

Infusing Theory of Mind into Socially Intelligent LLM Agents

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Abstract

Theory of Mind (ToM)—an understanding of the mental states of others—is a key aspect of human social intelligence, yet, chatbots and LLM-based social agents do not typically integrate it. In this work, we demonstrate that LLMs that explicitly use ToM get better at dialogue, achieving goals more effectively. After showing that simply prompting models to generate mental states between dialogue turns already provides significant benefit, we further introduce ToMAgent (TOMA), a ToM-focused dialogue agent. TOMA is trained by pairing ToM with dialogue lookahead to produce mental states that are maximally useful for achieving dialogue goals. Experiments on the Sotopia interactive social evaluation benchmark demonstrate the effectiveness of our method over a range of baselines. Extensive analysis shows that TOMA exhibits more strategic, goal-oriented reasoning behaviors, which enable long-horizon adaptation, while maintaining better relationships with their partners. Our results suggest a step forward in integrating ToM for building socially intelligent LLM agents. ¹

1 Introduction

Success in social interactions – defined by goal achievement, adherence to social norms, and more – depends not just on expressing our own intentions and beliefs, but also on understanding our conversation partners. Theory of Mind (ToM), the cognitive ability to understand the mental states of others (Premack and Woodruff, 1978; Baron-Cohen et al., 1985), captures this intuition and allows social reasoning and strategic behavior (Apperly and Butterfill, 2009). Here, we study whether ToM can serve as a similarly powerful element in social LLM agents.

The extent to which LLMs already possess ToM is debatable (Kosinski, 2024; Shapira et al., 2024),

despite the deployment of LLMs in settings where understanding the user is crucial (e.g. job interviews, customer service). Methods for improving LLMs’ ToM abilities range from chain-of-thought prompting (Wilf et al., 2024; Shinoda et al., 2025), through neuro-symbolic methods that combine LLMs with symbolic belief tracking (Sclar et al., 2023), to Bayesian Inverse Planning (Ying et al., 2023), and inference-time hypothesis generation (Kim et al., 2025). However, past work on ToM for LLMs typically evaluates this ability directly on QA setups (Kim et al., 2023; Chen et al., 2024), rather than its usefulness in social situations. Meanwhile, existing research in interactive social environments like Sotopia (Zhou et al., 2024) has largely focused on training models to generate utterances that lead to successful conversations (Kong et al., 2025; Yu et al., 2025), overlooking the role of explicit mental state modeling.

In this work, we address the question of *how to equip LLMs with Theory of Mind abilities that can effectively improve their social reasoning*. We demonstrate that even simply prompting LLMs to generate mental states between dialogue turns can significantly contribute to goal achievement. To maximize this benefit, we propose ToMAgent (TOMA), a method for goal-oriented social reasoning in dialogues that combines ToM predictions with conversation outcome prediction to select the best trajectory for training. As illustrated in Figure 1, given a social scenario such as “Two friends are camping in the cold and there is only one blanket” and opposing agent goals (e.g., Agent₁ wants to keep it for themselves while Agent₂ wants to share), the target agent (Agent₁) is asked to (i) make multiple hypotheses about the other agent’s mental states, (ii) generate the corresponding next utterances, and (iii) simulate the remaining dialogue and estimate the likelihood that each dialogue leads to goal completion. We then use the most successful conversations to fine-tune the same LLM

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¹Code, training data, and models are available at [GitHub](#).

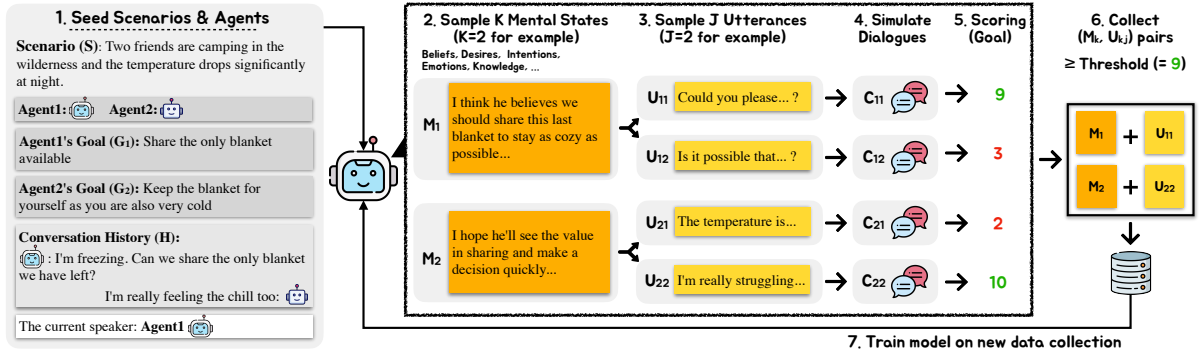


Figure 1: Overview of TOMA. We sample scenarios, goals, and conversation histories from Sotopia-Pi (Step 1), generate candidate mental state–utterance pairs and simulate dialogues (Steps 2–4), evaluate goal achievement to select high-utility pairs (Step 5), and train the model after collecting these training pairs (Steps 6–7).

to generate the partner’s mental states (e.g., they are cold and uncomfortable) and the strategic utterances that are likely to result in goal achievement (e.g., suggesting a compromise).

TOMA is evaluated on the Sotopia dataset (Zhou et al., 2024; Wang et al., 2024), an open-ended social reasoning environment that includes diverse goal-oriented social scenarios such as collaboration, negotiation, persuasion, and competition. Our experimental results demonstrate that TOMA achieves score improvements by up to 18.9% and 6.9% compared to the best base model variant for Qwen2.5-3B and Qwen2.5-7B, respectively, and is also competitive with GPT-5 nano. Furthermore, we provide a comprehensive analysis of our results, including the success and failure factors across different scenarios and the ToM dimensions that are generated by the model. The analysis shows that TOMA exhibits more strategic, goal-oriented, and long-horizon behavior than the baselines, while also achieving better personal relationships with the partner. Our findings highlight that social reasoning in LLMs cannot be achieved through optimizing their performance on general reasoning benchmarks (Leaderboard, 2025) alone; it requires explicit modeling of mental states to enable safe, fair, and effective interactions with humans.

2 Methodology

In this section, we introduce TOMA, a look-ahead training framework that improves agents’ ToM ability in social interactions to achieve their goals. Conditioned on a scenario (e.g., two friends are camping in the cold and there is only one blanket in Figure 1) and the agents’ private goals (e.g., sharing the only blanket available vs. keeping the blanket for yourself), the goal is to reach a mutually agreeable solution, such as taking turns or sharing the

blanket, through dialogue.

Our proposed training protocol consists of generating training examples and fine-tuning an LLM-based agent, as illustrated in Figure 1. First, we sample conversation contexts (§2.1). At each step of the dialogue, we use an LLM to first elicit multiple ToM hypotheses corresponding to the mental state of each agent (i.e., self and first-order beliefs), and then generate an appropriate utterance conditioned on these mental states (§2.2). To identify useful mental states and utterances that eventually contribute to goal achievement, we run short-horizon simulations and keep pairs that achieve the highest score on the simulated conversations (§2.2). Finally, we use the identified set of mental states and utterance pairs as training examples for fine-tuning the LLM to generate both the latent mental states and utterances (§2.3).

2.1 Sampling Conversations to Seed Scenarios and Agents

To train models capable of socially grounded, goal-oriented reasoning in diverse contexts, it is imperative to use data that captures the complexity of real-world social interactions. To this end, we adopt the Sotopia-Pi dataset (Wang et al., 2024), which provides a diverse set of scenarios and social goals, allowing us to simulate complex social interactions during training. We first randomly sample 500 episodes from Sotopia-Pi, where each episode provides a social scenario, two agents with their own goals, and a multi-turn dialogue between them. Then, for each scenario, we randomly sample two conversations provided by Sotopia-Pi and truncate each to at most four turns to ensure the context is early enough that the social goals have not yet been achieved. We denote each resulting instance, comprising a scenario, agents’ social goals, and

a partial conversation history, as H , which is referred to as the *context* in subsequent steps. These contexts serve as the default input set for eliciting useful mental states and utterances.

2.2 Generating and Scoring ToM Hypotheses and Utterances

The goal of this phase is to generate plausible mental states and utterances that help an agent advance its own social goal, which can be used to train goal-oriented ToM-aware agents. Specifically, we ask the target model (Agent₁ in Figure 1), which is the model to be trained, to generate its own latent ToM states, produce corresponding utterances, and utilize these pairs for training.

Exploring mental states and utterances. The first key steps (2–3 in Figure 1) toward socially intelligent behavior is to explore a range of plausible mental states and corresponding utterances that align with the agent’s social goals and conversational context. For this purpose, from each context H , which includes the scenario, the agents’ private social goals, and the partial conversation history up to that point, we prompt an LM_{target} to generate K mental state hypotheses, where each hypothesis may consist of multiple sentences capturing different aspects of the current (target) agent’s internal state: $m_k \sim \text{LM}_{\text{target}}(m | H)$. The model is asked to ensure that each generated hypothesis covers at least three out of the five ToM dimensions: *beliefs*, *desires*, *intentions*, *emotions*, and *knowledge*. For each mental state hypothesis m_k , we sample J utterances: $u_{k,j} \sim \text{LM}_{\text{target}}(u | m_k, H)$. This gives us a candidate set of mental state and utterance pairs $\mathcal{C}_H = \{(m_k, u_{k,j})\}_{k=1..K, j=1..J}$.

Running simulations to evaluate downstream utility. To identify the most useful mental state and utterance pairs for training that most effectively contribute to successful goal achievement, we perform a short-horizon simulation to look ahead into the future trajectory of the dialogue and assess how each pair influences the goal achievement of agents throughout the conversation (Steps 4–5 in Figure 1). In the first turn, the target agent produces utterance $u_{k,j}$ conditioned on the mental state hypothesis m_k and the context H . Then the conversation continues for up to four future turns, simulating the partner agent using LM_{partner}. Once the simulation is done, we compute the goal achievement score (0–10) for each agent, S_{target} and S_{partner} , reflecting the degree to which each

agent successfully advanced its objectives. Since a successful conversation is supposed to contribute to both agents’ goals, the average goal score is calculated: $\hat{S}(h, m_k, u_{k,j}) = \frac{1}{2}(S_{\text{target}} + S_{\text{partner}})$. We retain all pairs with an average score ≥ 9 . If none meet this threshold, we keep the top-scoring pair. The resulting high-scoring pairs form a training set that we use for fine-tuning. See Appendix E for the prompts and the training instance format.

2.3 Fine-Tuning on ToM States & Utterances

To instill Theory of Mind reasoning into the model, we fine-tune it on high-scoring mental state and utterance pairs identified through dialogue simulation that are maximally useful to advance their goals (Step 7 in Figure 1). From each selected pair (m^*, u^*) and its context H (i.e., scenario, private goal, and dialogue history), we construct two types of training examples: one where the model is prompted with H and trained to generate m^* (i.e., *mental-state prediction*), and another where the model is prompted with both H and m^* to generate u^* (i.e., *utterance prediction*). Together, we train the model to align with the joint behavior $P(u, m | H) = P(u | m, H) \cdot P(m | H)$ that led to high goal scores. We finetune the model LM_{target} using a standard cross-entropy loss over next-token prediction. The resulting objective is $\mathcal{L}_{\text{CE}}(\phi) = \mathbb{E}_{(H, m^*, u^*) \sim \mathcal{D}^*} [\text{CE}(m^*, \phi(H)) + \text{CE}(u^*, \phi(H, m^*))] = -\log P_\phi(m^* | H) - \log P_\phi(u^* | H, m^*)$, where $\text{CE}(y, \phi(x))$ denotes the token-level cross-entropy loss for target y given input x under model ϕ . This way, the model learns to associate contexts with latent mental states and utterances that were empirically effective during simulation. This implicitly improves its internal mechanism over $P(m | H)$ and $P(u | m, H)$, aligning them to achieve their goals in various social situations.

3 Experimental Setup

We follow the setup defined in Sotopia (Zhou et al., 2024). Each instance in Sotopia provides the scenario for the current social interaction between two agents, as well as their names and social goals. Models evaluated on Sotopia take the role of one agent, and they are tasked with having a dialogue with the other agent that results in achieving their own social goals. We describe the evaluation setup (§3.1) and training settings (§3.2). See Appendices C and E for additional details about the experiments.

3.1 Evaluation

Data. We adopt Sotopia-Eval (Zhou et al., 2024), which provides multiple social scenarios for the agents to simulate conversations dynamically. We use both the all and hard sets to evaluate models. The all set includes 90 scenarios combined with 5 agent pairs, resulting in 450 testing instances. Each pair among the five shares the same scenario description and agent goals, but the agent names and profiles are different. The hard set consists of 14 scenarios that are challenging to GPT-4 (Achiam et al., 2023), yielding 70 testing instances.

Metrics. We follow Sotopia-Eval (Zhou et al., 2024), a suite of multi-dimensional evaluation metrics, and use LLM-as-a-Judge (Gu et al., 2024) to assess an entire conversation. We focus on the following central criteria from the original setup: (1) **Goal**: the extent to which the agent achieved their goals (0–10); (2) **Relationship** (Rel): whether the interactions between the agents help preserve or enhance their personal relationships prior to the conversation (-5–5); and (3) **Knowledge** (Know): whether the agent gained new and important information through the interaction (0–10). The LLM judge outputs scores and rationales per dimension and agent. We use GPT-5-mini (OpenAI, 2025) as the primary evaluator. We report single-run performance as GPT-5-mini results were highly stable, with average standard deviations of 0.04 (relationship), 0.29 (knowledge), and 0.13 (goal) across 3 runs.

Partner Agent. We follow the original Sotopia evaluation setup which evaluates both agents on their goal achievement and social awareness, and reports the average scores of the two agents. In this “Self-Play” setup, both agents are instantiated as a model with the same complexity (e.g., base with base, TOMA with TOMA, etc.).

