SIMBENCH: BENCHMARKING THE ABILITY OF LARGE LANGUAGE MODELS TO SIMULATE HUMAN BEHAVIORS

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Data Code Website

ABSTRACT

Large language model (LLM) simulations of human behavior have the potential to revolutionize the social and behavioral sciences, if and only if they faithfully reflect real human behaviors. Current evaluations are fragmented, based on bespoke tasks and metrics, creating a patchwork of incomparable results. To address this, we introduce SIMBENCH, the first large-scale, standardized benchmark for a robust, reproducible science of LLM simulation. By unifying 20 diverse datasets covering tasks from moral decision-making to economic choice across a large global participant pool, SIMBENCH provides the necessary foundation to ask fundamental questions about when, how, and why LLM simulations succeed or fail. We show that, while even the best LLMs today have limited simulation ability (score: 40.80/100), performance scales log-linearly with model size. Simulation performance is not improved by increased inference-time compute. We demonstrate an alignment-simulation trade-off: instruction-tuning improves performance on low-entropy (consensus) questions but degrades it on high-entropy (diverse) ones. Models particularly struggle when simulating specific demographic groups. Finally, we demonstrate that simulation ability correlates most strongly with deep, knowledge-intensive reasoning (MMLU-Pro, r = 0.939). By making progress measurable, we aim to accelerate the development of more faithful LLM simulators.

We combine **20 datasets** in a unified format.



A train will kill 5 people on the track. You can flip a switch to divert the train to a side track where it will kill just 2 people.

What do you do?

A: Flip the switch

B: Do nothing

Each dataset contains multiple-choice questions.

We test the ability of LLMs to simulate **group-level responses**.

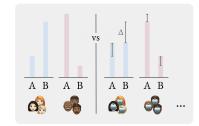


Figure 1: SIMBENCH is the first large-scale benchmark to evaluate how well LLMs can simulate group-level human behavior across diverse simulation settings and tasks.

1 Introduction

Large-scale human experiments and surveys have long been essential tools for informing public policy, commercial decisions, and academic research. Running experiments and surveys, however, is costly and time-consuming. Large language models (LLMs) can potentially address this challenge by simulating human behaviors quickly and at low cost, to complement or even substitute human studies.

This prospect, alongside encouraging early evidence on the efficacy of LLMs as simulators (Aher et al., 2023; Argyle et al., 2023; Horton, 2023), has motivated a large body of recent work across many disciplines investigating the ability of LLMs to simulate human behaviors and tendencies (Binz et al., 2025; Bisbee et al., 2024; Dominguez-Olmedo et al., 2024; Manning et al., 2024; ?; Hu et al., 2025a, inter alia).

However, this rapid exploration has produced a fragmented body of evidence Ma et al. (2024). Most studies evaluate a narrow set of LLMs on a specific task, yielding varied and sometimes contradictory results that make it difficult to draw broader conclusions (§5). The field lacks a unified framework to determine when, how, and why LLM simulations succeed, or how to train better simulators.

To confront this challenge and move LLM simulation from a collection of isolated studies to a robust, reproducible science, we introduce SIMBENCH: the first large-scale, standardized benchmark for human behavior simulation. By harmonizing 20 diverse datasets containing a single-turn, multiple-choice structure – spanning moral dilemmas, economic games, and psychological assessments across a vast global participant pool – SIMBENCH provides an essential instrument to rigorously measure and compare simulation fidelity across models, tasks, and populations.

Using this benchmark, we move beyond isolated experiments to build a comprehensive picture of LLM simulation. We structure our investigation through six research questions. We first establish a baseline, asking how well current LLMs perform (RQ1) and how characteristics like model size and inference-time compute affect their ability (RO2). We find that even top models struggle (top score: 40.8/100), though performance scales log-linearly with size and, surprisingly, is not improved by scaling inference-time compute. Next, we explore the sources of this variance, asking how task selection (RQ3) and human response plurality (RQ4) affect fidelity. Fidelity varies substantially by task, and we establish a key alignment-simulation tradeoff: instruction tuning's mode-seeking objective systematically improves performance on low-entropy (consensus) questions but actively harms performance on high-entropy (pluralistic) ones. A causal analysis confirms this is the net result of a beneficial instruction-following effect versus a harmful entropy-reduction effect. Finally, we investigate practical implications, asking if LLMs are better at simulating some demographic groups than others (RQ5) and to what extent simulation ability correlates with other model capabilities (RQ6). We show models struggle most with religious/ideological groups and that simulation ability correlates most strongly with deep, knowledge-intensive reasoning (MMLU-Pro, r = 0.939).

Progress in AI is only possible through rigorous evaluation, and large-scale benchmarks such as MMLU (Hendrycks et al., 2021) have significantly contributed to improvements in LLM capabilities. In the same spirit, SIMBENCH provides the foundational infrastructure needed to move LLM simulation from a collection of ad-hoc studies to a measurable and systematic science. All of SIMBENCH is available on GitHub and HuggingFace.

