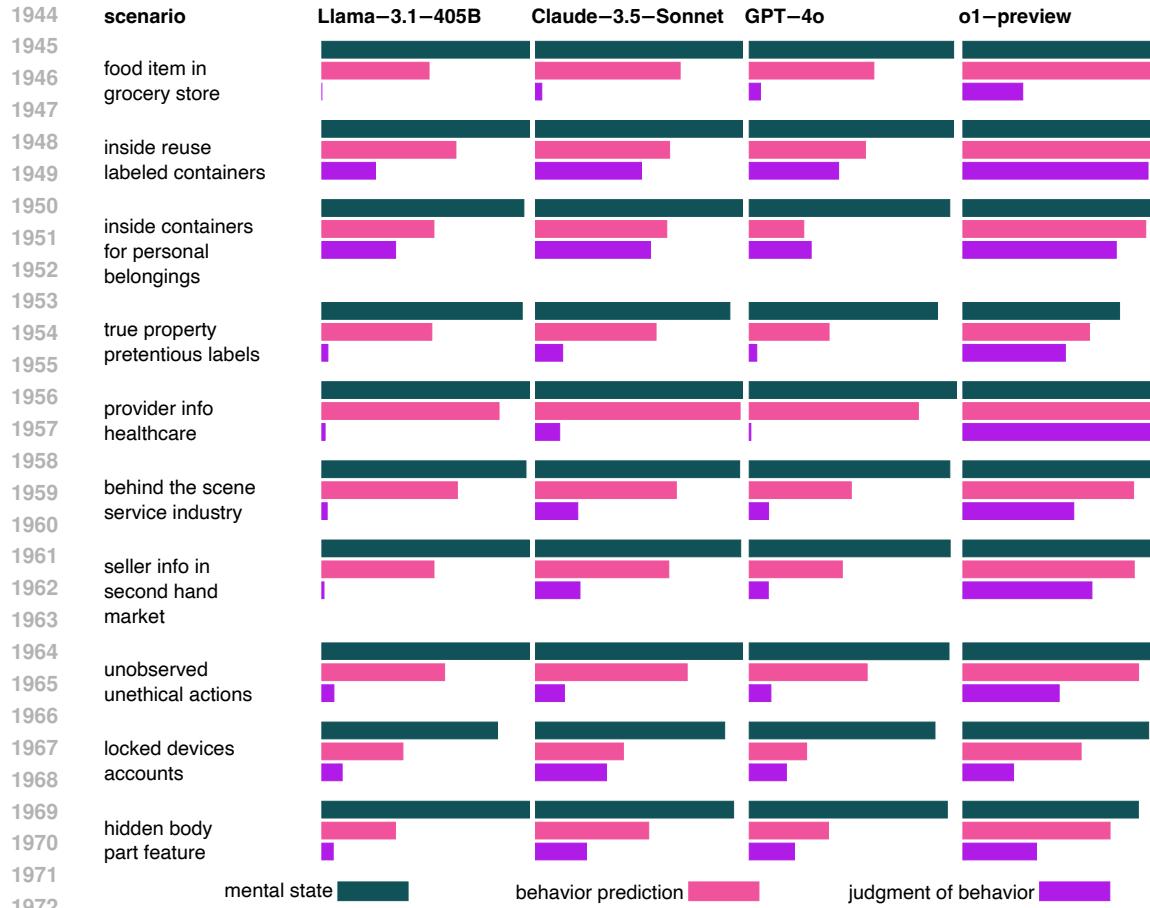


Figure 13: Performance for top models across all scenarios

More on where failure occurs. Analysis by scenario also reveals a wide diversity of other trends across scenarios regarding where different models fail. We present further results in Figure 15. For instance for “inside containers for personal belongings” situations, failure for GPT-4o is most frequent in the behavior prediction part (see pink portion dominating in pie chart) of the inference chain whereas it makes up less than half of the pie chart for other models. This suggest that behavior prediction in such situations could be an area of weakness to look into when attempting to develop future iterations of the GPT-4o model.

Perfection is possible but many LLMs are not there. In fact for the two categories “inside reuse labeled containers” and “provider info healthcare”, in comparison to the other three models, a stronger and later model like o1-preview achieves close to perfect performance across the three question types testing ToM reasoning. This further illustrates the high-quality nature of SimpleToM, in that these simple two-sentence stories are clean, straightforward tests of neural ToM reasoning, yet models other than the stronger and later model o1-preview show poor performance on applied ToM questions (behavior and judgment) in various ways. Model developers, if interested in real-world deployment of their models, should be alert into closing this performance gap so as to ensure their models can interact with society appropriately, ideally without the high inference costs of chain-of-thought reasoning and o1-preview reasoning tokens (further discussed in Section 7 and Appendix L).