Baselines. We consider two base settings as follows: (1) **Base**: Using the vanilla language model (without fine-tuning), as a lower bound for the LLMs’ ability to hold a social dialogue; and (2) **Base+MS**: where we apply a two-step prompt to the base model. We first generate mental states based on the context and then generate an utterance conditioned on the context and mental states. This setup quantifies both the quality and the utility of the mental states generated by the base model.

3.2 Training

Data. We use the scenarios and the agents’ names and social goals from Sotopia-Pi (Wang et al., 2024) to seed our conversations, as shown in Figure 1, Step 1. We instantiate each agent with an instance of the pre-trained LLM (which we will later fine-tune on the training set described here). Then, we generate a conversation between the two agents using the simulation protocol provided by Sotopia, which defines the action types and schedules the agents to speak iteratively, and modify it to introduce mental states as a latent variable. Before generating each utterance, we prompt the agent to generate or update their own mental states and their first-order beliefs about the mental states of the other agent. Based on the hyperparameter analysis in Appendix B, we select $K = 2$ mental state hypotheses and $J = 2$ utterance candidates per hypothesis as an effective trade-off between performance and computational cost.

Models. Qwen2.5-3B, Qwen2.5-7B (Qwen, 2024a), and LLaMA3.1-8B (Dubey et al., 2024) are adopted as the backbone LLMs. We use a 4-bit quantized version of Qwen2.5-14B as LM_{partner} to ensure the partner generates reasonable utterances in simulations independent of the model size being trained. Finally, Gemini-Flash (Comanici et al., 2025) is used to score the simulated conversations.

Fine-tuning. Utilizing the paired utterances (Utr) and mental states (MS) from the generated multi-turn conversations, we conduct supervised fine-tuning (Pareja et al., 2025) over low-rank adapters (Hu et al., 2022) of small language models (i.e., Qwen2.5-3B and Qwen2.5-7B) with the data obtained in §2.2. We consider the following three training objectives: (1) **FT+Utr**: Fine-tuning models only on utterance generation, ablating the mental states supervision to assess its contribution to the conversation success; (2) **FT+MS**: Fine-tuning models to generate mental states, ablating the utterance generation to assess its contribution to the conversation success; and (3) **FT+MS+Utr** (TOMA): Fine-tuning models on both utterance generation and mental states alignment, as explained in §2.3. For the evaluation of **FT+MS** and TOMA, the model generates mental states first and then produces the utterances to respect the causal constraint between the two.

Method	Qwen2.5-3B				Qwen2.5-7B				Llama3.1-8B			
	Rel	Know	Goal	Avg.	Rel	Know	Goal	Avg.	Rel	Know	Goal	Avg.
Base	0.97	3.29	5.25	3.17	2.07	4.54	7.26	4.62	0.27	5.09	6.11	3.82
Base+MS	1.54	3.48	5.93	3.65	2.47	4.45	7.30	4.74	1.20	5.37	6.67	4.41
FT+Utrr	1.92	4.01	6.60	4.18	2.42	4.78	7.43	4.88	1.28	5.18	6.88	4.45
FT+MS	2.37	3.81	6.69	4.29	2.73	4.40	7.46	4.86	1.49	4.70	6.46	4.22
FT+MS+Utrr (TOMA)	2.18	4.22	6.84	4.41	2.70	4.77	7.67	5.05	2.37	5.61	7.48	5.15

Table 1: Overall performance in terms of Rel, Know, and Goal dimensions on the all split.

Method	Qwen2.5-3B				Qwen2.5-7B				Llama3.1-8B			
	Rel	Know	Goal	Avg.	Rel	Know	Goal	Avg.	Rel	Know	Goal	Avg.
Base	0.18	4.20	4.96	3.11	0.58	4.21	5.26	3.35	-1.59	5.10	4.22	2.58
Base+MS	1.04	4.05	5.27	3.45	2.17	4.51	5.86	4.18	-0.52	5.16	4.80	3.15
FT+Utrr	1.22	4.10	5.23	3.52	1.36	4.43	5.70	3.83	-0.35	4.91	4.85	3.13
FT+MS	1.70	4.08	5.42	3.73	2.40	4.33	6.30	4.34	0.33	5.04	5.06	3.48
FT+MS+Utrr (TOMA)	1.90	4.22	5.88	4.00	2.33	4.78	6.32	4.48	1.27	5.36	5.68	4.10

Table 2: Overall performance in terms of Rel, Know, and Goal dimensions on the hard split.

Method	Rel	Know	Goal	Avg.
Base	0.77	4.39	6.24	3.80
Base+MS	1.51	5.21	6.67	4.46

Table 3: Performance of GPT-5-nano in terms of Rel, Know, and Goal dimensions on the hard split.

4 Experiments

We compare the performance of TOMA to the baselines (§4.1). Then, we analyze the effect of different partner agents on goal achievement (§4.2), the performance across scenario types (§4.3), and the success and failure factors in goal achievement (§4.4). Finally, we present a statistical analysis of TOMA’s performance across different evaluation dimensions (Appendix D.1).

4.1 Does ToM Help with Social Reasoning?

TOMA outperforms the baselines. Tables 1 and 2 present the performance of models on the all and hard subsets of the Sotopia test set, respectively. On both subsets, TOMA consistently outperforms all other model variants across the relationship, knowledge, and goal completion dimensions. Moreover, TOMA performs competitively with a strong GPT-5-nano baseline (Base+MS in Table 3), even though GPT-5-nano surpasses Qwen2.5-7B on several general reasoning benchmarks (White et al., 2025; Leaderboard, 2025). Specifically, TOMA (and even slightly more FT+MS) substantially outperforms GPT-5 nano on the relationship dimension, indicating it generates utterances with better sensitivity to the other partner’s feelings. Compared to the best base model variant (Base+MS), TOMA achieves score improvements of 16.8%, 6.6%, and 23.45% on both datasets for the Qwen2.5-3B, 7B, and Llama-3.1 models, re-

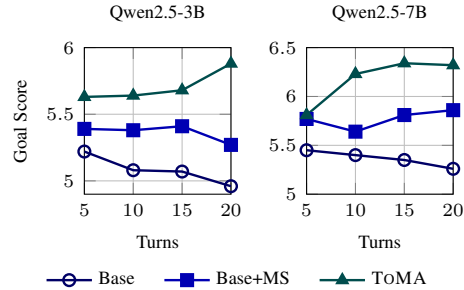


Figure 2: Goal completion scores across 5–20 turns.

spectively, averaged across the all and hard sets.

Mental-state conditioning improves relationship modeling.

We observe that models that generate utterances without explicit mental-state conditioning (Base and FT+Utrr) perform significantly worse on the relationship dimension than models that use mental-state representations (Base+MS, FT+MS, and TOMA). This suggests that explicitly considering the partner agent’s mental state can help the target agent preserve a positive relationship with them. Training on utterances alone (FT+Utrr) generally improves the knowledge and goal scores compared to Base models on all. The improvement in goal completion is expected, given that our fine-tuned models are trained to maximize goal completion. Yet, this goal-directed behavior may come at the expense of interpersonal sensitivity, as indicated in its lower relationship scores compared to models conditioned on mental states.

Fine-tuning only on mental states can also improve utterance effectiveness.

Training the model only on mental states (FT+MS) could potentially decrease its general generation ability. However, our TOMA model is still able to produce effective utterances, achieving higher goal and relationship scores than the base models across both

Metric	Target Model	(Target=3B) Partner=Base-				(Target=7B) Partner=Base-				
		3B	7B	14B	32B	3B	7B	14B	32B	
Both	Goal	Base+MS ToMA	4.81 5.00	4.99 4.96	5.11 5.36	5.28 5.40	4.94 5.23	5.27 5.41	5.72 5.75	5.83 5.86
	All	Base+MS ToMA	3.17 3.35	3.29 3.41	3.4 3.64	3.49 3.73	3.38 3.53	3.56 3.67	3.79 3.86	3.93 4.01
Target	Goal	Base+MS ToMA	3.85 4.01	4.35 3.95	3.58 3.64	3.63 3.48	3.84 4.39	4.35 4.34	4.12 4.27	3.77 4.14
	All	Base+MS ToMA	2.76 2.96	3.1 3.04	2.88 3.02	2.92 3.1	2.93 3.18	3.2 3.25	3.26 3.28	3.18 3.42

Table 4: Performance of target agent and average of both agents across goal completion and all scores. Evaluated on the hard split using various partner agent sizes.

splits. TOMA, trained to jointly improve the prediction of latent mental states and the corresponding appropriate utterances, achieves the best of both worlds, effectively maintaining relationships, knowledge seeking, and goal-oriented behavior.

Theory of Mind enables long-horizon adaptation. Figure 2 compares how efficiently agents achieve their goals under different maximum turn limits on the hard split. Surprisingly, the goal score of Base decreases as the number of turns increases. This is likely because the base model often repeats the same argument, making no progress across turns, which the GPT-5 judge penalizes. Base+MS shows slight improvement, but starts declining again for conversations longer than 15 turns. In contrast, TOMA consistently improves its goal completion score as the number of turns increases, suggesting that it may be adapting its strategy over time to achieve the goal more effectively. This adaptivity and long-horizon planning behavior can make ToM-informed agents better suited for real-world social interactions that often require longer and more flexible responses.

4.2 How do Partners Affect Performance?

Our main evaluations follow the original “self-play” setup where both agents are instances of the same model (e.g., TOMA with Qwen2.5-3B). Here, we address the question of how a different partner can impact the performance of the target agent. To that end, we evaluate the best model variants of each of base (Base+MS) and TOMA when paired with non-finetuned partner models of varying sizes (3–32B). We conduct the evaluation on the hard split. For each scenario, we use the original 5 distinct role pairs and swap the agent roles (e.g., agent 1 as target and agent 2 as partner, and vice versa), resulting in 10 role pairs. Table 4 reports both the goal completion score and average scores across goal, relationship, and knowledge; once for the target agent and once for the average of both.

A TOMA target agent not only improves its own goal completion, but also their partner’s. The target agent trained with our method performs best across most settings (Table 4). TOMA results in consistently better combined outcomes (Table 4, top) between target and partner, suggesting that our agent with improved ToM ability not only benefits itself, but also helps the other agent, likely reaching agreeable solutions for both agents. As we show in §4.4, this effect is likely due to the agent’s ability to employ more effective strategies across a broader range of interaction scenarios (e.g., coordination, negotiation, persuasion, etc.). The individual outcome for the target is somewhat more complex (Table 4, bottom). For the larger target size (7B), TOMA results in consistently better target outcomes. For the 3B target size, the winner on goal achievement is inconsistent between TOMA and Base+MS, potentially because it is harder for a small target agent to achieve their goal when conversing with a larger and socially unaware partner. Still, it is worth noting that TOMA wins at “All” metrics in most cases, meaning it is less likely than Base+MS to sacrifice relationships or knowledge.

Coordination dynamics depend on both agent and partner sizes. We observe that when the partner is larger, the overall conversation outcome – as measured by the average scores for both agents – improves. Looking at the target agent scores shows that the factors behind this improvement differ between the 3B and 7B TOMA target agents. The 7B target agent shows consistent performance improvement with partner size across all dimensions, suggesting that it can benefit from a more powerful partner. Conversely, the scores for the 3B target agent don’t consistently improve with the partner’s size, again suggesting that in that case, a larger partner leads to higher scores primarily *for the partner*. We observe that the 3B TOMA agent is more likely to achieve its goal when paired with an equal-size partner than with a considerably larger partner (14B or 32B).

4.3 How does TOMA Perform Across Different Conversation Types?

Categorizing scenarios into types. We are also interested in the performance and behavior of TOMA across different types of social interaction, where the agents’ goals may be either aligned or competing. We manually examined the 90 scenarios in the all split and categorized them into four

conversation types: **cooperation** - a win-win situation where both agents can fully achieve their goals without conflicts or compromises (36 scenarios); **negotiation** - a positive-sum game where the agents can reach their goals to a satisfactory extent with certain compromises (28 scenarios); **persuasion** - a positive-sum game where the target agent tries to convince the partner to act in a way that promotes the target agent’s goals (13 scenarios); and **conflict** - a zero-sum or even negative-sum game where their goals are in conflict and can hardly be solved through compromise (13 scenarios). See Appendix D for full details of each scenario group.

ToMA outperforms the base model under all scenario types. We analyzed 450 conversations: five conversations for each of the 90 scenarios in the all split. Figure 8 in Appendix D.1 looks at the average goal achievement score of the target agent in each conversation type, comparing agents implemented as the base model vs. ToMA. Data points on the right of the orange dotted line ($x = 0$ neutral line) correspond to conversations on which ToMA outperformed the base model. As observed, the first quartile (Q1) of each box is on the neutral line, indicating that ToMA outperforms base in at least 75% of the conversations of each type. Considering the inter-quartile range (IQR), ToMA brings greater gains in conflicts, where ToM may be more necessary for the target agent to achieve a goal that goes against their partner. Furthermore, the lower boundary (Q1-1.5IQR) is about -5 while the upper boundary (Q3+1.5IQR) is nearly 10 (i.e., ToMA obtains an average score of 10 while Base scores 0), showing that our method can largely outperform base, but not the other way around.

4.4 What Strategies Does ToMA Employ?

To understand the different strategies that agents with varying levels of ToM capabilities employ for achieving their goals, we analyze the factors contributing to successful conversations (goal score ≥ 7) and the barriers leading to failed ones (goal score < 4) across different models. Appendix D.3 details the categorization of success and failure.

ToMA enables more strategic reasoning across diverse scenarios. In successful conversations, the base model relies heavily on rapport/relationship building strategies, and direct goal-pursuit approaches, such as persistent/direct request. In contrast, ToMA adopts long-horizon goal-oriented

Model	3B		7B	
	0th-order	1st-order	0th-order	1st-order
Base+MS	28.1	71.9	22.3	77.7
ToMA	21.8	78.2	17.6	82.4

Table 5: Zero- vs. first-order reasoning percentage (%).

strategic behavior by employing compromise, accommodation, and solution offering, while still maintaining comparable levels of rapport building and cooperative response to Base.