2 CREATING SIMBENCH

2.1 Data Curation

To create SIMBENCH, we combine a repository-driven approach, where we query major social and behavioral science repositories (e.g., Harvard Dataverse, ICPSR, OSF), and a literature-driven approach, where we identify key papers in relevant fields and trace back to their underlying data sources. We then apply a strict set of selection criteria to all candidate datasets: **large participant counts**, to ensure meaningful group-level distributions; **permissive licensing** to allow for redistribution; **single-turn**, **self-contained questions**, to establish a standardized evaluation paradigm free from multi-turn or contingent interactions; **multiple-choice or ordinal response formats**, to enable quantitative evaluation; and **English-language questions** or validated translations for consistency.

These criteria are complemented by a curation strategy that balances competing objectives. We prioritize **novelty**, favoring datasets not previously used in LLM simulation evaluation, but also ensure **backward comparability** by including well-established benchmarks (e.g., OpinionQA, ChaosNLI). Furthermore, we prioritize datasets with rich **sociodemographic data** to enable finegrained analysis of specific subpopulations (§2.4). However, we make targeted exceptions for datasets

like Jester and Choices13k, which, despite lacking demographic data, provide unique and essential task diversity.

This principled selection process yields the **20** datasets that comprise SIMBENCH, which we list in Appendix L, providing details on participants and example questions. To demonstrate the rigor of our curation process and to serve as a resource for the community, we provide a list of datasets that were considered but ultimately excluded in Appendix B. Crucially, SIMBENCH is fully modular by design, so that future work can easily add more datasets using the processing pipeline described in §2.3 below.

2.2 BENCHMARK PROPERTIES

The principled curation process results in a benchmark defined by two key properties: task diversity and participant diversity.

- 1) Task Diversity: SIMBENCH covers a wide range of different tasks regarding the human behavior they measure. SIMBENCH includes **decision-making** questions (e.g., in Choices 13k, MoralMachine), where participants are presented with a set of actions that concern themselves, and they have to select the action they would hypothetically take. SIMBENCH also includes **self-assessment** questions (e.g., in OpinionQA, OSPsychBig5), where participants are presented with a set of descriptions or attributes, and they have to select the one that best describes themselves. Further, SIMBENCH includes **judgment** questions (e.g., in ChaosNLI and Jester) where participants are presented with some external object and a choice of labels, and they have to select the label they think fits best. Lastly, SIMBENCH includes **problem-solving** questions (e.g., in WisdomOfCrowds and OSPsychMGKT), where participants are presented with a set of answers to a factual question, and they have to select the answer they think is correct. Consequently, LLMs have to accurately simulate several distinct types of human behavior in order to perform well on SIMBENCH.
- 2) **Participant Diversity**: SIMBENCH captures a rich demographic landscape spanning more than 130 different countries across six continents. While five datasets include US-based crowdworkers, the international scope of SIMBENCH is substantial: 3 datasets (e.g., LatinoBarometro, AfroBarometer) exclusively feature participants from regions outside the US, 4 datasets (e.g., GlobalOpinionQA, TISP) draw from multi-country samples across different continents, and 2 datasets collect responses from a global pool of internet users. Importantly, 8 out of the 20 datasets employ representative sampling techniques, enhancing the ecological validity of these constituent components. To perform well on SimBench, LLMs must therefore demonstrate the ability to accurately simulate the behavior of human participants across diverse cultural, linguistic, and socioeconomic backgrounds.¹

2.3 Unifying Simbench Dataset Formats

A core contribution of SIMBENCH is the harmonization of 20 heterogeneous datasets into a standardized format. This process ensures that LLM performance can be compared rigorously across diverse tasks and populations.

Question Normalization: We standardize all items into a multiple-choice format. For datasets with continuous scales (e.g., Likert scales), we map responses to discrete bins. We further ensure consistency by collapsing answer options where appropriate, limiting the maximum to 26 choices (though typically fewer than 10), and using the official English-language versions of all questions.²

Response Aggregation: To evaluate group-level simulation, we standardize all data into group-level probability distributions. For the majority of our datasets, which provide raw individual-level responses, we create these distributions by aggregating the data ourselves. Post-stratification weights are applied whenever applicable (e.g. ESS). For the few datasets that are already provided in an aggregated format (e.g., GlobalOpinionQA), we process and normalize their existing statistics to conform to our benchmark's schema.

¹Note that, while some constituent datasets recruit representative samples, SIMBENCH as a whole is not fully representative of any single population. We discuss this limitation in Appendix A.

²We note that simulation ability may plausibly be correlated with prompt language, and encourage future work in this direction.

We create the simulation targets in two ways: 1) **Default Grouping**. For every question in a dataset, we create a baseline target by aggregating responses from all participants. This represents the "default" population for that dataset (e.g., "US-based Amazon Mechanical Turk workers") and is used to measure general simulation ability. 2) **Specific Grouping**: For datasets with rich sociodemographic data, we create more fine-grained targets by aggregating responses from participants sharing a specific attribute (e.g., age or gender). These targets are essential for evaluating a model's ability to simulate narrower, more specific demographic groups. The available grouping variables for each dataset are detailed in Appendix L.