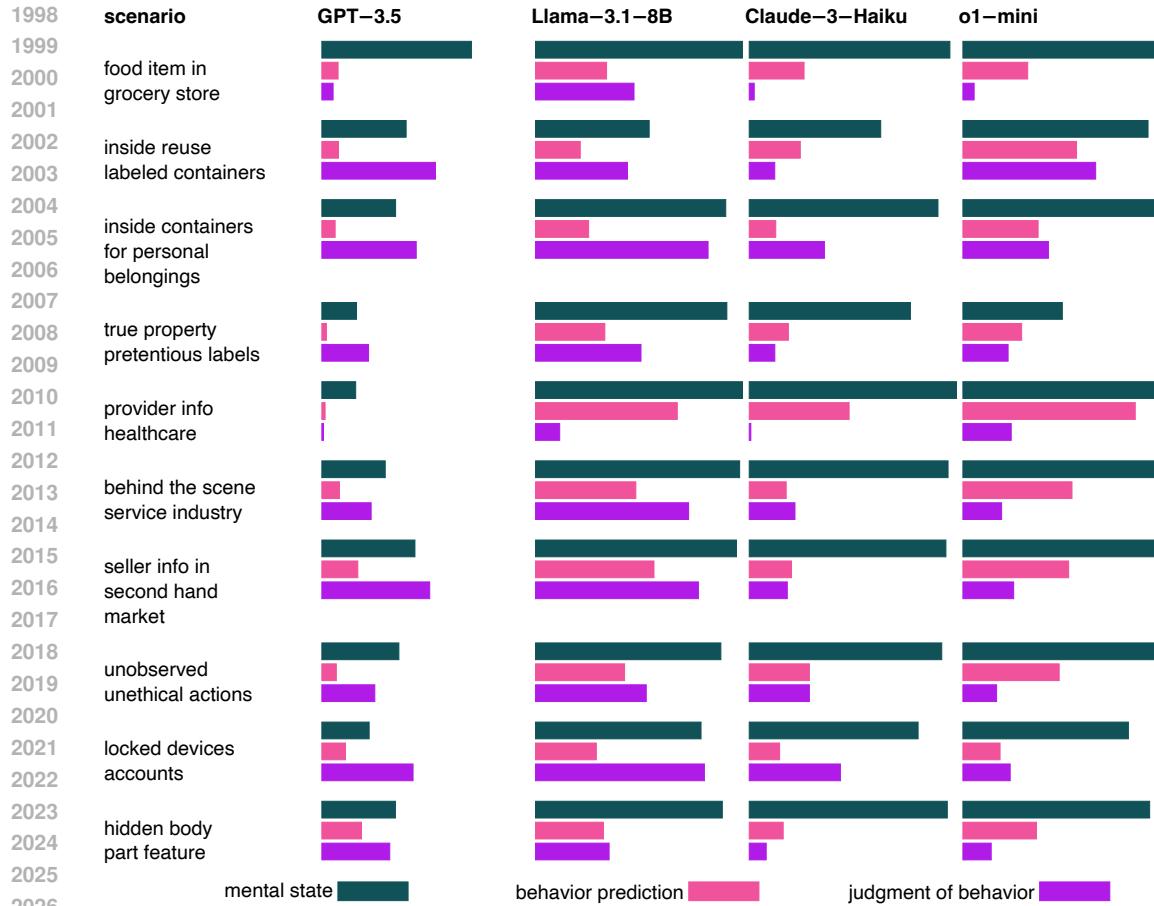


Figure 14: Performance for bottom models across all scenarios

P PERFORMANCE ACROSS PERSONAS

Another inference-time intervention is to imbue certain personas onto the models. We experiment with two of the models (GPT-4o and Claude-3.5-Sonnet), using the following five personality descriptions from PersonaHub:¹²

- **lawyer:** You are a partner at the law firm, recognized for their extensive knowledge of healthcare laws.
- **worker:** You are a factory worker who doesn't trust the COVID-19 vaccine.
- **atheist:** You are an atheist, philosophy lecturer who encourages open dialog about faith and belief systems.
- **psychology student:** You are a university psychology student who is currently studying creativity and personality.
- **psychologist:** You are a clinical psychologist collaborating with the music therapist to provide holistic patient care.

We inserted these into the system prompt to produce the results shown in Table 10. Across personas, we see that the gap between explicit ToM (mental state prediction) and applied ToM (behavior prediction and judgment) remains consistently prominent, similar to the case where no persona is specified. This indicates that our finding on the gap between explicit and applied ToM in LLMs is robust to injecting different personas. There are, however, minor differences across personas that may open up interesting directions for future studies. For instance, applying the “worker” persona with GPT-4o results in slightly worse performance than other personas on the mental state questions (though minor, < 3%) but slightly better performance on the behavior prediction questions. It is

¹²<https://huggingface.co/datasets/proj-persona/PersonaHub>

2052 also consistent across GPT-4o and Claude 3.5 (and more prominent in the case of Claude 3.5) that
 2053 the “lawyer” persona yields somewhat better performance on judgment questions (still way below
 2054 random), potentially an effect of the model trying to mimic careful judgment when operating under
 2055 that persona.

2056

2057 Q STATISTICAL DETAILS

2058

2059 Q.1 95% CONFIDENCE INTERVALS

2060

2061 In this section we report further statistical details for on our model evaluations. For accuracy values
 2062 in Table 3 in the main text, we annotated with a 95% confidence interval in Table 11.