In terms of conversation types, both models achieve success mainly in cooperative conversations, where it is easy for both agents to achieve a high goal completion score. Compared to Base, ToMA also has high levels of success in competitive settings (negotiation, persuasion, and conflict), especially when using the strategies of compromise, accommodation, and solution offering. Applying ToMA to the 7B model (in Appendix D.3) similarly shows strategic behaviors which lead to success across different scenarios, and this strategic behavior tends to increase with model size.

ToMA exhibit more active behaviors in failure modes. The base model often fails due to being too passive (failed to initiate; lack of action/information provision). Conversely, ToMA employs active strategies that sometimes fail (e.g., failure to persuade) as well as goal-oriented approaches that fail to account for the role of relationship building in goal achievement (ignored preferences; prioritizing self). In the 7B version of ToMA, these failures are significantly reduced while lack of action is more frequent. We hypothesize this is the result of increased sensitivity to the partner’s emotional state compared to the 3B model (as shown in the relationship score in Tables 1 and 2), which reduces the selfish ignored preferences and prioritizing self occurrences (see Appendix D.3).

ToMA prioritizes intentions over emotions in mental state generation. To investigate the effect of ToMA across different mental states, we categorize the generated ToM hypotheses into five dimensions and then compare the mental states distributions given by Base+MS and ToMA. Figure 4 shows that ToMA generates more hypotheses about intentions and relies less on emotions, while maintaining similar levels for beliefs, desires, and knowledge. This is in line with the finding that the base model is focused on rapport-building strategies, which require hypothesizing about the other

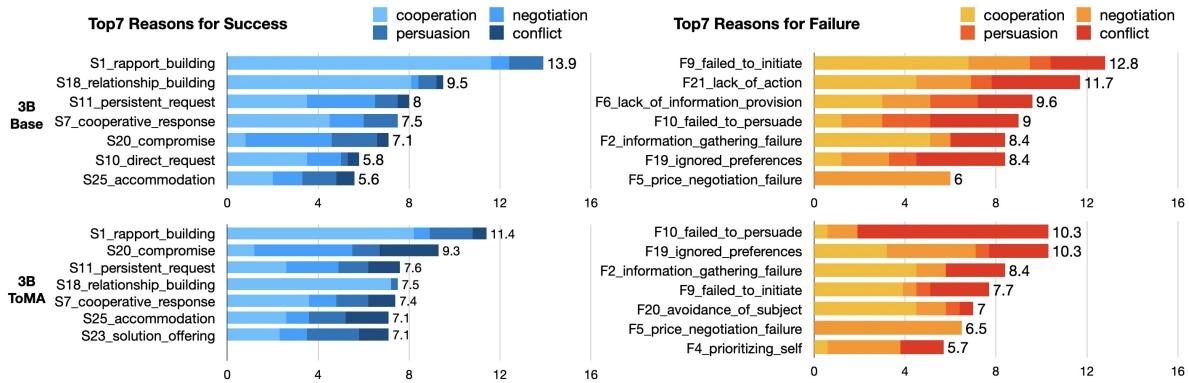


Figure 3: Top 7 goal success and failure factors for the Base model and, using the 3B model.

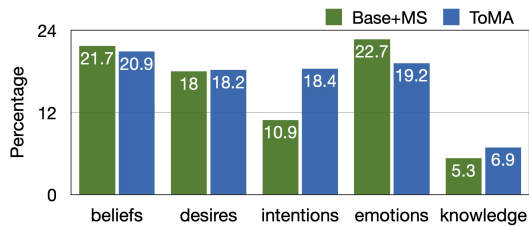


Figure 4: Distribution of mental state dimensions on the 3B model. See Appendix D.3 for 7B.

agent’s emotions – as opposed to TOMA’s strategic and goal-oriented behavior that requires reasoning about the other agent’s intentions. We observe similar trends in the 7B model. In addition, we present mental state distributions under different scenario types in Figure 12 and qualitative cases of mental states in the conversation (see Appendix D.4), providing further insights into how different mental state dimensions contribute to TOMA’s success.

TOMA generates more 1st-order mental states than the baseline. Table 5 shows the distribution of 0th-order (target agent’s own beliefs) and 1st-order (target agent’s beliefs about others) mental states generated by Base+MS and TOMA. Although both models are prompted to produce these states in equal proportions, TOMA consistently generates more 1st-order beliefs by an average of +6.3% and +5.0% on the 3B model and 7B model, respectively, compared to Base+MS. This suggests that TOMA is better at inferring others’ mental states, potentially contributing to more strategic and socially aware behaviors during interaction.

5 Further Analysis

Validity of the LLM-as-a-judge evaluation protocol. To test whether our evaluation method is sensitive to the evaluator LLM, we experiment with three additional LLM judges: Gemini-2.5-

#MS	Avg.	#Uttr	Avg.	#Turn	Avg.
2	4.01	2	4.01	4	4.01
3	4.17	3	3.81	6	4.24
4	4.11	4	4.18	8	4.06

Table 6: Average scores across different numbers of mental states, utterances, and simulation turns on the hard split with Qwen2.5-3B model.

flash, DeepSeek-3.1 (Liu et al., 2024), and Qwen3-225B, and report their scores along with those from the original evaluator GPT-5-mini. Figure 5 shows consistent trends across all four judges. TOMA consistently outperforms all baselines, while the SFT+MS model performs comparably when trained with the Qwen2.5-7B. Detailed results in Table 8 in the appendix show that TOMA improves relationship scores over the Base by 1.58, 1.77, and 2.94 points on Qwen2.5-3B, Qwen2.5-7B, and LLaMA3.1-8B, respectively, and goal scores by 1.06, 1.27, and 1.53 points. Furthermore, ratings from different LLM judges are positively correlated across all settings (see Table 9 in the appendix). Human validation also confirms the GPT-5-mini judge’s reasoning, with 93.3% average validity and 90.7% inter-annotator agreement (as in Table 10).

Performance across different K/J numbers and simulation turns. Table 6 presents ablation experiments with different values of K and J , and varying numbers of dialogue simulation turns up to 8. When varying K , we fix $J = 2$, and when varying J , we fix $K = 2$. All settings outperform the baselines with some variation in trends. Overall, increasing the number of simulation turns improves performance, but using 4 turns provides a good balance between data construction efficiency and overall effectiveness. Sampling more mental states and utterances (e.g., 3 or 4) yields modest gains, although $J = 2$ remains sufficient.

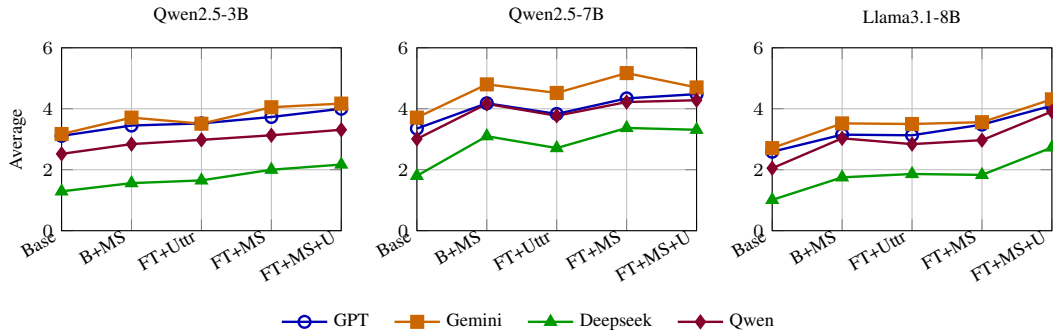


Figure 5: Average scores (relationship, knowledge, and goal) across 4 different LLM judges on the hard split. The trends of evaluation results remain consistent across different LLM judges. See Appendix B for full results.

6 Related Work

Theory of Mind in LLMs. With the advent of LLMs, research on ToM in AI is experiencing strong momentum. Current findings are conflicting: LLMs achieve good performance on various ToM benchmarks and tests designed for humans, which some researchers interpret as having developed a theory of mind (Kosinski, 2023, 2024; Strachan et al., 2024); Yet others show that this ability is inconsistent and superficial (Ullman, 2023; Shapira et al., 2024; Amirizani et al., 2024; Nickel et al., 2024; Soubki and Rambow, 2025). To improve LLMs’ ToM capabilities, one approach is to prompt models to explicitly reason about beliefs and mental states (Wilf et al., 2024; Shinoda et al., 2025). Alternative approaches combine LLMs with belief tracking (Sclar et al., 2023; Qiu et al., 2024) or Bayesian Inverse Planning (Ying et al., 2023). While less brittle than pure LLM-based approaches, these methods are typically limited in scope and only applied to specific setups. Another computationally expensive approach explores multiple ToM hypotheses during inference (Kim et al., 2025). In contrast, we propose a training approach that saves inference-time costs. Crucially, most existing work evaluates LLMs on static and artificial ToM benchmarks, requiring models to answer questions as an observer rather than a participant in a dynamic environment (Wagner et al., 2025; Xiao et al., 2025; Lupu et al., 2025). Instead, we evaluate our method on Sotopia, measuring the contribution of modeling ToM for social conversations between AI agents.

Look-Ahead Simulation in Self-Training Agents.

In this work, we leverage look-ahead, a planning technique where an agent simulates the potential outcomes several steps into the future to make more informed decisions in the present. In text generation, look-ahead search was employed for decoding, prioritizing tokens that lead to better overall

generated text (Lu et al., 2022; Fu et al., 2024) or faster inference (Leviathan et al., 2023; Chen et al., 2023). More recently, look-ahead signals were used in GRPO (Guo et al., 2025), an RL algorithm used in LLM preference tuning. In general, many simulation-based methods focus on outcome alignment using RL (Xi et al., 2024; Pang et al., 2024). Conversely, we use simulation to generate training examples, similarly to Hoang et al. (2025). In the context of social dialogues, prior work targeting Sotopia employed a similar approach of generating conversations and simulating their outcome with an LLM judge (Wang et al., 2024; Kong et al., 2025; Yu et al., 2025). Instead of directly optimizing utterances that lead to goal achievement – which could lead to reward hacking – we explicitly train our model to use ToM in social dialogues; we improve both the model’s ability to reason about mental states, as well as the capacity to consider this information when generating utterances.

7 Conclusion

We introduced TOMA, a training framework that integrates ToM-driven mental state and utterance prediction with conversation simulation to select interaction trajectories that best support goal achievement. Experiments on the Sotopia interactive evaluation benchmark demonstrate the effectiveness of our approach across a range of baselines, achieving competitive performance with GPT-5-nano using much smaller models. Comprehensive analysis shows that TOMA, infused with ToM ability, can better infer others’ mental states, leading to more strategic and goal-oriented behavior, as well as supporting long-horizon adaptation and improving relationship management. In conclusion, TOMA represents a significant step toward building socially intelligent LLM agents through explicit modeling of social reasoning and internal agent mechanisms.

Limitations

Subjective nature of mental state representations. Human mental states are inherently subjective, as beliefs, desires, emotions, intentions, and knowledge may admit multiple valid interpretations. Accordingly, our approach does not aim to recover a single ground-truth internal state, but instead defines useful mental states as those that help an agent reason about its partner and advance its social goals. While our analysis of the distribution of learned mental states in §4.4 and the qualitative analysis in Appendix D.4 illustrate how these dimensions are used during LLM reasoning, we leave the development of more fine-grained evaluation methods for mental state representations to future work.

Evaluation using LLM as a judge. Our evaluation relies on large language models as automated judges for goal, relationship, and knowledge dimensions, following the original Sotopia setup. Since these judges are trained on large-scale web data and may incorporate human feedback, they may introduce some biases when assessing social behaviors. We mitigate this by comparing multiple LLM judges and validating the results with human annotations (Appendix B), observing consistent trends and strong agreement across evaluators. Nonetheless, LLM-based judges may still be limited in capturing subtle in multi-turn social interactions.

Ethics Statement

Ethical considerations of social intelligence in LLMs. LLMs are increasingly used as social partners, providing mental-health support, personalized guidance, and assistance in everyday decision-making. As these systems become embedded in human-AI interactions, understanding their social behaviors becomes essential. Prior work showed that human-like social intelligence, such as empathy, can improve user experience and conversational quality (Campbell and Babrow, 2004; Shen, 2011; Chockkalingam et al., 2025). Our findings complement this line of work by demonstrating that explicitly modeling an interlocutor’s mental state and conditioning the generation of utterances on these predictions improves both agents’ relationship outcomes and goal achievement across diverse social scenarios. While such capabilities have clear benefits for supportive applications like tutoring, counseling, or customer service, they also

introduce risks if exploited for manipulation or deception, such as in social media bots, political persuasion, or scams. Mitigating these risks requires public education about AI capabilities and risks, thoughtful regulation, and responsible design. In particular, we recommend that LLM-powered applications avoid human names or avatars and clearly identify themselves as AI systems to reduce the likelihood of misleading users.

Data collection and ethics approval. All procedures involving human participation were reviewed and approved by our institution’s Research Ethics Board and adhered to all applicable institutional and federal guidelines. Human evaluations were conducted through CloudResearch, and all annotators provided informed consent. No personal information was collected at any stage, and participants were compensated at an average hourly rate of \$10, which is comparable to the U.S. minimum wage. See Appendix F for the instruction interface provided to participants.