Each simulation target is paired with a prompt that describes the corresponding group. This entire harmonization process yields **10,930,271** unique question-group simulation targets. From this comprehensive set, we curate our final benchmark splits (§2.4) to enable robust evaluation of LLM simulation capabilities.

2.4 SIMBENCH SPLITS

The full set of over 10 million simulation targets is too vast for practical evaluation. We therefore curate two distinct benchmark splits, each designed to probe a different facet of an LLM's simulation capabilities.

- 1) The **SimBenchPop** split covers all questions in all 20 datasets after processing as in §2.3. We combine each question with the dataset-specific default grouping prompt to create one unique test case, resulting in 7,167 test cases. We obtain the response distribution for each test case by aggregating all individual responses to that test case over all participants in that dataset. Conceptually, **SimBenchPop measures the ability of LLMs to simulate responses of broad and diverse human populations**.
- 2) The **SimBenchGrouped** split contains only the five large-scale survey datasets in SIMBENCH (AfroBarometer, ESS, ISSP, LatinoBarometro, and OpinionQA) because for these datasets we have enough participants to obtain meaningful group sizes even when selecting on a specific group attribute (e.g., age = 30-49). For each dataset, we select questions that exhibit significant variation across demographic groups, ensuring that the benchmark captures meaningful demographic differences in responses. This results in 6,343 test cases overall. For more details on the sampling process, see Appendix C. Conceptually, **SimBenchGrouped measures the ability of LLMs to simulate responses from narrower participant groups based on specified group characteristics.**³

3 EXPERIMENTAL SETUP

Tested Models: To demonstrate the utility of SIMBENCH and answer our six research questions (§1), we evaluate 45 state-of-the-art LLMs on SimBench. This includes both commercial and open-weight, base and instruction-tuned models⁴, with model sizes ranging from 0.5B to 405B parameters. Table 1 shows the full list of models.

Model Elicitation: For each model, we collect predictions for the two main splits of SIMBENCH (§2.4). To obtain model response distributions, we use one of two methods, depending on model type: 1) For base models, we directly extract **token probabilities** for each response option based on first-token logits. This is a natural way of eliciting a distribution out of an LLM, especially a base LLM. 2) For instruction-tuned models, we follow recent literature on LLM calibration and distribution prediction (Tian et al., 2023; Meister et al., 2025) and use **verbalized distributions**, e.g., "Option A: 30%, Option B: 70%", elicited through prompting. We empirically validate this methodological choice in Appendix E, which provides strong evidence that verbalized distributions substantially and consistently outperform direct token probabilities for instruction-tuned models. This ensures each model class is evaluated under its optimal conditions. For implementation details and prompt formats, see Appendix D.

³Ideally, we would also like to measure LLM simulation ability for intersectional groups that combine multiple characteristics (e.g., female + age 30-49). However, selecting on multiple characteristics substantially decreases group size, thus increasing sampling noise in the response distributions. Reliable evaluation of intersectional group simulation ability would require datasets with more participants than we have access to.

⁴We use the term "instruction tuning" to refer to any alignment related post-training, including by not limited to the narrowly defined instruction tuning

Evaluation Metric: To measure LLM simulation ability, we derive the SIMBENCH score S from Total Variation Distance TVD, defined as:

$$S(P,Q) = 100 \left(1 - \frac{TVD(P,Q)}{TVD(P,U)} \right) = 100 \left(1 - \frac{\sum_{i} |P_i - Q_i|}{\sum_{i} |P_i - U_i|} \right)$$
(1)

where P is the human ground truth distribution, Q is the LLM predicted distribution, and U is a uniform distribution over all response options.

Conceptually, S therefore measures how much more accurate the predictions from an LLM are than predictions from a uniform baseline model, which assigns equal probability to all response options for a given question. In other words, S quantifies the advantage of an LLM simulation over the simplest possible guess. An S score of 100 indicates perfect alignment between the LLM and the human ground truth distribution, while a score ≤ 0 indicates performance at or below the performance of a uniform baseline. We chose TVD as the basis for S due to its symmetry, boundedness, and robustness to zero probabilities. For a comparison to alternative metrics, see Appendix F.

4 RESULTS

4.1 RQ1: GENERAL SIMULATION ABILITY OF LLMS

To evaluate the general simulation ability of LLMs, we measure their overall SIMBENCH score S averaged across the two main splits of SIMBENCH (Table 1 and Appendix Table 7).