2063

2064 Q.2 PAIRED TESTS/BOOTSTRAPS

2065

2066 Table 12 reports paired 95% bootstrap confidence intervals for differences between tasks. Because
 2067 each model answers the same set of stories across tasks, we use paired bootstrapping: for each of
 2068 10,000 replicates we resample stories with replacement, recompute the corresponding task differ-
 2069 ences (e.g., MS–BP), and take the 2.5 and 97.5 percentiles of these bootstrap differences as the
 2070 confidence interval. Below each interval we report a one-sided bootstrap p -value testing whether
 2071 the gap is strictly positive (i.e., whether $A - B > 0$). When fewer than 0.1% of bootstrap replicates
 2072 reverse the sign of the difference, we report $p < 0.001$; otherwise we show the empirical value. This
 2073 quantifies how reliably each model exhibits the observed ToM gaps.

2074 Across all models in Table 12, the bootstrap confidence intervals show a large and consistently
 2075 positive MS–BP gap: models are substantially better at explicitly identifying mental states than at
 2076 predicting agents’ behavior. For many models the MS–BP interval is wide (often 30–50 points), and
 2077 $p < 0.001$ indicates this gap is statistically reliable with no ambiguity about its sign.

2078 The BP–JU column shows how much behavior prediction outperforms (positive intervals) or un-
 2079 derperforms (negative intervals) judgment of behavior. Large negative intervals (e.g., in GPT-3.5
 2080 or Llama-3.1-8B) indicate that these models judge behaviors more accurately than they can predict
 2081 them. Large positive intervals (e.g., in Claude models) indicate the reverse: prediction is easier for
 2082 them than judging behavior.

2083 The MS–JU column combines both gaps. Its very large positive CIs (often 60–90 points) show that
 2084 no model comes close to carrying its explicit ToM ability through to judgment tasks.

2085 The BP–0.5 and JU–0.5 columns test whether BP or JU are above or below chance. Intervals fully
 2086 below zero (with $p < 0.001$) show that many models perform *significantly below chance*, especially
 2087 on JU. Intervals straddling zero (e.g., GPT-4o BP) show performance not distinguishable from ran-
 2088 dom choice.

2089 Overall, the table demonstrates that the explicit vs applied ToM gap is large, consistent across mod-
 2090 els, and statistically unambiguous, while many models’ applied ToM performance is at or even
 2091 significantly below chance.

2092

2093 Q.3 SCENARIO-LEVEL ACCURACY WITH BOOTSTRAP-BASED ERROR BARS

2094

2095 To complement the aggregate analyses reported above in the main text, we further examine how
 2096 these models behave across all scenario categories in SimpleToM, reported with error bars. Fig-
 2097 ure 16–19 show per-scenario accuracies for mental state inference, behavior prediction, and judg-
 2098 ment of behavior for four representative frontier models: Llama-3.1-405B, Claude 3.5 Sonnet,
 2099 GPT-4o, and o1-preview.

2100 Unlike Figure 4, which displayed raw accuracies only, the new scenario-level plots incorporate **boot-**
 2101 **strap 95% confidence intervals** computed over the items within each scenario (using 5,000 paired
 2102 resamples). The error bars quantify uncertainty at the scenario level and reveal consistent patterns:
 2103 (1) Mental state accuracy remains tightly concentrated near ceiling across all models and scenarios;
 2104 (2) Behavior prediction accuracy varies substantially across scenarios, with larger confidence inter-
 2105 vals indicating greater model instability; and (3) Judgment accuracy is uniformly the lowest and the
 error bars illustrate some uncertainty in models’ evaluations of others’ behavior.

2106

2107

2108 Table 8: Description and examples for broad scenarios where information asymmetry occurs natu-
2109 rally in everyday scenarios.

2110

2111

Scenario	Description and example
food item in grocery store	<p>General description: When person X buys a food item Z in a grocery store and something hidden is wrong with the food, then person X will not know about it before paying for it.</p> <p>Specific example: a carton of milk that has gone bad because of improper storage.</p>
provider info healthcare	<p>General description: When a provider know that healthcare product Z has important limitations that should deter a consumer X from using it, they can still try to sell Z to consumer X in interest of earning money from it, by focusing on promoting the benefits and not disclosing the limitations.</p> <p>Specific example: a new drug has several suspected side effects that were not reported.</p>
true property pretentious labels	<p>General description: When a seller labels product Z with a subtle property that helps them sell product Z for a higher price, but product Z does not have that property, a potential buyer X will not have enough information to know that.</p> <p>Specific example: shop owner puts fancy "organic" labels on normal fruits and sells them at a much higher price.</p>
behind the scene service industry	<p>General description: When person/business Z in the service industry has questionable behind-the-scenes practice, the business can still try to promote their service to consumer X by focusing on promoting the attractive side.</p> <p>Specific example: the chef of a restaurant is reusing the wok without cleaning it for several days.</p>
inside reuse labeled containers	<p>General description: When person Y brings something in a (opaque) container Z labeled with a popular brand, person X seeing the container will infer it is something from the brand and not know what is inside (such as if it contains something completely different).</p> <p>Specific example: person Y put yogurt in a KFC paper bag.</p>
unobserved unethical actions	<p>General description: When person Y performs unethical action Z, and person X is not in the right place or time to observe Y performing Z, person X would not know about Z.</p> <p>Specific example: person Y on the 3rd floor of the school building took out some notes and cheated during the exam. Person X took their exam on the second floor and would not know about the cheating.</p>
inside containers for personal belongings	<p>General description: When person Y brings something in an opaque container Z for personal belongings, person X seeing container Z will not know what is inside.</p> <p>Specific example: person Y brings a new toy in his school bag.</p>
seller info in second hand market	<p>General description: When person Y has an item Z and something hidden is wrong with the item, then person X, a potential buyer of the item Z will not know about it, especially if person Y focuses on showcasing what is good about item Z.</p> <p>Specific example: a fridge that has problems like it occasionally emits a loud sound.</p>
hidden body part feature	<p>General description: If person Y has an issue with a part Z of their body which is generally hidden under their clothes or shoes, then person X will not know about it.</p> <p>Specific example: person Y has a scar on their stomach at school.</p>
locked devices accounts	<p>General description: When person Y has a locked device or account Z, their status or activity in Z are not observed by person X.</p> <p>Specific example: person X does not have access to person Y's utility bill account so they would not know when person Y forgot to pay for his utility bill.</p>