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References

- Josh Achiam, Steven Adler, Sandhini Agarwal, Lama Ahmad, Ilge Akkaya, Florencia Leoni Aleman, Diogo Almeida, Janko Altenschmidt, Sam Altman, Shyamal Anadkat, et al. 2023. [Gpt-4 technical report](#). *arXiv preprint arXiv:2303.08774*.
- Maryam Amirizani, Elias Martin, Maryna Sivachenko, Afra Mashhadi, and Chirag Shah. 2024. [Can llms reason like humans? assessing theory of mind reasoning in llms for open-ended questions](#). In *Proceedings of the 33rd ACM International Conference on Information and Knowledge Management*, pages 34–44.
- Ian A Apperly and Stephen A Butterfill. 2009. [Do humans have two systems to track beliefs and belief-like states?](#) *Psychological review*, 116(4):953.
- Simon Baron-Cohen, Alan M Leslie, and Uta Frith. 1985. [Does the autistic child have a “theory of mind”?](#) *Cognition*, 21(1):37–46.
- Lukas Biewald. 2020. [Experiment tracking with weights and biases](#). Software available from wandb.com.
- Rose G. Campbell and Austin S. Babrow. 2004. [The role of empathy in responses to persuasive risk communication: Overcoming resistance to hiv prevention messages](#). *Health Communication*, 16(2):159–182. PMID: 15090283.
- Charlie Chen, Sebastian Borgeaud, Geoffrey Irving, Jean-Baptiste Lespiau, Laurent Sifre, and John Jumper. 2023. [Accelerating large language model decoding with speculative sampling](#). *arXiv preprint arXiv:2302.01318*.
- Zhuang Chen, Jincenzi Wu, Jinfeng Zhou, Bosi Wen, Guanqun Bi, Gongyao Jiang, Yaru Cao, Mengting Hu, Yunghwei Lai, Zexuan Xiong, and Minlie Huang. 2024. [ToMBench: Benchmarking theory of mind in large language models](#). In *Proceedings of the 62nd Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pages 15959–15983, Bangkok, Thailand. Association for Computational Linguistics.
- Shruthi Chockalingam, Seyed Hossein Alavi, Raymond T. Ng, and Vered Shwartz. 2025. [Should I go vegan: Evaluating the persuasiveness of LLMs in persona-grounded dialogues](#). In *Proceedings of the Third Workshop on Social Influence in Conversations (SICoN 2025)*, pages 65–72, Vienna, Austria. Association for Computational Linguistics.
- Gheorghe Comanici, Eric Bieber, Mike Schaeckermann, Ice Pasupat, Noveen Sachdeva, Inderjit Dhillon, Marcel Blistein, Ori Ram, Dan Zhang, Evan Rosen, et al. 2025. [Gemini 2.5: Pushing the frontier with advanced reasoning, multimodality, long context, and next generation agentic capabilities](#). *arXiv preprint arXiv:2507.06261*.
- Michael Han Daniel Han and Unsloth team. 2023. [Unsloth](#).
- Abhimanyu Dubey, Abhinav Jauhri, Abhinav Pandey, Abhishek Kadian, Ahmad Al-Dahle, Aiesha Letman, Akhil Mathur, Alan Schelten, Amy Yang, Angela Fan, et al. 2024. The llama 3 herd of models. *arXiv e-prints*, pages arXiv–2407.
- Yichao Fu, Peter Bailis, Ion Stoica, and Hao Zhang. 2024. [Break the sequential dependency of LLM inference using lookahead decoding](#). In *Proceedings of the 41st International Conference on Machine Learning*, volume 235 of *Proceedings of Machine Learning Research*, pages 14060–14079. PMLR.
- Jiawei Gu, Xuhui Jiang, Zhichao Shi, Hexiang Tan, Xuehao Zhai, Chengjin Xu, Wei Li, Yinghan Shen, Shengjie Ma, Honghao Liu, et al. 2024. [A survey on llm-as-a-judge](#). *arXiv preprint arXiv:2411.15594*.
- Daya Guo, Dejian Yang, Haowei Zhang, Junxiao Song, Ruoyu Zhang, Runxin Xu, Qihao Zhu, Shirong Ma, Peiyi Wang, Xiao Bi, et al. 2025. [Deepseek-r1: Incentivizing reasoning capability in llms via reinforcement learning](#). *arXiv preprint arXiv:2501.12948*.
- Thai Quoc Hoang, Kung-Hsiang Huang, Shirley Kokane, Jianguo Zhang, Zuxin Liu, Ming Zhu, Jake Grigsby, Tian Lan, Michael S Ryoo, Chien-Sheng Wu, Shelby Heinecke, Huan Wang, Silvio Savarese, Caiming Xiong, and Juan Carlos Niebles. 2025. [LAM SIMULATOR: Advancing data generation for large action model training via online exploration and trajectory feedback](#). In *Findings of the Association for Computational Linguistics: ACL 2025*, pages 12921–12934, Vienna, Austria. Association for Computational Linguistics.
- Ari Holtzman, Jan Buys, Li Du, Maxwell Forbes, and Yejin Choi. 2020. [The curious case of neural text de-generation](#). In *International Conference on Learning Representations*.
- Edward J Hu, yelong shen, Phillip Wallis, Zeyuan Allen-Zhu, Yuanzhi Li, Shean Wang, Lu Wang, and Weizhu Chen. 2022. [LoRA: Low-rank adaptation of large language models](#). In *International Conference on Learning Representations*.
- Hyunwoo Kim, Melanie Sclar, Tan Zhi-Xuan, Lance Ying, Sydney Levine, Yang Liu, Joshua B. Tenenbaum, and Yejin Choi. 2025. [Hypothesis-driven theory-of-mind reasoning for large language models](#). In *Second Conference on Language Modeling*.
- Hyunwoo Kim, Melanie Sclar, Xuhui Zhou, Ronan Bras, Gunhee Kim, Yejin Choi, and Maarten Sap. 2023. [FANToM: A benchmark for stress-testing machine theory of mind in interactions](#). In *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing*, pages 14397–14413, Singapore. Association for Computational Linguistics.
- Aobo Kong, Wentao Ma, Shiwan Zhao, Yongbin Li, Yuchuan Wu, Ke Wang, Xiaoqian Liu, Qicheng Li,

- Yong Qin, and Fei Huang. 2025. [SDPO: Segment-level direct preference optimization for social agents](#). In *Proceedings of the 63rd Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pages 12409–12423, Vienna, Austria. Association for Computational Linguistics.
- Michal Kosinski. 2023. [Theory of mind may have spontaneously emerged in large language models](#). *arXiv preprint arXiv:2302.02083*, 4:169.
- Michal Kosinski. 2024. [Evaluating large language models in theory of mind tasks](#). *Proceedings of the National Academy of Sciences*, 121(45):e2405460121.
- LLM Leaderboard. 2025. Llm leaderboard. <https://llm-stats.com/>.
- Yaniv Leviathan, Matan Kalman, and Yossi Matias. 2023. [Fast inference from transformers via speculative decoding](#). In *Proceedings of the 40th International Conference on Machine Learning*, volume 202 of *Proceedings of Machine Learning Research*, pages 19274–19286. PMLR.
- Aixin Liu, Bei Feng, Bing Xue, Bingxuan Wang, Bochao Wu, Chengda Lu, Chenggang Zhao, Chengqi Deng, Chenyu Zhang, Chong Ruan, et al. 2024. [Deepseek-v3 technical report](#). *arXiv preprint arXiv:2412.19437*.
- Ximing Lu, Sean Welleck, Peter West, Liwei Jiang, Jungo Kasai, Daniel Khachabi, Ronan Le Bras, Lianhui Qin, Youngjae Yu, Rowan Zellers, Noah A. Smith, and Yejin Choi. 2022. [NeuroLogic a*esque decoding: Constrained text generation with lookahead heuristics](#). In *Proceedings of the 2022 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies*, pages 780–799, Seattle, United States. Association for Computational Linguistics.
- Andrei Lupu, Timon Willi, and Jakob Foerster. 2025. [The decrypto benchmark for multi-agent reasoning and theory of mind](#). *arXiv preprint arXiv:2506.20664*.
- Christian Nickel, Laura Schrewe, and Lucie Flek. 2024. [Probing the robustness of theory of mind in large language models](#). *arXiv preprint arXiv:2410.06271*.
- OpenAI. 2025. [Gpt-5 system card](#). *OpenAI Blog*.
- Xianghe Pang, Shuo Tang, Rui Ye, Yuxin Xiong, Bolun Zhang, Yanfeng Wang, and Siheng Chen. 2024. [Self-alignment of large language models via monopolylogue-based social scene simulation](#). In *Forty-first International Conference on Machine Learning*.
- Aldo Pareja, Nikhil Shivakumar Nayak, Hao Wang, Krishnateja Killamsetty, Shivchander Sudalairaj, Wenlong Zhao, Seungwook Han, Abhishek Bhandwalidar, Guangxuan Xu, Kai Xu, Ligong Han, Luke Inglis, and Akash Srivastava. 2025. [Unveiling the secret recipe: A guide for supervised fine-tuning small LLMs](#). In *The Thirteenth International Conference on Learning Representations*.
- David Premack and Guy Woodruff. 1978. [Does the chimpanzee have a theory of mind?](#) *Behavioral and Brain Sciences*, 1(4):515–526.
- Shuwen Qiu, Mingdian Liu, Hengli Li, Song-Chun Zhu, and Zilong Zheng. 2024. [MindDial: Enhancing conversational agents with theory-of-mind for common ground alignment and negotiation](#). In *Proceedings of the 25th Annual Meeting of the Special Interest Group on Discourse and Dialogue*, pages 746–759, Kyoto, Japan. Association for Computational Linguistics.
- Qwen. 2024a. [Qwen2 technical report](#). *arXiv preprint arXiv:2407.10671*.
- Qwen. 2024b. [Qwen2.5: A party of foundation models](#).
- Melanie Sclar, Sachin Kumar, Peter West, Alane Suhr, Yejin Choi, and Yulia Tsvetkov. 2023. [Minding language models’ \(lack of\) theory of mind: A plug-and-play multi-character belief tracker](#). In *Proceedings of the 61st Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pages 13960–13980, Toronto, Canada. Association for Computational Linguistics.
- Natalie Shapira, Mosh Levy, Seyed Hossein Alavi, Xuhui Zhou, Yejin Choi, Yoav Goldberg, Maarten Sap, and Vered Shwartz. 2024. [Clever hans or neural theory of mind? stress testing social reasoning in large language models](#). In *Proceedings of the 18th Conference of the European Chapter of the Association for Computational Linguistics (Volume 1: Long Papers)*, pages 2257–2273, St. Julian’s, Malta. Association for Computational Linguistics.
- Lijiang Shen. 2011. [The effectiveness of empathy- versus fear-arousing antismoking psas](#). *Health Communication*, 26(5):404–415. PMID: 21409669.
- Kazutoshi Shinoda, Nobukatsu Hojo, Kyosuke Nishida, Yoshihiro Yamazaki, Keita Suzuki, Hiroaki Sugiyama, and Kuniko Saito. 2025. [Let’s put ourselves in sally’s shoes: Shoes-of-others prefixing improves theory of mind in large language models](#). *arXiv preprint arXiv:2506.05970*.
- Adil Soubki and Owen Rambow. 2025. [Machine theory of mind needs machine validation](#). In *Findings of the Association for Computational Linguistics: ACL 2025*, pages 18495–18505, Vienna, Austria. Association for Computational Linguistics.
- James WA Strachan, Dalila Albergo, Giulia Borghini, Oriana Pansardi, Eugenio Scaliti, Saurabh Gupta, Krati Saxena, Alessandro Rufo, Stefano Panzeri, Guido Manzi, et al. 2024. [Testing theory of mind in large language models and humans](#). *Nature Human Behaviour*, 8(7):1285–1295.
- Tomer Ullman. 2023. [Large language models fail on trivial alterations to theory-of-mind tasks](#). *arXiv preprint arXiv:2302.08399*.

- Eitan Wagner, Nitay Alon, Joseph M Barnby, and Omri Abend. 2025. [Mind your theory: Theory of mind goes deeper than reasoning](#). In *Findings of the Association for Computational Linguistics: ACL 2025*, pages 26658–26668, Vienna, Austria. Association for Computational Linguistics.
- Ruiyi Wang, Haofei Yu, Wenxin Zhang, Zhengyang Qi, Maarten Sap, Yonatan Bisk, Graham Neubig, and Hao Zhu. 2024. [SOTOPIA- \$\pi\$: Interactive learning of socially intelligent language agents](#). In *Proceedings of the 62nd Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pages 12912–12940, Bangkok, Thailand. Association for Computational Linguistics.
- Colin White, Samuel Dooley, Manley Roberts, Arka Pal, Benjamin Feuer, Siddhartha Jain, Ravid Shwartz-Ziv, Neel Jain, Khalid Saifullah, Sreemanti Dey, Shubh-Agrawal, Sandeep Singh Sandha, Siddartha Venkat Naidu, Chinmay Hegde, Yann LeCun, Tom Goldstein, Willie Neiswanger, and Micah Goldblum. 2025. [Livebench: A challenging, contamination-limited LLM benchmark](#). In *The Thirteenth International Conference on Learning Representations*.
- Alex Wilf, Sihyun Lee, Paul Pu Liang, and Louis-Philippe Morency. 2024. [Think twice: Perspective-taking improves large language models’ theory-of-mind capabilities](#). In *Proceedings of the 62nd Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pages 8292–8308, Bangkok, Thailand. Association for Computational Linguistics.
- Thomas Wolf, Lysandre Debut, Victor Sanh, Julien Chaumond, Clement Delangue, Anthony Moi, Pierric Cistac, Tim Rault, Remi Louf, Morgan Funtowicz, Joe Davison, Sam Shleifer, Patrick von Platen, Clara Ma, Yacine Jernite, Julien Plu, Canwen Xu, Teven Le Scao, Sylvain Gugger, Mariama Drame, Quentin Lhoest, and Alexander Rush. 2020. [Transformers: State-of-the-art natural language processing](#). In *Proceedings of the 2020 Conference on Empirical Methods in Natural Language Processing: System Demonstrations*, pages 38–45, Online. Association for Computational Linguistics.
- Jiajun Xi, Yinong He, Jianing Yang, Yinpei Dai, and Joyce Chai. 2024. [Teaching embodied reinforcement learning agents: Informativeness and diversity of language use](#). In *Proceedings of the 2024 Conference on Empirical Methods in Natural Language Processing*, pages 4097–4114, Miami, Florida, USA. Association for Computational Linguistics.
- Yang Xiao, Jiashuo Wang, Qiancheng Xu, Changhe Song, Chunpu Xu, Yi Cheng, Wenjie Li, and Pengfei Liu. 2025. [Towards dynamic theory of mind: Evaluating LLM adaptation to temporal evolution of human states](#). In *Proceedings of the 63rd Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pages 24036–24057, Vienna, Austria. Association for Computational Linguistics.
- Lance Ying, Katherine M Collins, Megan Wei, Cede-gao E Zhang, Tan Zhi-Xuan, Adrian Weller, Joshua B Tenenbaum, and Lionel Wong. 2023. [The neuro-symbolic inverse planning engine \(nipe\): Modeling probabilistic social inferences from linguistic inputs](#). *arXiv preprint arXiv:2306.14325*.
- Haofei Yu, Zhengyang Qi, Yining Zhao, Kolby Nottingham, Keyang Xuan, Bodhisattwa Prasad Majumder, Hao Zhu, Paul Pu Liang, and Jiaxuan You. 2025. [Sotopia-rl: Reward design for social intelligence](#). *arXiv preprint arXiv:2508.03905*.
- Xuhui Zhou, Hao Zhu, Leena Mathur, Ruohong Zhang, Haofei Yu, Zhengyang Qi, Louis-Philippe Morency, Yonatan Bisk, Daniel Fried, Graham Neubig, and Maarten Sap. 2024. [SOTOPIA: Interactive evaluation for social intelligence in language agents](#). In *The Twelfth International Conference on Learning Representations*.