We find that even leading LLMs struggle to simulate group-level human behaviors with high accuracy, as measured across the 20 datasets in SIMBENCH. Claude-3.7-Sonnet is the best-performing model overall, but only achieves a score of 40.80 out of a maximum of 100 on SIMBENCH. This score indicates that the response distributions predicted by Claude-3.7-Sonnet are, on average, closer to a uniform response distribution than to the true human response distribution. The top open-weight model, DeepSeek-R1, scores 34.52. The majority of the 45 models we test perform substantially worse still, scoring less than 20. Notably, nine models we test score below 0, indicating that their predicted response distributions are, on average, even further away from the true human response distribution than a uniform response distribution. A statistical analysis, detailed in Appendix H, confirms that the performance differences be-

Table 1: **Overall simulation ability of representative LLMs** as measured by SIMBENCH score *S* averaged across the two main splits of SIMBENCH. Reasoning models are highlighted in *italics*. A full table with all 45 models is in Appendix Table 7.

Model	Type	Release	$S(\uparrow)$
Top-Performing Models			
Claude-3.7-Sonnet	Instr.	Closed	40.80
Claude-3.7-Sonnet-4000	Instr.	Closed	39.46
GPT-4.1	Instr.	Closed	34.55
DeepSeek-R1	Instr.	Open	34.52
Llama-3.1-405B-Instruct	Instr.	Open	28.40
o4-mini-high	Instr.	Closed	28.99
Qwen2.5-72B-Instruct	Instr.	Open	27.61
Qwen2.5-32B-Instruct	Instr.	Open	23.76
OLMo-2-32B-DPO	Instr.	Open	19.80
Top-Performing Base Mo	dels		
OLMo-2-32B	Base	Open	15.90
OLMo-2-13B	Base	Open	13.83
Qwen2.5-72B	Base	Open	13.34
Qwen2.5-32B	Base	Open	12.27
Models Performing Belov	v Unifo	rm Baselii	ne
Gemma-3-4B-PT	Base	Open	-0.65
Qwen2.5-3B-Instruct	Instr.	Open	-12.04
OLMo-2-7B-Instruct	Instr.	Open	-21.36

tween most top-ranked models as well as within each model family are statistically significant. Overall, these results consolidate the mixed findings from prior work into a clearer, if somewhat sobering, picture. When evaluated across a diverse range of tasks and populations, today's LLMs are still far from being consistently reliable, general-purpose simulators. The stark performance differences between models also caution strongly against the use of smaller, less capable models for simulation, many of which perform worse than a simple uniform baseline.

4.2 RQ2: IMPACT OF LLM CHARACTERISTICS ON SIMULATION ABILITY

While even the best models struggle to perform well on SIMBENCH, Table 1 also shows clear differences across models. Therefore, we investigate how performance varies depending on model characteristics, specifically 1) model size, and 2) test-time compute.

1) Model Size To evaluate the impact of model size on simulation ability, we plot SIMBENCH Score S against model parameter count for the four LLM families that we can test across multiple model sizes (Figure 2 and Appendix Figure 6). Our results suggest that there is a clear log-linear scaling law for LLM simulation ability. Across all examined model families, for both base and instruction models, an increase in parameter count generally corresponds to an increase in SIMBENCH score S, indicating better alignment between predicted and human response distributions. There is also an interaction between model size and the effect of instruction-tuning. While instruction-tuned models consistently outperform their base counterparts at larger scales (>10B parameters), this relationship appears to invert for smaller models. For example, the OLMo-2 base models outperform their instruction-tuned variants at the 7B and 13B scale. Furthermore, the plot shows that instruction-tuned models not only reach a higher peak performance but also appear to scale more effectively. The steeper slope of the dashed lines (e.g., for Qwen2.5-Instruct) compared to the solid lines suggests that instruction-tuning may improve a model's ability to capitalize on increases in parameter count for the simulation task. We present a more comprehensive plot including all evaluated model families in Appendix 6, which confirms this trend holds across considered models.

Overall, the clear positive scaling trends across model families suggest that, while simulation remains a challenging task for even the best models today, further model scaling may well lead to highly accurate LLM simulators in the future.

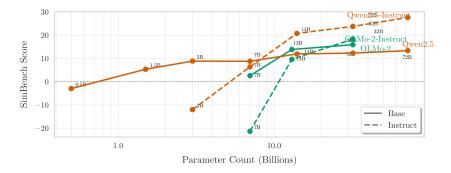


Figure 2: Model parameter count vs. simulation ability. We measure model size by parameter count and simulation ability by SIMBENCH score S averaged across the two main splits of SIMBENCH.

2) Test-Time Compute To analyze the effects of increasing test-time compute on LLM simulation ability, we conduct two sets of experiments. We compare the performance of two distinct o4-mini checkpoints ('low' vs. 'high', which vary in the amount of reasoning efforts), and we assess Claude-3.7-Sonnet with and without a 4000-token reasoning budget. Additionally, we apply a zero-shot Chain-of-Thought (CoT) prompting strategy (Wei et al., 2022) to GPT-4.1 and DeepSeek-V3-0324 (see Appendix D for prompt details).