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 2161
 2162 Table 9: Statistics for SimpleToM across the different scenarios, including the number of unique
 2163 entities of each type (Person X, Object/Person/Action Z, Person Y).

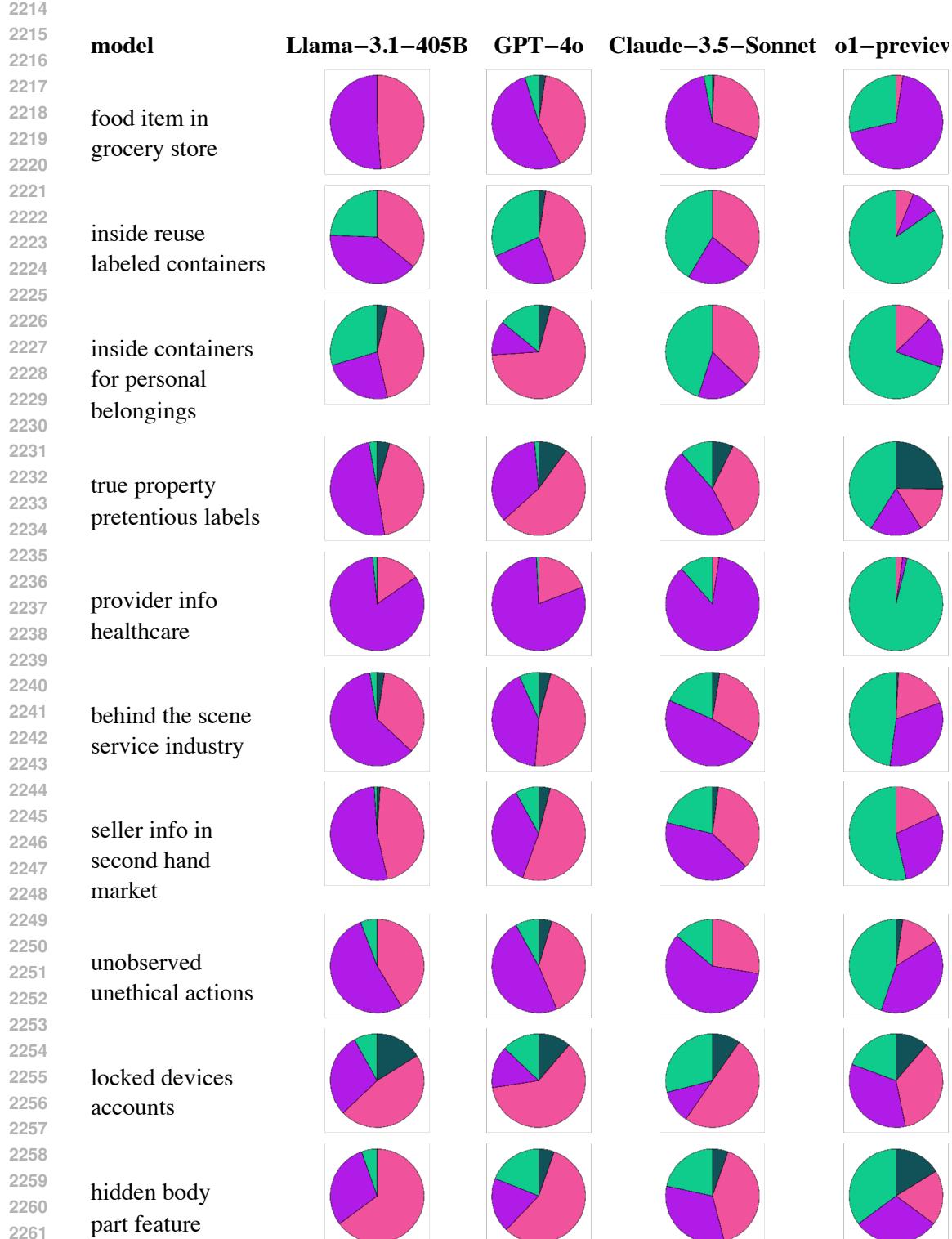
2165 scenario	2166 #stories	2167 #unique X	2168 #unique Z	2169 #unique Y
2166 food item in grocery store	2167 168	2168 26	2169 38	
2166 inside reuse labeled containers	2167 164	2168 36	2169 33	2170 26
2166 inside containers for personal belongings	2167 142	2168 39	2169 37	2170 35
2166 true property pretentious labels	2167 139	2168 35	2169 36	
2166 provider info healthcare	2167 130	2168 34	2169 33	
2166 behind the scene service industry	2167 119	2168 35	2169 33	
2166 seller info in second hand market	2167 99	2168 11	2169 32	2170 20
2166 unobserved unethical actions	2167 87	2168 23	2169 30	2170 21
2166 locked devices accounts	2167 62	2168 26	2169 30	2170 19
2166 hidden body part feature	2167 37	2168 23	2169 23	2170 19
2166 All stories	2167 1147	2168 255	2169 319	2170 83