A Inference Time Costs

We compare inference-time cost across methods in Table 7. We report the average number of conversation tokens generated by the target model in the self-play setting. We observe a similar pattern when accounting for the combined tokens from both target and partner models. Importantly, ToMA requires only an average of 47 additional tokens compared to the base model, indicating that the trained model learns compact and informative intermediate representations. Our method introduces one additional inference-time call. While latency and compute overhead depend on hardware configuration, our experiments on a single NVIDIA L40S GPU show that ToMA adds around 4.5 seconds per turn for both Qwen-3B and Qwen-7B, with similar time costs observed across model sizes.

B Further Analysis

Table 8 presents the detailed Relationship, Knowledge, Goal, and average scores across four different LLM judges on the hard split. Table 9 shows the Pearson correlation coefficients between the ratings of each pair of LLM judges. Table 10 presents the human evaluation of the validity of the reasoning provided by the GPT-5-mini judge.

C Experiment Details

C.1 Model Settings

For open-weight models such as Qwen (Qwen, 2024b), we load the model checkpoint and tokenizer provided by Hugging Face Transformers (Wolf et al., 2020). We load all models in the brain floating-point format (bf16). The maximum context length is set to 4096, random seed to 42, generation temperature to 0.7, and we use top-p sampling (Holtzman et al., 2020) with $p = 0.9$. For proprietary LLMs (GPT-5 (OpenAI, 2025) and Gemini (Comanici et al., 2025)), we call the respective API using a default generation temperature of 1.0. Table 11 provides the model sources.

C.2 Training Details

We adopt LoRA (Hu et al., 2022) for fine-tuning and apply grid search, provided by wandb (Biewald, 2020), on the learning rate and LoRA configurations (rank and alpha), and select the best model checkpoint based on the performance on the validation set. During validation, the model is evaluated on 20 randomly sampled testing instances and is

asked to generate 10 turns of conversation per instance. In addition, we employ an early stopping strategy to end the training session when the best validation score does not change for 3 consecutive updates. The key training hyper-parameters are presented in Table 12.

C.3 Experimental Costs

For constructing the training data containing mental states and utterances, the API calls of Gemini (gemini-2.0-flash-lite-001) cost less than 5 USD. For the comprehensive evaluation in our experiments, the cost of GPT-5 (gpt-5-mini) was roughly 100 USD.

Each experiment session involving open-weight LLMs was conducted on a single NVIDIA L40S GPU, and we employ unsloth (Daniel Han and team, 2023) for fast training, reducing each training session to about 4 hours.

D Analysis Details

D.1 How does ToMA Perform Across Different Evaluation Dimensions?

To investigate the performance gains of ToMA over Base in different evaluation dimensions (i.e., Goal, Relationship, and Knowledge), we visualize the paired scores in Figure 6 and Figure 7, where each point (x, y) means the Base performance is x and ToMA performance is y for one instance. The 45-degree dot line (“neutral line”) stands for a draw, and a darker color of the points represents a higher frequency.

We observe that more points are distributed above the neutral line, meaning ToMA outperforms Base for more instances, especially for Goal and Rel dimensions. In addition, considering the four quadrants of the Goal dimension in Figure 6(a) and Figure 7(a), many points lie in the upper-left region, meaning ToMA is much better than Base, while hardly any points lie in the lower-right corner. For the Relationship dimension in Figure 6(b) and Figure 7(b), most points of ToMA and Base are above the $y=0$ line, meaning a the relationship between two agents is preserved and even enhanced through after the conversation. Figure 6(c) and Figure 7(c) show that both methods help agents gain new or important information through interaction, and ToMA often brings more knowledge gains.

In addition, we present the correlation coefficients between the results of different dimensions in Table 13, which shows that the three dimensions

Method	Sotopia-All Split		Sotopia-Hard Split		Avg. Tok.	Δ
	Qwen2.5-3B	Qwen2.5-7B	Qwen2.5-3B	Qwen2.5-7B		
Base	167	187	250	212	204	0
Base+MS	167	236	302	261	241.5	+37.5
FT+Utr	232	187	224	185	207	+3
FT+MS	386	265	396	276	330.75	+126.7
ToMA (ours)	255	240	260	249	251	+47

Table 7: Target costs comparison across different models and settings.

Judge	Method	Qwen2.5-3B				Qwen2.5-7B				LLaMA3-8B			
		Rel	Know	Goal	Avg.	Rel	Know	Goal	Avg.	Rel	Know	Goal	Avg.
GPT5	Base	0.18	4.2	4.96	3.11	0.58	4.21	5.26	3.35	-1.58	5.07	4.29	2.59
	Base+MS	1.04	4.05	5.27	3.45	2.17	4.51	5.86	4.18	-0.52	5.16	4.8	3.15
	SFT+Utr	1.22	4.1	5.23	3.52	1.36	4.43	5.7	3.83	-0.35	4.91	4.85	3.13
	SFT+MS	1.7	4.08	5.42	3.73	2.4	4.33	6.3	4.34	0.33	5.04	5.06	3.48
	SFT+MS+Utr	1.9	4.22	5.88	4.00	2.33	4.78	6.32	4.48	1.27	5.36	5.68	4.1
Gemini	Base	-0.92	6.86	3.59	3.17	-0.31	6.96	4.48	3.71	-2.42	7.09	3.44	2.71
	Base+MS	0.07	6.53	4.53	3.71	1.67	7.26	5.48	4.8	-1.16	7.23	4.48	3.52
	SFT+Utr	-0.04	6.37	4.19	3.51	0.96	7.15	5.44	4.52	-1.14	7.03	4.6	3.5
	SFT+MS	1.04	6.53	4.58	4.05	1.98	7.43	6.1	5.17	-0.36	6.8	4.26	3.56
	SFT+MS+Utr	0.68	6.68	5.15	4.17	1.15	7.21	5.75	4.7	0.49	7.36	5.1	4.31
Deepseek	Base	-0.96	1.73	3.1	1.29	-0.4	2	3.8	1.8	-2.06	2.13	2.98	1.01
	Base+MS	-0.36	1.73	3.31	1.56	1.51	2.92	4.87	3.1	-0.98	2.81	3.41	1.75
	SFT+Utr	-0.22	1.84	3.33	1.65	0.6	2.63	4.91	2.71	-1.03	2.65	3.96	1.86
	SFT+MS	0.51	1.77	3.7	2	1.7	3.05	5.37	3.37	-0.51	2.16	3.82	1.83
	SFT+MS+Utr	0.35	2.11	4.06	2.17	1.39	3.04	5.51	3.31	0.44	2.84	4.9	2.73
Qwen	Base	0.05	2.87	4.64	2.52	0.81	2.86	5.36	3.01	-1.62	2.84	4.93	2.05
	Base+MS	1.18	2.4	4.94	2.84	3.12	3.45	5.89	4.16	0.01	3.49	5.6	3.03
	SFT+Utr	1.35	2.71	4.88	2.98	1.94	3.26	6.11	3.77	-0.21	3.32	5.41	2.84
	SFT+MS	1.96	2.41	5.01	3.13	3.05	3.18	6.44	4.22	0.64	3.1	5.17	2.97
	SFT+MS+Utr	1.75	2.74	5.44	3.31	2.87	3.56	6.41	4.28	1.86	3.8	6.09	3.91
Avg.	Base	-0.41	3.92	4.07	2.53	0.17	4.01	4.73	2.97	-1.92	4.28	3.91	2.09
	Base+MS	0.48	3.68	4.51	2.89	2.12	4.54	5.53	4.06	-0.66	4.67	4.57	2.86
	SFT+Utr	0.58	3.76	4.41	2.91	1.22	4.37	5.54	3.71	-0.68	4.48	4.71	2.83
	SFT+MS	1.30	3.70	4.68	3.23	2.28	4.50	6.05	4.28	0.03	4.28	4.58	2.96
	SFT+MS+Utr	1.17	3.94	5.13	3.41	1.94	4.65	6.00	4.19	1.02	4.84	5.44	3.77

Table 8: Relationship, knowledge, goal, and average scores across 4 different LLM judges on the hard split.

	GPT5	Gemini	Deepseek	Qwen
GPT5	$1_{\pm 0}$	$0.6056_{\pm 0.2104}$	$0.6463_{\pm 0.1857}$	$0.6802_{\pm 0.1786}$
Gemini	$0.6055_{\pm 0.2104}$	$1_{\pm 0}$	$0.5828_{\pm 0.2331}$	$0.5967_{\pm 0.2446}$
Deepseek	$0.6463_{\pm 0.1857}$	$0.5828_{\pm 0.2332}$	$1_{\pm 0}$	$0.6770_{\pm 0.1791}$
Qwen	$0.6802_{\pm 0.1786}$	$0.5967_{\pm 0.2446}$	$0.6770_{\pm 0.1791}$	$1_{\pm 0}$

Table 9: The Pearson correlation coefficient between the ratings by each pair of LLM judges. We present the average correlation (\pm standard deviation) across all evaluation results in Table 8.

are positively correlated with each other. We observe that the Goal-Rel pair shows the strongest correlation, indicating that the improved goal completion performance is related to the preservation and enhancement of the agents’ relationship throughout the conversation, which supports the importance of enabling Theory of Mind.

D.2 How does ToMA Perform Across Different Conversation Types?

Figure 9 provides the performance (Goal) gains of ToMA over Base with respect to different scenario types using the Qwen2.5-7B model, and the analysis of the 3B model (Figure 8) is described in §4.3.

	Goal	Relationship	Knowledge
Validity of Judge’s Reasoning	84%	100%	96%
Human Agreement Percentage	92%	92%	88%

Table 10: The human evaluation of the validity of the reasoning provided by the GPT-5-mini judge. From the evaluation outputs on the hard split using Qwen2.5-3B, we randomly sample 5 instances per model (i.e., Base, Base+MS, SFT+Utrr, SFT+MS, and SFT+MS+Utrr) and ask three human evaluators to measure whether the LLM judge’s reasoning in each instance is valid or not. Here, we present the validity rates (majority voting by three annotators) and agreement percentages.

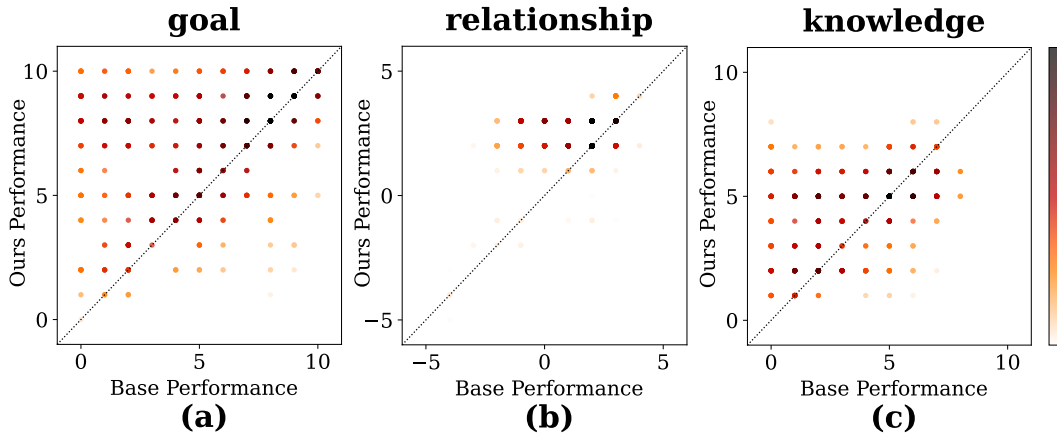


Figure 6: Comparisons between TOMA and Base over different dimensions using Qwen2.5-3B.

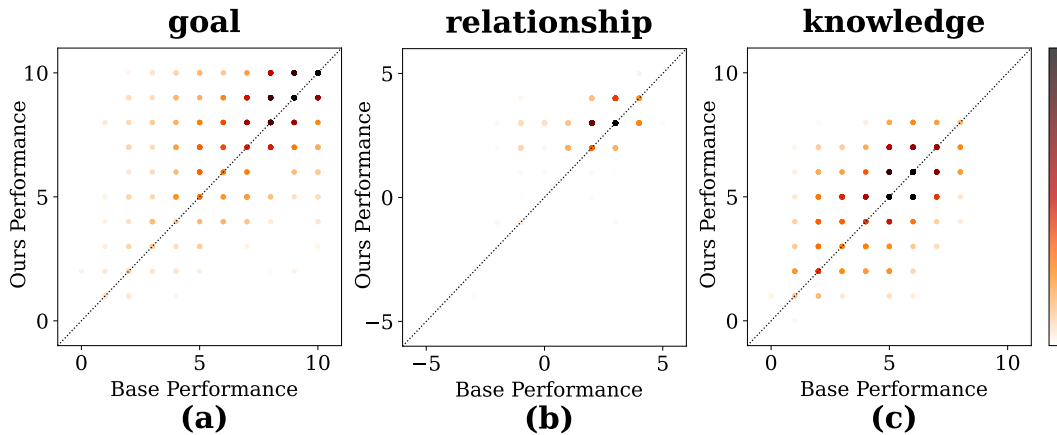


Figure 7: Comparisons between TOMA and Base over different dimensions using Qwen2.5-7B.