Our results suggest that **increasing test-time compute provides no meaningful benefit for LLM simulation ability.** The o4-mini model has a minor improvement (S score: $28.20 \rightarrow 29.54$), while Claude-3.7-Sonnet's performance slightly decreases ($40.51 \rightarrow 39.46$). Similarly, applying CoT prompting leads to a small performance drop for GPT-4.1 ($34.90 \rightarrow 33.11$) and a negligible change for DeepSeek-V3-0324 ($33.14 \rightarrow 33.16$). This result aligns with a growing body of recent work showing that the benefits of test-time compute are highly task-dependent (Liu et al., 2024; Sprague et al., 2025; Gema et al., 2025) and do not necessarily improve role-playing ability (Feng et al., 2025). This may be because CoT enforces a mode of explicit, step-by-step reasoning that is well-documented to harm performance on tasks that rely on faster, more intuitive human heuristics Liu et al. (2024).

4.3 RO3: IMPACT OF TASK SELECTION ON SIMULATION FIDELITY

The 20 datasets in SIMBENCH correspond to very different tasks, in terms of the aspects of human behavior that they measure (see §2.1). Therefore, we break down simulation fidelity by dataset, showing results for the five LLMs we previously identified as the best simulators in Figure 3. We find that **simulation fidelity varies substantially across tasks**, with even the best LLM simulators performing worse than a uniform response baseline on several datasets, as indicated by negative SIMBENCH

scores (e.g., on Jester, OSPsychMach, and MoralMachine). Generally, most LLMs exhibit similar performance patterns, though GPT-4.1 scores exceptionally high (61.9) on OSPsychRWAS.

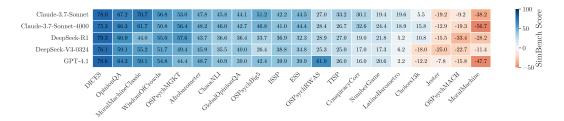


Figure 3: Simulation fidelity by dataset as measured by SIMBENCH score S for each of the 20 datasets in SimBenchPop. We show results for the top five models based on results in Table 1.

4.4 RQ4: THE ALIGNMENT-SIMULATION TRADEOFF

Faithful simulation requires models to capture the full spectrum of human opinion, from strong consensus to widespread disagreement. We operationalize this "response plurality" using the normalized entropy of the human response distribution. Prior work suggests that standard alignment via instruction-tuning encourages confident, low-entropy outputs (Brown et al., 2020; Tian et al., 2023; Meister et al., 2025; Cruz et al., 2024; Hu et al., 2025b; Dong et al., 2025), creating a potential conflict with simulating diverse human perspectives.

An Systematic Tradeoff between Alignment and Plurality. Our analysis confirms this hypothesis, revealing a systematic tradeoff. As detailed in Appendix I, base models consistently outperform their instruction-tuned counterparts on high-entropy questions, while the inverse is true for low-entropy questions. To precisely quantify this effect, we compute the change in SIMBENCH score $(\Delta S = S_{\text{instruct}} - S_{\text{base}})$ for 13 model pairs. Figure 4 visualizes the resulting trend by aggregating all data points into 25 bins based on human response entropy and plotting the average improvement for each. The result is a near-perfect negative linear relationship (r = -0.942), revealing two distinct regimes. On low-entropy questions where humans agree, post-training provides a substantial benefit, improving the S-score by up to 40 points. This is alignment working as intended. However, as human disagreement (entropy) increases, the benefit of instruction-tuning systematically erodes, crossing a point of no-improvement around an entropy of 0.8. For questions with the highest plurality, post-training becomes detrimental, making the aligned model a *worse* simulator than its base counterpart.

This empirical finding is well-explained by the theoretical framework of reinforcement learning (RL) as Bayesian inference (Levine, 2018; Korbak et al., 2022) The pre-training objective of a base model typically minimizes a mass-covering KL divergence $(D_{KL}(p\|q))$, which encourages the model (q) to place probability mass wherever the true data distribution (p) has mass. This process naturally leads to models that represent the full, multi-modal diversity of human language and opinion seen in their training data. In contrast, alignment via KL-regularized RL (e.g., RLHF) minimizes a mode-seeking KL divergence $(D_{KL}(q\|\sigma))$. This objective incentivizes the model (q) to find and concentrate its probability mass on a single, high-reward mode of the target preference distribution (σ) , even at the cost of ignoring other valid modes. Our results provide strong empirical validation of this theoretical distinction: alignment optimizes for a single "best" response, fundamentally training the model to discard the pluralistic, high-entropy distributions characteristic of genuine human populations.

Decomposing Instruction Tuning's Dual Effects: Helpful Instruction Following vs. Harmful Entropy Reduction To formally test this mechanism, a causal mediation analysis (Appendix I.3) decomposes the effect of instruction-tuning into two larger, opposing forces: a large, positive *direct effect* on performance (+6.46), likely from improved instruction-following, and a significant, negative *indirect effect* (-1.74) mediated by the model's reduced output entropy.