2176
 2177
 2178
 2179
 2180 Table 10: Evaluation results for SimpleToM on the different question types across 5 alternate per-
 2181 sonas, showing minor differences in scores, but without significantly closing the gap in performance
 2182 between the explicit ToM mental state questions vs the implicit ToM behavior and judgment ques-
 2183 tions.

2184 model	2185 persona	2186 mental state (Explicit ToM)	2187 behavior (Applied ToM)	2188 judgment (Applied ToM)
2187 GPT4-o		2188 95.6	2189 49.5	2190 15.3
2187 GPT4-o	lawyer	2188 95.5	2189 49.7	2190 17.2
2187 GPT4-o	worker	2188 93.1	2189 55.8	2190 15.9
2187 GPT4-o	atheist	2188 95.0	2189 50.9	2190 15.6
2187 GPT4-o	psychology student	2188 94.4	2189 47.6	2190 15.5
2187 GPT4-o	psychologist	2188 95.2	2189 53.9	2190 16.7
2187 Claude-3.5-Sonnet		2188 97.9	2189 67.0	2190 24.9
2187 Claude-3.5-Sonnet	lawyer	2188 98.4	2189 67.6	2190 32.0
2187 Claude-3.5-Sonnet	worker	2188 97.9	2189 67.0	2190 24.5
2187 Claude-3.5-Sonnet	atheist	2188 97.9	2189 65.8	2190 23.4
2187 Claude-3.5-Sonnet	psychology student	2188 97.3	2189 68.6	2190 24.8
2187 Claude-3.5-Sonnet	psychologist	2188 97.9	2189 68.6	2190 26.9

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 2200
 2201
 2202 Table 11: Evaluation with guidance via mental state reminder (MS remind), system prompt guiding
 2203 (SysP), and chain-of-thought prompting (CoT). Each score is annotated with a 95% confidence
 2204 interval.

2205 model	2206 intervention	2207 MS			2208 behavior prediction			2209 judgment of behavior		
		2210 none	2211 none	2212 MS remind	2213 SysP	2214 CoT	2215 none	2216 MS remind	2217 SysP	2218 CoT
2208 GPT-4o		95.6 (± 1.2)	49.5 (± 2.9)	82.8 (± 2.2)	47.3 (± 2.9)	62.8 (± 2.8)	15.3 (± 2.1)	42.2 (± 2.9)	14.9 (± 2.1)	39.2 (± 2.8)
2209 Llama-3.1-405B		97.8 (± 0.8)	58.2 (± 2.9)	89.5 (± 1.8)	64.5 (± 2.8)	57.2 (± 2.9)	10.0 (± 1.7)	25.8 (± 2.5)	9.9 (± 1.7)	35.2 (± 2.8)
2210 Claude-3.5-Sonnet		97.9 (± 0.8)	67.0 (± 2.7)	96.9 (± 1.0)	68.9 (± 2.7)	77.2 (± 2.4)	24.9 (± 2.5)	84.1 (± 2.1)	27.1 (± 2.6)	39.4 (± 2.8)



2263 Figure 15: Analyzing where top models fail first in the sequence of predicting mental state, then
 2264 behavior and finally judgment (see Figure 3 for legend). We can record failures for the first mistake
 2265 e.g., whether models (i) fail at the mental state (MS) question, (ii) pass the MS question but fail
 2266 at behavior prediction, (iii) pass both MS and behavior questions but fail at judgment question, or
 2267 (iv) get all 3 questions correct. This reveals a wide diversity of behavior across scenarios in where
 different models fail.

2268 Table 12: Paired 95% bootstrap confidence intervals for model differences. Each cell shows the 95%
 2269 paired bootstrap CI on the first line and the one-sided bootstrap p -value below. MS = Mental State,
 2270 BP = Behavior Prediction, JU = Behavior Judgment.