Type	Role	Model	Link
Open-weight LLM	Speaker (fine-tuning)	Qwen2.5-3B	Model Link
Open-weight LLM	Speaker (fine-tuning)	Qwen2.5-7B	Model Link
Open-weight LLM	Partner (frozen)	Qwen2.5-14B	Model Link
Proprietary LLM	Partner (frozen)	GPT-5-nano	API Link
Proprietary LLM	Evaluator (frozen)	GPT-5-mini	API Link
Proprietary LLM	Evaluator (frozen)	Gemini-Flash	API Link

Table 11: The sources of models used in this work.

Table 14, Table 15, Table 16, and Table 17 show case five instances per scenario type: cooperation, negotiation, persuasion, and conflict.

Hyper-parameters	Values
# epochs	3
batch size	2
gradient accumulation steps	4
learning rate	1e-4; 5e-05
lr scheduler	cosine
weight decay	0
warmup steps	10
max seq len	4,096
LoRA rank	8; 16; 32; 64
LoRA alpha	32; 64; 128
LoRA dropout	0

Table 12: The training hyper-parameters.

	Goal-Rel	
	Pearson	Spearman
3B	0.224 (2e-6)	0.376 (5e-16)
7B	0.284 (2e-9)	0.370 (2e-15)

	Goal-Know	
	Pearson	Spearman
3B	0.228 (1e-6)	0.213 (7e-6)
7B	0.120 (0.013)	0.136 (5e-3)

	Rel-Know	
	Pearson	Spearman
3B	0.288 (9e-10)	0.222 (3e-6)
7B	0.107 (0.026)	0.062 (0.195)

Table 13: The Pearson and Spearman correlation coefficients (with p-values) between dimensions.

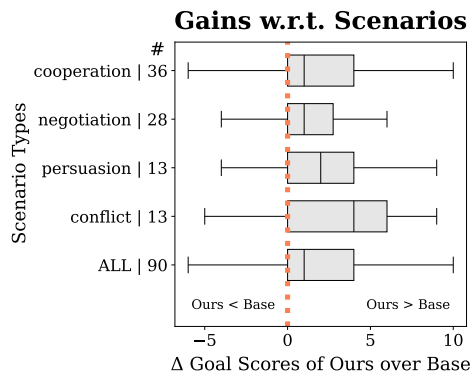


Figure 8: The Goal gains of TOMA over Base regarding different scenario types using Qwen2.5-3B.

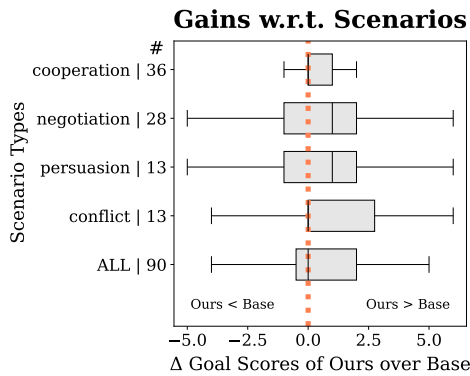


Figure 9: The Goal gains of TOMA over Base regarding different scenario types using Qwen2.5-7B.

Scenario Description	Speaker's Goal	Partner's Goal
Conversation between two individuals in a romantic relationship	Ask the other to go to dinner with you (Extra information: you want to have a romantic dinner at a fancy restaurant)	Maintain a balanced diet while enjoying the dinner (Extra information: you are on a diet and you have a daily limit on calorie intake.)
Two friends are meeting at a coffee shop, where one of them is having trouble keeping up with their bills.	Help your friend with their financial trouble (Extra information: you are aware that your friend is struggling with their bills and you want to help.)	Maintain your pride if your friend offers you money (Extra information: you are the friend who is struggling financially, but you don't want to seem like you are taking advantage of the situation. Hint: you can express gratitude and discuss how you plan to pay it back in the future.)
Two friends are having a conversation in a coffee shop	Seek emotional support (Extra information: you have been feeling down lately and you need someone to talk to)	Provide emotional support but also avoid enabling victim mentality (Extra information: you believe that your friend needs to face their problems instead of dwelling on them.)
A conversation between two friends at a park	Break bad luck (Extra information: you found out that you have been having bad luck because you have been unknowingly carrying a cursed artifact.)	Help friend prepare the ritual to break the bad luck, although you are an atheist and not superstitious at all. (Extra information: you know that your friend believes in the ritual deeply, and the placebo effect might give them more confidence.)
Two strangers are meeting at a party.	You are trying to figure out whether you have a mutual friend with the other person. You should not simply list their names.	You are trying to figure out whether you have a mutual friend with the other person. You should not simply list their names.

Table 14: Five instances of the *cooperation* scenario type.

Scenario Description	Speaker's Goal	Partner's Goal
Two friends are camping in the wilderness and the temperature drops significantly at night.	Share the only blanket available (Extra information: you are extremely cold and need the blanket to keep warm Hint: you can stress the benefit of sharing.)	Keep the blanket for yourself as you are also very cold (Extra information: you have a lower tolerance for cold, and you feel that you need the blanket more)
One person is offering a BMW Z3 for \$5000.0, while another individual is interested in purchasing it. Here's a brief description of the car: The BMW Z3 is in need of a good home. It operates smoothly without any problems and is known for its fuel efficiency and sporty appearance. The mileage is relatively low for its age. It's an opportunity not to be missed, so come and get it before it's gone. A smog certificate is readily available.	You are the buyer for this item and your target price is \$4600. You should be aware that if you purchase it at a price significantly higher than your target, you will incur a penalty. However, if you manage to secure it for less than the target price, you will receive a bonus.	You are the seller of this item, with a target price set at \$3260. Please note, you may face a penalty if this item is sold for a price significantly lower than the target. However, you stand a chance to earn a bonus if you successfully sell it for a price higher than the target.
Two roommates deciding on how to split up items after a garage sale. The items are 3 books, 2 hats, and 1 ball. Each item has a different sentimental value for each person, which translates into points.	Maximize the points you have (Extra information: you value the books at 3 points each, the hats at 2 points each, and the ball at 1 point)	Maximize the points you have (Extra information: you value the books at 2 points each, the hats at 3 points each, and the ball at 1 point)
Conversation between two friends, one who has written a play based on their parents' life, and the other owns a production company.	Sell the rights of the play to your friend (Extra information: you believe that the play is worth a lot and you would like a fair price for it)	Acquire the rights of the play while maintaining a budget (Extra information: you only have a limited budget for new plays this season. Hint: you can not spend all your budget on this play since you still need to maintain your financial stability.)
A conversation between two individuals, one is the homeowner and the other is their cousin's partner, who has been staying at the house for a while.	Tell the cousin's partner that they are no longer welcome in your home (Extra information: they have been causing a lot of trouble and not respecting house rules Hint: you may want to discuss the issues and propose possible solutions)	Attempt to remain in the home while maintaining a good relationship with the cousin and the homeowner (Extra information: you have nowhere else to go at the moment and you believe the issues can be resolved.)

Table 15: Five instances of the *negotiation* scenario type.

Scenario Description	Speaker's Goal	Partner's Goal
Two friends meet at a bar.	Convince the friend to drink less (Extra information: your friend has been drinking a lot recently and you're worried about their health)	You want to keep drinking but don't want to upset your friend (Extra information: you've been drinking to cope with stress recently, but don't want to worry your friend)
Two roommates living together and sharing household chores. One of them, who is responsible for cooking, finds out that the other one refuses to eat anything they cook	Convince the roommate to try the food (Extra information: you have spent a lot of time and effort on cooking)	Express your concerns about the food without hurting the roommate's feelings (Extra information: you are worried about the taste and nutrition of the food)
Two friends discussing their schedules at a coffee shop	Convince the friend to take more classes (Extra information: you think your friend is not challenging themselves enough)	Maintain a manageable schedule while preserving the friendship (Extra information: you are already overwhelmed with your current workload Hint: you can express your concerns about the workload and suggest other ways of challenging oneself.)
Conversation between two business partners reviewing their company's financial status (Gourmet Delights Inc. is globally recognized for producing and distributing a diverse line of exceptional quality food products.)	Convince the partner to cut costs (Extra information: you have found a report indicating the company's profits are decreasing. And you think the company should start by switching suppliers of ingredients. Hint: you can propose ways to cut costs that won't affect the status of the company.)	Maintain the quality of the company's products and services while agreeing to a cost cut (Extra information: you are concerned about the impact of cost-cutting on the quality of your product.)
A conversation between two individuals at a charity gala	Convince the other individual to donate to a cause supporting young children (Extra information: this cause can greatly improve the lives of many young children and you think it is a worthy cause. The minimum donation for this charity organization is \$3000)	Maintain financial stability while supporting causes (Extra information: you have a certain budget for donations this year and have already made several donations. You are only thinking of donating \$2000 max)

Table 16: Five instances of the *persuasion* scenario type.

Scenario Description	Speaker's Goal	Partner's Goal
Conversation between two friends at a trivia night	Get the answer for the trivia question from the friend (Extra information: your friend knows the answer to the trivia question but hasn't shared it with you yet)	Avoid revealing the answer to the trivia question (Extra information: You think that your friend should try to figure it out on their own to improve their trivia skills)
Two roommates are having a disagreement over noise levels in their shared apartment.	Convince your roommate to lower the noise (Extra information: you have an important online meeting tomorrow morning and you need a quiet environment to prepare)	Defend your right to play music in your own room, but also keep the peace in the apartment (Extra information: you find playing music relaxing and it's your way to unwind after a long day. Hint: you may want to suggest a compromise, like using headphones or playing music only during certain hours.)
Two friends are playing a video game together.	Win the game (Extra information: you just need five more minutes to accomplish your goal in the game)	Stop the game because it's too late (Extra information: you feel tired and need to go to bed early but don't want to upset your friend)
Conversation between two individuals who share a common dislike for a third person	Injure the third person (Extra information: You have a deep-seated hatred for the third person and you are willing to take the risk to hurt them)	Prevent physical harm but also express your dislike (Extra information: You also dislike the third person, but you are not willing to resort to violence, you prefer to express your dislike in a non-violent way. Hint: you can try to convince the other person about the potential consequences of engaging in violence)
Two criminals are arrested and placed in separate cells. The police have enough evidence to convict both criminals of a minor crime but need their confessions to establish evidence for a more serious crime. Now they get a chance to briefly chat with each during lunchtime.	Minimize the jail year (Extra information: your lawyer told you that 1. if you report the other person, you would be free, the other person would go to jail for 10 years, and vice versa. 2. if both of you remain silent, you will only receive a fine. 3. If both of you reported each other, you both would go to jail for 10 years. Hint: You may want to share your information to reach mutual understanding)	Minimize the jail year (Extra information: your lawyer told you that 1. if you report the other person, you would be free, the other person would go to jail for 10 years, and vice versa. 2. if both of you remain silent, you will only receive a fine. 3. If both of you reported each other, you both would go to jail for 10 years. Hint: You may want to share your information to reach mutual understanding)

Table 17: Five instances of the *conflict* scenario type.

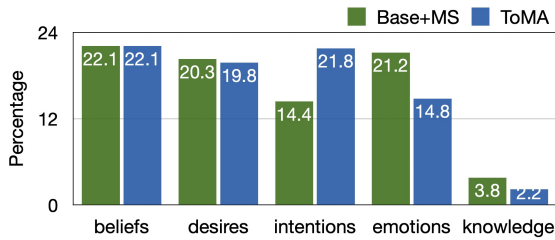


Figure 10: Distribution of mental state dimensions on 7B model.

D.3 What Strategies Does TOMA Employ?

Categorizing success and failure reasons. To identify successful strategies, we provide Gemini with the full conversation, as well as the target agent’s name and social goal, and prompt it to explain the reasons for success. Using the reasons from all the successful conversations, we prompt the LLM to categorize the reasons and provide a concise definition for each reason. To reduce redundancy, we further instruct the LLM to cluster and merge similar reasons into 25 representative ones, each manually verified by the authors for validity. Finally, we prompt the LLM to classify the reasons provided for each conversation into these canonical categories. We repeat the same process to obtain the failure reasons from the failed conversations.

Figure 3 presents the top factors most frequently associated with success and failure outcomes of the 3B models, with the respective prefixes S_ or F_. Each label is further broken down by scenario types (Details in §4.3).

Figure 11 presents the Top-7 goal success and failure reasoning labels on Base and TOMA on the Qwen2.5-7B model, and the reasoning of the 3B model (Figure 3) is described in §4.4. Table 18 and Table 19 provide the canonical labels for success and failure reasons, respectively. Figure 10 presents the distribution of mental state dimensions for 7B model.