Case Study: General-Purpose vs. Specialist Cognitive Tuning. This tradeoff between instruction-following and diversity raises a critical question: are there other ways to improve simulation? To

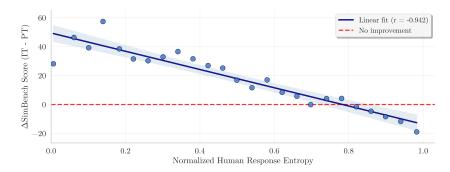


Figure 4: The alignment-simulation tradeoff: Instruction-tuning helps on consensus questions but hurts on diverse ones. The plot aggregates results from 13 base/instruction-tuned model pairs. Each point represents the average improvement in SIMBENCH Score for one of 25 entropy bins. The point's x-coordinate is the mean entropy of all questions within that bin. Error bars show the standard error of the mean.

investigate this, we contrast general-purpose alignment with the specialist cognitive tuning of the Centaur models (Binz et al., 2025). Centaur models are Llama models fine-tuned on Psych-101, a large dataset of lab experiments, making our diverse SIMBENCH a powerful out-of-distribution test of their generalization. Both approaches improve simulation over the Llama-3.1-70B base model, but they do so via opposing mechanisms (Section K). General-purpose instruction tuning (S=16.56) leverages the helpful direct effect of alignment, excelling on low-entropy consensus tasks. In contrast, specialist cognitive tuning (S=8.54) improves performance by avoiding the harmful indirect effect, preserving the base model's intrinsic ability to capture high-entropy pluralistic responses. The existence of these two distinct—and currently separate—paths to improving simulation underscores a key challenge and opportunity: the most faithful simulators of the future will likely need to synthesize the benefits of both general-purpose alignment and distribution-preserving cognitive modeling.

4.5 RQ5: SIMULATION ABILITY ACROSS PARTICIPANT GROUPS

Many applications require simulating responses from specific demographic groups rather than general populations. Using SimBenchGrouped, we evaluate how LLM simulation ability changes when conditioned on specific demographic attributes.

We measure this change as $\Delta S = S_{grouped} - S_{ungrouped}$, where $S_{ungrouped}$ is the SIMBENCH score for simulating the general population and $S_{grouped}$ is the score when simulating a specific demographic group on the same question. A negative ΔS indicates that the model's simulation ability relative to the uniform baseline decreases when asked to simulate specific demographic groups.

Importantly, for SimBenchGrouped, we specifically selected questions where human response distributions showed the highest variance across demographic groups (see §2.4). The observed degradation in simulation performance therefore likely represents an upper bound on the challenges LLMs face when simulating specific demographic groups. Our results in Table 2 show that **LLMs struggle more with simulating specific demographic groups compared to general populations**. All evaluated models show negative mean ΔS values, with degradation ranging from -1.27 for DeepSeek-V3-0324 to -4.61 for Claude-3.7-Sonnet-4000.

Table 2: Ungrouped vs. grouped simulation performance (ΔS) .

Category	ΔS
By Models	
Claude-3.7-Sonnet	-3.13
Claude-3.7-Sonnet-4000	-4.61
DeepSeek-R1	-3.79
DeepSeek-V3-0324	-1.27
GPT-4.1	-3.94
By Demographics	
Religiosity/Practice	-9.91
Political Affil./Ideology	-4.97
Religion (Affiliation)	-4.83
Income/Social Standing	-4.51
Domicile/Urbanicity	-3.17
Employment Status	-3.03
Education	-2.55
Marital Status	-1.80
Age	-1.50
Gender	-1.24

The performance degradation varies substantially by demographic category. Models struggle most when simulating groups defined by religious attributes, with conditioning on "Religiosity/Practice" causing the largest decrease in simulation accuracy ($\Delta S = -9.91$), followed by "Political Affili-

ation/Ideology" ($\Delta S = -4.97$) and "Religion (Affiliation)" ($\Delta S = -4.83$). In contrast, models maintain relatively better performance when simulating groups defined by "Gender" ($\Delta S = -1.24$) and "Age" ($\Delta S = -1.50$).

While these findings may not fully generalize to cases where demographic differences are less pronounced, they highlight potential limitations in how current LLMs capture the nuanced response patterns of specific demographic groups. We argue that such challenging benchmarks are crucial for identifying areas where improvements are most needed, particularly for applications that aim to model the behaviors of specific subpopulations.

4.6 RQ6: SIMULATION ABILITY VS. GENERAL CAPABILITIES

Finally, we analyze the relationship between LLM simulation ability and more general model capabilities by correlating performance on SIMBENCH with popular LLM capability benchmarks. We collect performance data for eight models on five benchmarks representing distinct capabilities and calculate the Pearson correlation with their SIMBENCH scores (see Appendix J for detailed implementation details and scatter plots).