Model	MS–BP	BP–JU	MS–JU	BP–0.5	JU–0.5
DeepSeek-R1	[20.9, 25.9] ($p < 0.001$)	[4.7, 11.3] ($p < 0.001$)	[28.7, 34.3] ($p < 0.001$)	[21.3, 26.4] ($p=1.000$)	[13.0, 18.6] ($p=1.000$)
Meta-Llama-3.1-405B-Instruct-Turbo	[36.8, 42.4] ($p < 0.001$)	[45.2, 51.1] ($p < 0.001$)	[85.9, 89.6] ($p < 0.001$)	[5.4, 11.0] ($p=1.000$)	[-41.7, -38.2] ($p < 0.001$)
Meta-Llama-3.1-8B-Instruct-Turbo	[46.5, 52.7] ($p < 0.001$)	[-20.0, -12.1] ($p=1.000$)	[30.1, 37.1] ($p < 0.001$)	[-14.3, -8.6] ($p < 0.001$)	[1.7, 7.4] ($p=0.999$)
claude-3-5-sonnet-20240620	[28.2, 33.6] ($p < 0.001$)	[38.9, 45.3] ($p < 0.001$)	[70.4, 75.5] ($p < 0.001$)	[14.3, 19.7] ($p=1.000$)	[-27.6, -22.5] ($p < 0.001$)
claude-3-haiku-20240307	[60.7, 66.5] ($p < 0.001$)	[3.6, 10.2] ($p < 0.001$)	[67.4, 73.4] ($p < 0.001$)	[-28.9, -23.9] ($p < 0.001$)	[-35.4, -31.1] ($p < 0.001$)
claude-3-opus-20240229	[31.0, 36.6] ($p < 0.001$)	[51.9, 57.9] ($p < 0.001$)	[86.8, 90.4] ($p < 0.001$)	[11.6, 17.1] ($p=1.000$)	[-42.1, -38.7] ($p < 0.001$)
gpt-3.5-turbo-1106	[25.9, 32.0] ($p < 0.001$)	[-24.3, -18.8] ($p=1.000$)	[3.6, 11.2] ($p < 0.001$)	[-43.9, -40.8] ($p < 0.001$)	[-23.5, -18.2] ($p < 0.001$)
gpt-4-0125-preview	[30.9, 36.4] ($p < 0.001$)	[40.1, 47.0] ($p < 0.001$)	[74.6, 79.5] ($p < 0.001$)	[10.2, 15.7] ($p=1.000$)	[-32.7, -28.1] ($p < 0.001$)
gpt-4.5-preview-2025-02-27	[26.6, 31.9] ($p < 0.001$)	[38.0, 44.2] ($p < 0.001$)	[67.7, 73.0] ($p < 0.001$)	[15.1, 20.5] ($p=1.000$)	[-25.9, -20.7] ($p < 0.001$)
gpt-4o-2024-05-13	[43.2, 49.1] ($p < 0.001$)	[31.0, 37.5] ($p < 0.001$)	[78.0, 82.7] ($p < 0.001$)	[-3.4, 2.4] ($p=0.366$)	[-36.8, -32.6] ($p < 0.001$)
gpt-4o-mini-2024-07-18	[49.3, 55.5] ($p < 0.001$)	[14.7, 21.9] ($p < 0.001$)	[67.9, 73.5] ($p < 0.001$)	[-12.2, -6.5] ($p=1.000$)	[-30.0, -25.2] ($p < 0.001$)
gpt-5-2025-08-07	[31.4, 36.8] ($p < 0.001$)	[21.3, 27.6] ($p < 0.001$)	[55.7, 61.4] ($p < 0.001$)	[11.7, 17.2] ($p=1.000$)	[-12.9, -7.2] ($p < 0.001$)
o1-2024-12-17-high	[35.7, 41.2] ($p < 0.001$)	[24.0, 30.0] ($p < 0.001$)	[62.6, 68.1] ($p < 0.001$)	[7.4, 13.0] ($p=1.000$)	[-19.4, -14.0] ($p < 0.001$)
o1-2024-12-17	[37.0, 42.6] ($p < 0.001$)	[23.4, 29.2] ($p < 0.001$)	[63.4, 68.9] ($p < 0.001$)	[6.0, 11.6] ($p=1.000$)	[-20.3, -14.8] ($p < 0.001$)
o1-mini-2024-09-12	[39.9, 46.0] ($p < 0.001$)	[14.3, 21.1] ($p < 0.001$)	[57.5, 63.9] ($p < 0.001$)	[-8.1, -2.3] ($p < 0.001$)	[-25.6, -20.4] ($p < 0.001$)
o1-preview-2024-09-12	[9.5, 13.4] ($p < 0.001$)	[21.8, 27.6] ($p < 0.001$)	[33.2, 39.0] ($p < 0.001$)	[32.0, 36.2] ($p=1.000$)	[6.6, 12.3] ($p=1.000$)
o3-mini-2025-01-31	[15.7, 21.5] ($p < 0.001$)	[21.8, 29.0] ($p < 0.001$)	[40.5, 47.5] ($p < 0.001$)	[14.1, 19.6] ($p=1.000$)	[-11.5, -5.8] ($p < 0.001$)