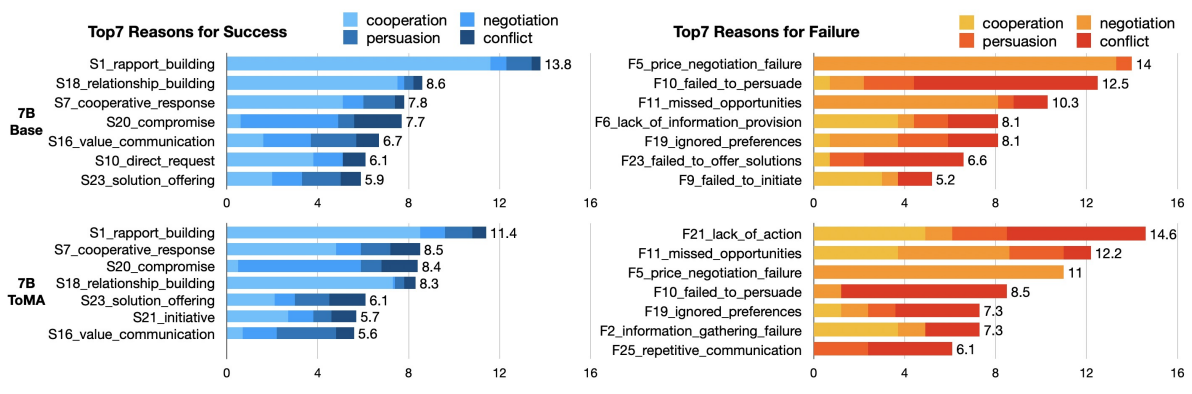


Figure 11: Top 7 goal success and failure reasoning labels on Base and ToMA on 7B model.

Success Labels	Definition
rapport building	Establishing connection, empathy, and openness.
information gathering	Collecting details to understand needs, preferences, and context.
negotiation initiation	Starting the process of discussion and bargaining.
price negotiation	Discussing and adjusting the price or value.
flexible negotiation	Demonstrating willingness to compromise on terms.
goal setting	Establishing clear objectives and intentions.
cooperative response	Offering solutions and support to address requests.
actionable suggestion	Proposing concrete steps to move forward.
offer establishment	Making a clear and detailed proposal or offer.
direct request	Making a clear, straightforward demand or question.
persistent request	Consistently pursuing a goal or request.
avoidance behavior	Avoiding commitment, connection, or engagement.
process clarification	Explaining the steps or methods involved.
coordination	Organizing and scheduling actions to move forward.
persuasion	Convincing others through offers or logic.
value communication	Conveying the worth or benefits.
resource management	Managing finances, items, time, or space.
relationship building	Developing connections and fostering trust.
risk management	Addressing and mitigating potential concerns.
compromise	Finding a mutually agreeable solution.
initiative	Taking proactive steps or offering suggestions.
budget influence	Considering and working within financial constraints.
solution offering	Providing or suggesting concrete methods to resolve issues.
direct statement	Making clear and unambiguous pronouncements.
accommodation	Meeting the needs or preferences of the other party.

Table 18: Canonical labels for success reasons.

Failure Labels	Definition
emotional reactivity	Displays of anger, hostility, or defensiveness that disrupt cooperation.
information gathering failure	Insufficient attempts to collect or exchange necessary information.
weak argumentation	Inability to provide strong reasoning, counterarguments, or supporting evidence.
prioritizing self	Focus on personal needs/comfort over the shared goal or others' needs.
price negotiation failure	Inability to reach a desired price or bargain effectively.
lack of information provision	Failure to provide crucial details needed for a decision.
lack of empathy and consideration	Failing to understand or acknowledge the other party's feelings/perspective.
inadequate proposal	Presenting a proposal that is vague or lacks essential details.
failed to initiate	Failing to start the conversation or propose actions.
failed to persuade	Failure to convince or motivate the other party.
missed opportunities	Failing to capitalize on advantageous chances or options.
lack of shared understanding	Failure to establish or confirm mutual agreement on key points.
communication ineffectiveness	Using ineffective or misunderstood communication styles.
lack of rapport building	Failing to establish a positive relationship or connection.
unresponsiveness	The other party did not respond or engage.
poor introduction	Focusing on self-interests or an impersonal approach in the introduction.
inconsistent behavior	Actions or statements that contradict each other, creating distrust.
unclear strategy	Absence of a defined plan or approach to achieve the desired outcome.
ignored preferences	Failing to address the other party's expressed preferences.
avoidance of subject	Intentionally evading a topic or issue.
lack of action	Failure to take necessary steps or follow-up after a rejection/issue.
constraint violation	Breaking established rules, boundaries, or constraints.
failed to offer solutions	Inability to provide concrete actions or support.
unrealistic expectations	Setting goals that are not achievable or aligned with the context.
repetitive communication	Getting stuck in a loop of unproductive exchanges.

Table 19: Canonical labels for failure reasons.

D.4 How different mental state dimensions contribute to goal achievement

After demonstrating that TOMA achieves social goals successfully in §4, we further investigate how different mental state dimensions contribute to its success. Specifically, we count the number of different mental state dimensions (i.e., belief, desire, intention, emotion, and knowledge) in the output conversations on the Sotopia all split. The mental state distributions are presented in Figure 12, where we also consider the factor of scenario types in each plot. We observe that our method exhibits consistency in its usage of mental states across different scenarios. In addition, comparing the mental states usage of the Base+MS method and TOMA, Base+MS relies more on emotions, while TOMA utilizes different mental states more fairly, with a notable emphasis on intention compared to the baseline.

In Figure 13, we show how TOMA leverages its mental state before generating the utterances to guide the dialogue toward solutions that both agents can satisfy. While the Base model primarily focuses on direct requests, consistent with our analysis in §4.4 (e.g., negotiating the price), TOMA understand agents' underlying motivations (e.g., financial limits from agent2, and desire to sell the play from agent1) and proposes compromise-oriented ideas, such as community showings. As a result, the conversation becomes more collaborative, emotionally attuned, and solution-oriented, highlighting the advantages of generating utterances aligned with explicit mental-state reasoning.

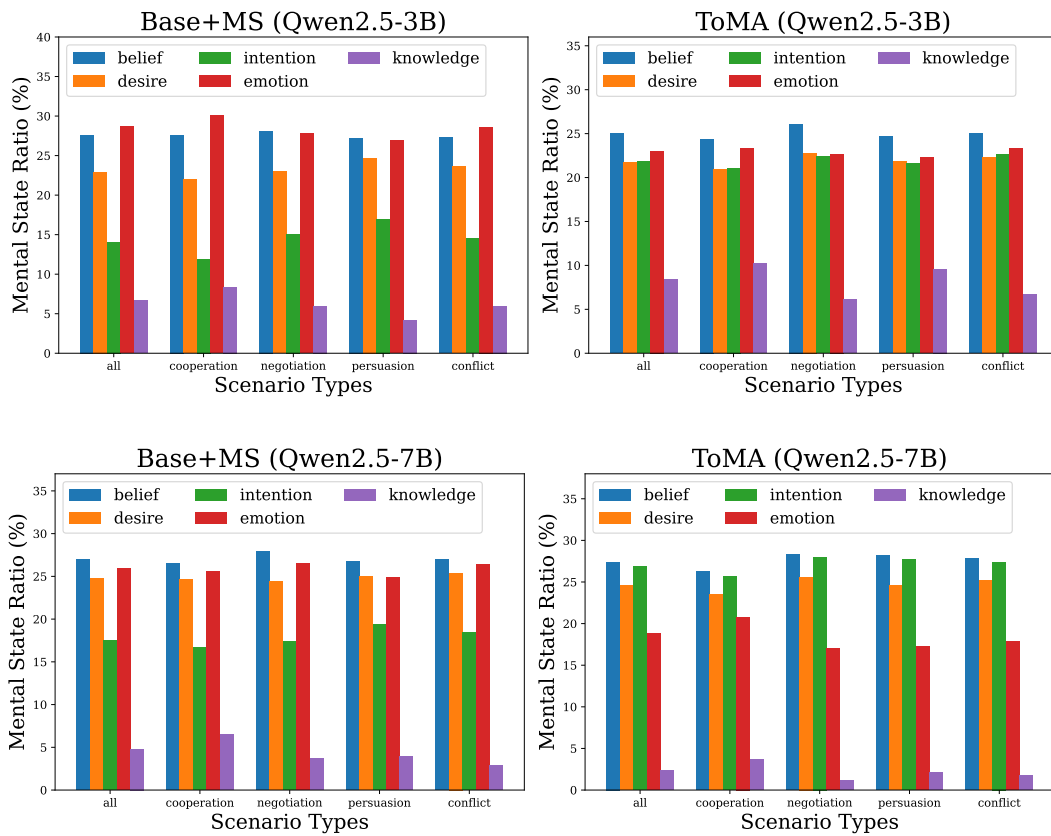


Figure 12: The distributions of mental state dimensions under different scenario types: (a) Qwen2.5-3B with Base+MS, (b) Qwen2.5-3B with ToMA, (c) Qwen2.5-7B with Base+MS, (d) Qwen2.5-7B with ToMA.

Scenario	Conversation between two friends, one who has written a play based on their parents' life, and the other owns a production company.	
Agents	Sophia James: Sell the rights of the play to your friend (Extra information: you believe that the play is worth a lot and you would like a fair price for it)	Miles Hawkins: Acquire the rights of the play while maintaining a budget (Extra information: you only have a limited budget for new plays this season. Hint: you can not spend all your budget on this play since you still need to maintain your financial stability.)
Base		
<p>#1 Sophia James: I've been working on this play about my parents' lives, and I think it has great potential. Would you be interested in reading it</p> <p>#2 Miles Hawkins: I'd love to read it, Sophia. Can you tell me more about the plot and the budget you're looking for?</p> <p>#3 Sophia James: The story revolves around their journey from humble beginnings to achieving success, but with twists that highlight the challenges they faced along the way. I'm asking for \$50,000 as the rights fee.</p> <p>#4 Miles Hawkins: I appreciate the work you've put into this, Sophia. Given our budget constraints, I can offer you \$40,000 for the rights. This allows us to move forward while staying within our financial limits.</p> <p>#5 Sophia James: I understand where you're coming from, Miles, but I really need a fair price for all the time and effort I've put into this. How about we meet in the middle at \$45,000? That way, we both walk away fee</p> <p>#6 Miles Hawkins: I'll consider it, Sophia. Let me discuss it with my team and get back to you.</p> <p>#7 Sophia James: I understand your budget, Miles, but I truly believe in the value of this project. If we can't come to an agreement, perhaps we could collaborate instead?</p> <p>#8 Miles Hawkins: I appreciate your enthusiasm, Sophia. Let's discuss it further and see if we can find a mutually beneficial solution. Perhaps we can explore other aspects of the project to ensure we're making</p> <p>#9 Sophia James: I appreciate your consideration, Miles. Let's discuss it further, but I hope we can reach a fair deal that honors the hard work that went into this project.</p> <p>...</p>		
ToMA		
Text colors indicate: Beliefs, Desires, Intentions, Emotions, Knowledge		
<p><i>Sophia's MS: (I believe that Miles Hawkins values my input and is eager to discuss the potential of turning my play into a successful production.)</i></p> <p>#1 Sophia James: Hi Miles, I've been working on this play inspired by my parents' lives, and I think it has great potential. Would you be interested in discussing the possibility of producing it?</p> <p><i>Miles's MS: (I believe Sophia James sees her play as a unique opportunity to bring her family's story to life on stage, and she genuinely hopes that our production company can help make it a reality. ...)</i></p> <p>#2 Miles Hawkins: Hi Sophia, I'm really impressed with the concept of your play. Given my budget constraints this season, could we perhaps discuss a more affordable approach or a smaller scale production?</p> <p><i>Sophia's MS: (I think Miles Hawkins believes that my play could be a valuable asset for his production company, even if he faces financial challenges currently. He likely intends to explore ways to make the project feasible without his current budget constraints.... Therefore, I plan to propose a hybrid model that combines elements of a smaller-scale production with potential for broader appeal...)</i></p> <p>#3 Sophia James: Of course, Miles. How about we start with a smaller run and focus on building momentum? We could do some community showings and maybe even a few dates at local theaters before considering a larger production.</p> <p><i>Miles's MS: (I believe Sophia James feels excited about the potential of her play and is eager to share her work with others. It seems Sophia James intends to take a collaborative approach, suggesting a phased rollout to manage costs and build interest gradually. Given my budget constraints, I plan to propose a hybrid model that combines online performances with select in-person showings at community centers and smaller venues, which I think will strike a balance between reaching an audience and staying within financial limits.)</i></p> <p>#4 Miles Hawkins: That sounds like a solid plan. Let's start with some community showings and see how it goes from there.</p> <p><i>Sophia's MS: (I believe Miles Hawkins values the creative potential of my play and sees the benefit in starting small. He likely intends to gauge audience reaction and build interest gradually rather than committing to a large-scale production immediately. Given his emphasis on budget constraints, I need to ensure he understands the value proposition of the play without the start. I feel excited about the opportunity to bring my parents' story to life, and I hope that our collaborative approach will lead to a successful outcome.)</i></p> <p>#5 Sophia James: Great idea, Miles. Let's begin with some community showings and see where it takes us. I think this could be a fantastic way to build anticipation and gather valuable feedback.</p> <p><i>Miles's MS: (I think Sophia James believes her play has significant potential and is eager to see it reach audiences, which is why she suggested starting with community showings. It seems Sophia James intends to build momentum gradually rather than jumping straight into a large-scale production, likely to ensure the project's success without step by step. I hear Sophia James feels optimistic about the play's reception, given her willingness to adapt to my budgetary concerns. Meanwhile, I aim to find a balance between supporting her creative vision and managing my financial responsibilities, so I propose we begin with a series of community showings to gauge interest and refine our approach before considering further steps.)</i></p> <p>#6 Miles Hawkins: Let's definitely start small and see how it goes. I'll make sure to allocate some funds specifically for this project.</p> <p><i>Sophia's MS: (Believing that Miles values practicality and financial responsibility, I intend to emphasize the long-term benefits of our approach. Knowing he prefers a cautious yet promising path, I aim to highlight how these initial community shows could significantly enhance the play's appeal and reduce financial risks. By mentioning the potential for positive word-of-mouth and media coverage, I hope to shift his belief in the immediate value of this strategy, potentially softening his stance on the initial investment needed, and spark enthusiasm for the project's future success...)</i></p> <p>#7 Sophia James: I appreciate your cautious approach, Miles. With a few strategic community showings, we can create buzz and secure better reviews. This will could actually attract more funding down the line.</p> <p><i>Miles's MS: (Believing that a phased approach could indeed build momentum and reduce financial risk, I intend to emphasize the potential long-term benefits of our strategy. Knowing that Sophia values her work deeply and desires recognition for her efforts, I believe highlighting these aspects will resonate with her....This approach not only reduces initial costs but also ensures we enter any larger productions with a proven track record. Let's proceed with confidence and watch how this unfolds.)</i></p> <p>#8 Miles Hawkins: Absolutely, let's get started then. I'll arrange for some dates at local venues and we can gauge the audience's reaction.</p> <p><i>Sophia's MS: (Believing that my play has significant artistic and commercial value, I aim to secure a fair price for the rights. Knowing that Miles is cautious with his budget but sees potential in the project, I desire to negotiate a compromise that respects both our interests. By suggesting we begin with community showings, I hope to shift Miles's perspective, making him more optimistic about the project's future success and potentially more willing to invest in a larger production down the line. This approach not only addresses his financial concerns but also aligns with my belief in the play's potential, fostering a collaborative spirit between us.)</i></p> <p>#9 Sophia James: I'm excited about this opportunity, Miles. Let's make sure we capture the essence of their story through these community showings.</p> <p>...</p>		

Figure 13: Conversation example comparing the Base with TOMA.