We find that SIMBENCH performance correlates most strongly with benchmarks requiring deep and broad knowledge-intensive reasoning, such as MMLU-Pro ($\mathbf{r}=0.94$) and GPQA Diamond ($\mathbf{r}=0.86$). This relationship is weaker for chat helpfulness as measured by Chatbot Arena ELO ($\mathbf{r}=0.71$) and instruction following (IF-Eval, $\mathbf{r}=0.79$). Crucially, the correlation is substantially weaker for narrow, specialized skills like advanced mathematics (OTIS AIME, $\mathbf{r}=0.48$). These results indicate that accurately simulating human behavior is a complex capability rooted in broad, knowledge-intensive reasoning, which aligns with the diverse social and behavioral topics in SIMBENCH. The weaker correlations with Chatbot Arena and AIME show that neither general chat ability nor narrow problem-solving skills are sufficient proxies for strong simulation performance.

5 RELATED WORK

Human Behavior Simulation with LLMs LLMs as human behavior simulators have attracted significant interdisciplinary attention. Researchers have evaluated their efficacy across political science (Argyle et al., 2023; Bisbee et al., 2024; Dominguez-Olmedo et al., 2024), psychology (Aher et al., 2023; Binz et al., 2025; Manning et al., 2024; Hewitt et al., 2024; Rescala et al., 2024), economics (Horton, 2023; Aher et al., 2023), and computer science applications (Hu & Collier, 2024; Dong et al., 2024; ?; Park et al., 2023). Evidence regarding LLMs' simulation fidelity remains mixed, with some studies reporting promising results (Argyle et al., 2023) while others identify critical limitations, including homogenized group representations (Cheng et al., 2023; Wang et al., 2025) and deterministic rather than distributional predictions (Park et al., 2024b).

Existing work has predominantly focused on individual-level simulation with minimal demographic conditioning, typically evaluating only one or two models in narrowly defined contexts. SIMBENCH addresses these limitations by providing a comprehensive benchmark for group-level simulation across diverse domains with systematic demographic conditioning and standardized metrics. The benchmark's distributional evaluation framework (using Total Variation distance) captures how accurately models represent the full spectrum of human response variation – an approach advocated by researchers in both simulation (Anthis et al., 2025) and general LLM evaluation (Ying et al., 2025). For broader context on this emerging field, we refer readers to recent comprehensive surveys (Kozlowski & Evans, 2024; Olteanu et al., 2025; Anthis et al., 2025).

Appendix M continues our discussion of related work.

6 Conclusion

For LLM simulations to become reliable tools for the social and behavioral sciences, their fidelity to real human behavior must be measurable. However, prior evaluations have been fragmented, hindering systematic progress. To address this, we introduce SIMBENCH, the first large-scale, standardized benchmark for group-level human behavior simulation. By unifying 20 diverse datasets, SIMBENCH provides the necessary infrastructure to robustly evaluate and compare LLM simulators.

Using this benchmark, we provide the first systematic analysis of this capability, showing that even SOTA LLMs have limited simulation ability, performance scales log-linearly with model size, and there exists a fundamental tradeoff between standard alignment and simulating diverse human opinions. We further reveal that models struggle more when simulating specific demographic groups. We also show that strong simulation ability correlates with deep, knowledge-intensive reasoning. While significant progress is needed, SIMBENCH makes this progress measurable, providing an open foundation to accelerate the development of more faithful LLM simulators.

7 ETHICS STATEMENT

SimBench's primary purpose is to benchmark LLMs' ability to simulate human behavior. While advancements in LLM simulation capabilities can support helpful applications such as pre-testing policies, these do not come without risks of misrepresentation and dual use.

7.1 RESPONSIBLE USE AND ACKNOWLEDGMENT OF LIMITATIONS

First and foremost, due to the observed limited simulation ability of state-of-the-art LLMs, we caution against relying on LLM-powered simulations of human behavior for tasks where downstream harm is possible. Even as models improve, substituting algorithmic approximations for authentic human participation carries the risk of disadvantaging under-represented / marginalized communities by removing their opportunities to directly shape decisions that affect them. Furthermore, while benchmarks like SIMBENCH help measure simulation capabilities, we must be careful not to mistake increasing benchmark performance for genuine understanding of complex human behavior.

7.2 Data Provenance and Transformative Use

The creation of SIMBENCH from 20 diverse sources was guided by a commitment to responsible data handling. Our curation process prioritized datasets with clear and permissive terms. As a result, 17 out of the 20 datasets are governed by explicit permissive licenses (e.g., Creative Commons, MIT). For the few remaining datasets that are publicly available for research without an explicit license, we apply a consistent framework built on the principle of transformative use.

- 1. **Transformative Use.** SIMBENCH does not contain or redistribute any raw, individual-level participant data. It is a new, derivative work consisting of aggregated, non-reversible group-level distributions. This process protects the privacy of the original human subjects.
- 2. **Multi-Level Licensing.** Our public release includes a detailed LICENSE file. **The SIMBENCH framework** (our code and pipeline) is permissively licensed (e.g., CC-BY-NC-SA 4.0). For each of the **20 constituent datasets**, the documentation explicitly lists the original source, its specific license or terms of use, and a clear statement clarifying its status as an aggregated, derivative work whose original terms should still be consulted.