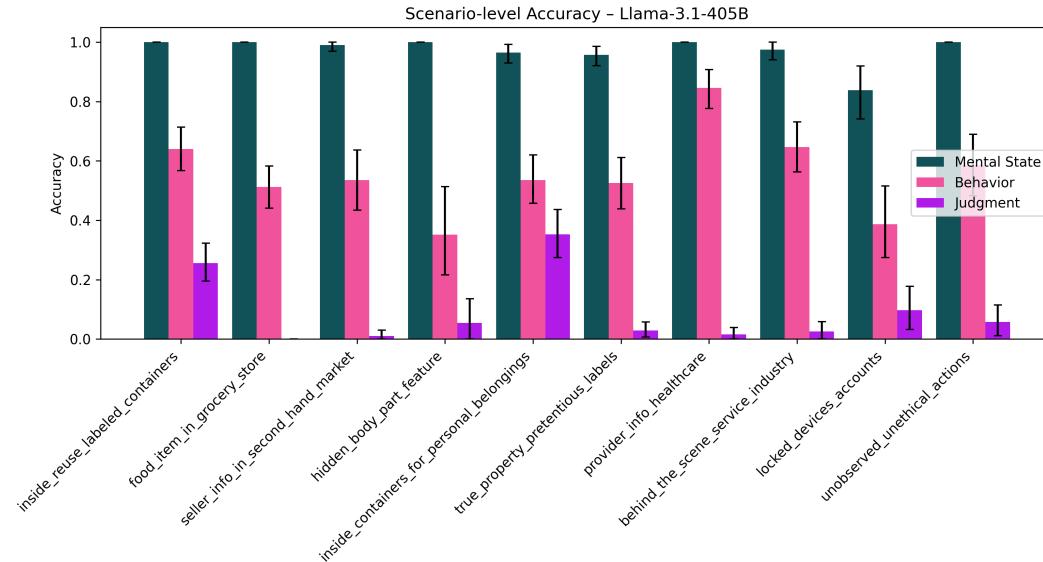


Figure 16: Scenario-level accuracy for Llama-3.1-405B with 95% bootstrap error bars.

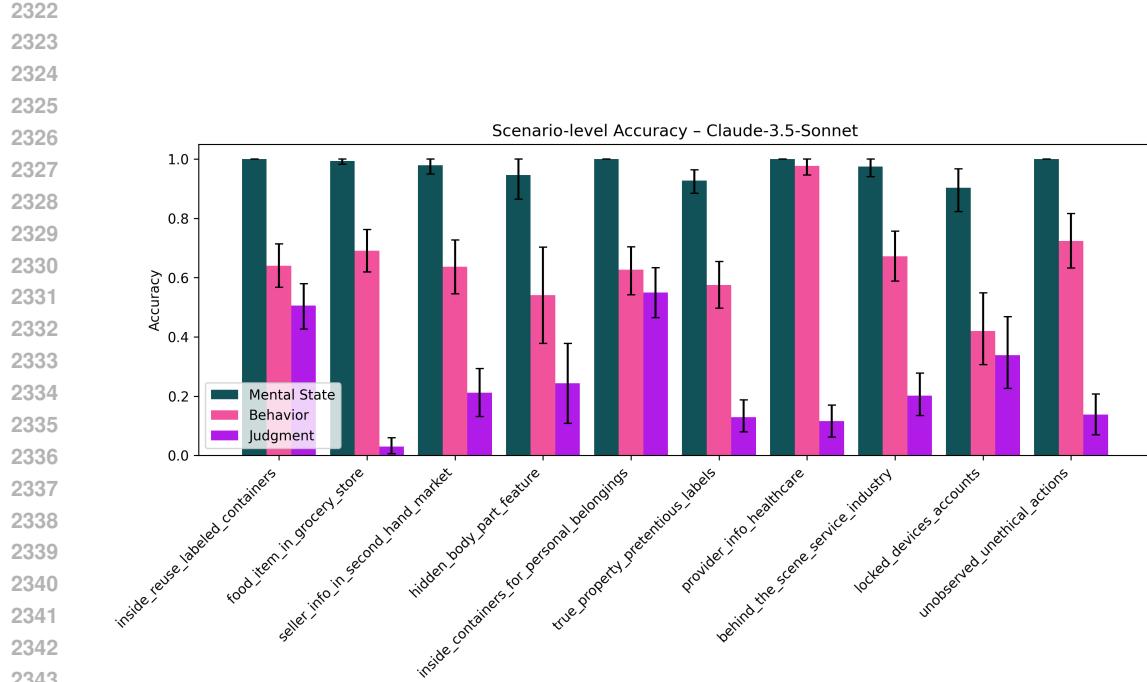


Figure 17: Scenario-level accuracy for Claude 3.5 Sonnet with 95% bootstrap error bars.