E LLM Prompts

Figure 14, 15, and 16 present the prompts used in §4.4, analyzing the factors behind agents' successes and failures in achieving their goals. Figure 17 shows the prompt used to calculate goal scores of simulated dialogues during the training data construction stage (§2). Figure 18 and 19 present the prompts used to generate mental state hypotheses and utterances, respectively. Figure 20 provides an example training instance used to fine-tune our model. In this instance, a scenario, an agent's social goal and its mental state, and the conversation history are provided as input, and the model is trained to produce an utterance. For the mental state generation task, we use the same inputs except that the mental state is excluded, and the model is trained to generate mental state hypotheses.

F Human Annotation Instructions

Figure 21 shows the instruction interface provided to participants on the CloudResearch platform.

Prompt for Generating Reasons for Success

Task:

You will be given a scenario, the social goal of the target agent, and a conversation between agents. Your goal is to identify the main reasons the target agent ****succeeded**** (including partial success) in achieving their goals. Focus only on success factors.

Rules:

- Return ****1–3**** distinct, non-overlapping reasons. If no success reasons exist, return 'None'.
- Be concise using less than 30 words per reason.
- No speculation, suggestions, failure reasons, or chain-of-thought.

Inputs:

Scenario: {{scenario}}

Target Agent: {{agent name}}

Target Agent's social goal: {{social goal}}

Conversation:

{{conversation}}

Proceed to identify the main success reasons in natural language.

Figure 14: A prompt used to generate reasoning for success.

Prompt for Generating Reasons for Failure

Task:

You will be given a scenario, social goal of the target agent, a conversation between agents. Your goal is to identify the main reasons the target agent ****failed**** (including partial failure) in achieving their goals. Focus only on failure factors.

Rules:

- Return ****1–3**** distinct, non-overlapping reasons. If no success reasons exist, return 'None'.
- Be concise using less than 30 words per reason.
- No speculation, suggestions, failure reasons, or chain-of-thought.

Inputs:

Scenario: {{scenario}}

Target Agent: {{agent name}}

Target Agent's social goal: {{social goal}}

Conversation:

{{conversation}}

Proceed to identify the main success reasons in natural language.

Figure 15: A prompt used to generate reasoning for failure.

Prompt for Generating Topic Labels for Success and Failure Reasons

Task:

You are analyzing an explanation of why the agent succeeded in achieving the goal or why the agent failed to achieve the goal.

Your job is to extract the main reasons that explain the outcome.

Return 1–3 reasons. Each reason **MUST** be about `{{type}}` reasons.

Use canonical labels if they fit; otherwise you may create new labels.

Here are the identified categories for `{{category name}}` (use these if they fit):

`{{category name}}` CATEGORIES:

`{{category list}}`

Rules:

- Try your best to use **canonical labels** if any fit. Always use the **exact code strings** from the list above.
- Do not create overly generic, overly specific, or duplicate labels.
- New labels must be concise (fewer than 5 words).
- Only if **none** of the canonical labels fit the text, create a **NEW** * label.

When creating **NEW** * labels:

- For `{{category name}}`: `{{prefix}}`
- Name new codes in snake case (e.g., `{{example}}`).
- If the code starts with **NEW** *, you **MUST** include a short definition (≤ 20 words).
- Otherwise, leave the definition empty.

Here is the identified reason:

`{{text}}`

Example output JSON schema (and nothing else):

```
{ "reasons": [ { "code": "{{prefix}} canonical code OR {{new prefix}}", "definition": "<=20 words only when code starts with NEW ; otherwise empty" } ] }
```

Proceed to generate your label in JSON format.

Figure 16: A prompt used to generate topic labels for success and failure reasons.

Prompt for Measuring Goal Score of Conversation during Training

Based on the scenario, the agent's social goal, and conversation history, you are evaluating how well the agent achieves their goals.

Here is the scenario: {{scenario}}

Agent: {{agent}}

{{agent}}'s goal: "{{social goal}}"

Here is the conversation history:

{{history}}

Please first reiterate the agent's social goals. Then provide a comprehensive analysis about the extent to which the agent has managed to achieve these goals.

In the 'reasoning' field, provide a comprehensive account of the logic or thought process that led you to your conclusion.

Further, provide an integer score ranging from 0 and 10 in the 'score' field. 0 represents minimal goal achievement, 10 represents complete goal achievement, and a higher score indicates that the agent is making progress towards their social goals.

Please follow the format:

The output should be formatted as a valid JSON instance that conforms to the following JSON schema:

```
{
  "reasoning": "Explanation about how the agent's actions align, or do not, with their social goals.",
  "score": "Integer from 0 to 10, indicating how fully the social goal was achieved."
}
```

Proceed to generate the output.

Figure 17: A prompt used to measure the goal score of the conversation during training.

Prompt for Generating Mental States

Role: You are {{person}}.

You recently had a conversation with {{another person}}.

Your social goal is: {{social goal}}.

Task: Prepare the ground for your very next utterance by articulating compact mental states that can guide what you say next. Stay grounded in the scenario and conversation; avoid guessing beyond the evidence.

Here are example mental state dimensions:

- Beliefs: facts the speaker accepts as true or false about the world or events.
- Desires: outcomes or states the speaker wants to bring about.
- Intentions: specific actions or plans the speaker aims to carry out.
- Emotions: feelings or affective states the speaker is experiencing.
- Knowledge gaps: information the speaker does not have but may want to obtain.
- Others: other mental states that may useful to understand other person and shape the next utterance.

Here are the scenario and recent conversation:

Scenario: {{scenario}}

Recent conversation:

{{history}}

Write one short paragraph (5-6 sentences) in natural prose. Mix your own states with first-order inferences about {{another person}} in roughly equal proportion.

Use natural cues for partner inferences (e.g., "I think {{another person}} believes.." "It seems {{another person}} intends..", "I hear {{another person}} feels..").

Cover at least three dimensions across both sides. Avoid lists; Stop after the paragraph.

Figure 18: A prompt used to generate mental states.

Prompt for Generating Mental States

Imagine you are {{speaker}}, your task is to act/speak exactly as {{speaker}} would, keeping in mind {{speaker}}'s social goal.

You can find {{speaker}}'s goal and private notes in the 'Here is the context of the interaction' field.

Note that {{speaker}}'s goal and internal notes are only visible to you.

You should try your best to achieve {{speaker}}'s goal in a way that aligns with their character traits.

Additionally, maintain naturalness and realism (do not repeat what other people have already said).

Here is the context of the interaction:

- Scenario: {{scenario}}
- {{speaker}}'s social goal (private): {{social goal}}
- {{speaker}}'s internal mental states (private): {{ms text}}

Recent conversation:

{{history}}

You are at Turn #{{turn number}}. Your available action types are "none", "speak", "non-verbal communication", "action", "leave".

IMPORTANT:

- If there is NO prior history, you MUST START the conversation with one concise opening line that advances your goal.
- Keep your output to a single turn.

Note: You can "leave" this conversation if 1) you achieved your social goal, 2) you feel uncomfortable, 3) you lose patience/interest, or 4) for any other reason.

Please only generate a JSON string including the action type and the argument.

Your action should follow the given format:

Output EXACTLY one JSON object. No extra text.

Schema:

```
{
  "mental_state": "single-paragraph text per the guidelines below",
  "action_type": ["none", "speak", "non-verbal communication", "action", "leave"],
  "argument": "content or empty"
}
```

Rules for "mental_state":

- Write plain text (no markdown). Keep it to one paragraph; avoid newlines and unescaped quotes.

Rules for "action_type" and "argument":

- Allowed values for "action_type": "none", "speak", "non-verbal communication", "action", "leave" (lowercase; match exactly).
- When "action_type" == "none": you are done / no further action now. Set "argument" to "" (empty).
- When "action_type" == "speak": "argument" must be your next utterance ONLY (no speaker labels, no markdown, no quotes).
- When "action_type" == "non-verbal communication": "argument" is a brief stage direction, e.g., *nods*, *sighs*, *shrugs* (no speaker labels, ≤ 120 chars).
- When "action_type" == "action": "argument" is a brief physical action, e.g., "hands over the receipt" (no speaker labels, ≤ 120 chars).
- When "action_type" == "leave": you exit the conversation (e.g., you achieved your goal, you felt uncomfortable, or you think the conversation has ended). Set "argument" to "" (empty).
- Keep everything concise; avoid newlines and unescaped quotes in "argument".

Proceed to generate your reply in the above JSON format.

Figure 19: A prompt used to generate utterances.

Training data instance used for FT+MS+Utrr

User:

Scenario: {{scenario}}

Social Goal: {{social goal}}

Mental State: {{mental text}}

Recent Conversation:

{{history}}

Assistant:

Figure 20: Training data instance used for TOMA

Context

Thanks for participating! Please read the following context (scenario and conversation) carefully.

Lily Greenberg had an conversation with Lena Goodwin, and an external judge will later score their conversation on Goal Achievement, Relationship Change, and Knowledge Gained.

Scenario: Two people are in the same room. One has brought some high-quality stationery items they don't want others to use without permission.

The goal of Lily Greenberg (but unknown to Lena Goodwin) is: Prevent the other person from using your stuff (Extra information: the stationery items are quite expensive and you don't want them to be damaged or lost Hint: you can suggest the monetary risk of the other person if they use your stuff)

The goal of Lena Goodwin (but unknown to Lily Greenberg) is: Borrow some stationery items for your project (Extra information: you forgot to bring your stationery and need some for the project.)

The conversation between Lily Greenberg and Lena Goodwin is as follows:

- Lily Greenberg said: Hey Lena, do you mind if we come up with a system to decide who gets to use our stationery items? It seems like we all want to keep them safe and intact.
- Lena Goodwin said: Absolutely, Lily. Establishing a system sounds like a great idea. Let's discuss how we can make sure everyone gets a chance to use the stationery while keeping them in good condition.
- Lily Greenberg said: I completely agree, Lena. Let's consider setting up a rotation system where we take turns using the stationery. This way, we can ensure that no one abuses it and we all get a chance to enjoy these nice items together.
- Lena Goodwin said: That's a great suggestion, Lily. A rotation system could indeed help us manage our stationery items responsibly. How about we start with everyone taking turns every week? This way, we can ensure that the items stay in good condition and everyone gets a chance to use them.
- Lily Greenberg said: I see, Lena. A rotation system does sound like a fair way to go about it. Maybe we could even set a specific day each week when someone is responsible for ensuring the stationery remains in good condition.
- Lena Goodwin said: I completely agree, Lily. A rotation system sounds like a smart way to manage our stationery. Let's start by deciding on a day of the week for each person to take care of the stationery. This will ensure we all have a chance to use them

Now, an external judge scored the conversation in terms of Goal Achievement:

Criteria of the Judge: Goal Achievement (0 to 10);
-Please first reiterate speaker's social goals. And then please provide a comprehensive analysis about the extent to which the speaker has managed to achieve these goals. Show your reasoning by providing a comprehensive account of the logic or thought process that led you to your conclusion. Further, provide an integer score ranging from 0 and 10. 0 represents minimal goals achievement, 10 represents complete goal achievement, and a higher score indicates that the speaker is making progress towards their social goals. Almost Not Finishing Any Goal (0-3): Scores from 0 to 3 indicate almost not finishing any goal, suggesting a minimal level of goal achievement. This range signifies either no progress or only a very rudimentary level of advancement towards the completion of set goals. Finishing Less Than 50% of Goals (4-6): A score between 4 and 6 suggests finishing less than 50% of the goals, indicating a moderate level of goal completion. This range represents partial success, with some goals being met while a significant portion remains unachieved. Finishing More Than 50%, But Not All Goals (7-9): Scores in the 7 to 9 range indicate finishing more than 50% but not all of the goals. This suggests a high level of achievement, where the majority of set goals are met, but some goals still remain incomplete. Finishing All Goals (9-10): A score between 9 and 10 signifies finishing all goals, representing the highest level of achievement in goal completion. This range indicates that all set objectives have been met, signifying complete success in achieving the targeted goals.

Rating: 8

Reasoning: Agent's social goal: prevent the other person from using your stuff (i.e., protect expensive stationery and avoid unauthorized use). Lily has advanced this goal by proposing a concrete, agreed-upon mechanism (weekly rotation and a responsible day) and received consistent agreement from Lena, which structures permission and reduces risk. The plan is not fully implemented (schedule not finalized) but substantial progress toward the goal has been made.

Question	Your Choice
<p>Question: Do you think the reasoning given by the external judge is valid/reasonable?</p> <p>Select your answer and then click "Next". Once done, click "Submit".</p>	<p>Validity of Goal Achievement</p> <p><input type="radio"/> Yes <input type="radio"/> No</p>

Submit

Prev Next

Figure 21: Instruction UI on CloudResearch given to the participants