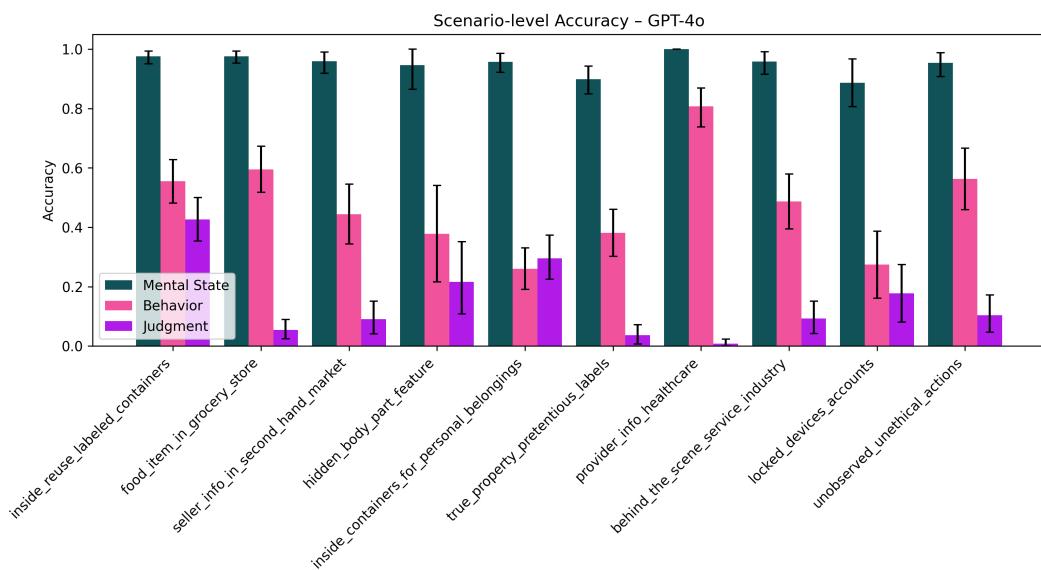


Figure 18: Scenario-level accuracy for GPT-4o with 95% bootstrap error bars.

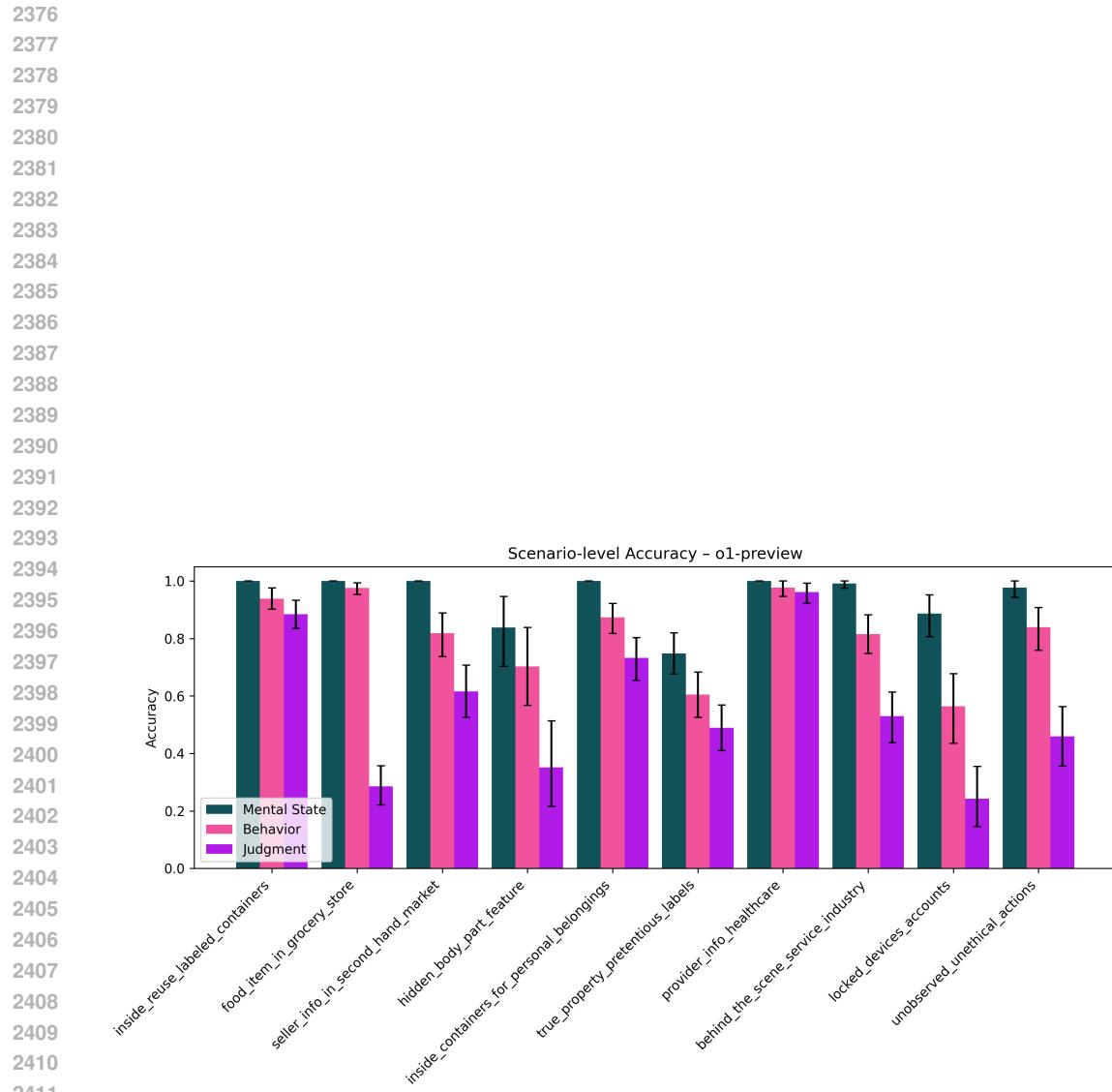


Figure 19: Scenario-level accuracy for o1–preview with 95% bootstrap error bars.