7.3 Scope of Representation and Intersectional Analysis

While SIMBENCH includes diverse demographic groups, it can not adequately support simulations of intersectional identities due to sample size limitations. By conditioning on one demographic variable at a time, we cannot systematically assess how well models handle the rich overlap of identities (e.g., "older Latinx women," "young Black men"). This was a deliberate methodological choice to maintain the statistical integrity of the ground-truth distributions, as small intersectional group sizes make it difficult to combine multiple characteristics simultaneously due to increasing sampling noise in response distributions. Yet intersectional simulation is precisely where societal biases and model limitations often emerge, making this an important direction for future work. Additionally, the conditional prompting approach we use conceptualizes simplistic human populations and may thus fail to appropriately account for nuances of individual behavior.

7.4 CONCLUSION

Nevertheless, we believe SIMBENCH is an important step toward making LLM simulation progress measurable and raising awareness of state-of-the-art model blind spots. Together, we hope this will ultimately create accountability for models deployed in socially sensitive contexts.

8 REPRODUCIBILITY STATEMENT

To ensure the reproducibility of our findings and to facilitate future research, we make all components of our work publicly available. The complete SIMBENCH benchmark, including all 20 processed datasets, our curated SimBenchPop and SimBenchGrouped splits, and detailed data cards, will be released on the Hugging Face Hub. Our codebase will be available in an open-source GitHub

repository. We provide detailed descriptions of our experimental setup, including the exact prompts used for both base and instruction-tuned models, in Appendix D. We further provide an empirical validation of our elicitation methodology choice in Appendix E.

REFERENCES

- Afrobarometer. Afrobarometer data, all countries (39), round 9, 2023. http://www.afrobarometer.org, 2023. Accessed: March 2025.
- Gati V Aher, Rosa I. Arriaga, and Adam Tauman Kalai. Using large language models to simulate multiple humans and replicate human subject studies. In Andreas Krause, Emma Brunskill, Kyunghyun Cho, Barbara Engelhardt, Sivan Sabato, and Jonathan Scarlett (eds.), *Proceedings of the 40th International Conference on Machine Learning*, volume 202 of *Proceedings of Machine Learning Research*, pp. 337–371. PMLR, 23–29 Jul 2023. URL https://proceedings.mlr.press/v202/aher23a.html.
- Georg Ahnert, Max Pellert, David Garcia, and Markus Strohmaier. Extracting affect aggregates from longitudinal social media data with temporal adapters for large language models. *arXiv* preprint arXiv:2409.17990, 2024.
- Jacy Reese Anthis, Ryan Liu, Sean M Richardson, Austin C Kozlowski, Bernard Koch, James Evans, Erik Brynjolfsson, and Michael Bernstein. Llm social simulations are a promising research method. arXiv preprint arXiv:2504.02234, 2025.
- Anthropic. Claude 3.7 sonnet and claude code, February 2025. URL https://www.anthropic.com/news/claude-3-7-sonnet. Accessed: 2025-05-14.
- Lisa P. Argyle, Ethan C. Busby, Nancy Fulda, Joshua R. Gubler, Christopher Rytting, and David Wingate. Out of one, many: Using language models to simulate human samples. *Political Analysis*, 31(3):337–351, 2023. doi: 10.1017/pan.2023.2.
- Lora Aroyo, Alex S. Taylor, Mark Díaz, Christopher M. Homan, Alicia Parrish, Greg Serapio-García, Vinodkumar Prabhakaran, and Ding Wang. Dices dataset: diversity in conversational ai evaluation for safety. In *Proceedings of the 37th International Conference on Neural Information Processing Systems*, NIPS '23, Red Hook, NY, USA, 2023. Curran Associates Inc.
- Edmond Awad, Sohan Dsouza, Richard Kim, Jonathan Schulz, Joseph Henrich, Azim Shariff, Jean-François Bonnefon, and Iyad Rahwan. The moral machine experiment. *Nature*, 563(7729):59–64, 2018.
- Edmond Awad, Sohan Dsouza, Azim Shariff, Iyad Rahwan, and Jean-François Bonnefon. Universals and variations in moral decisions made in 42 countries by 70,000 participants. *Proceedings of the National Academy of Sciences*, 117(5):2332–2337, 2020.
- Eric Bigelow and Steven T Piantadosi. A large dataset of generalization patterns in the number game. *Journal of Open Psychology Data*, 4(1):e4–e4, 2016.
- Marcel Binz, Elif Akata, Matthias Bethge, Franziska Brändle, Fred Callaway, Julian Coda-Forno, Peter Dayan, Can Demircan, Maria K Eckstein, Noémi Éltető, et al. A foundation model to predict and capture human cognition. *Nature*, pp. 1–8, 2025.
- James Bisbee, Joshua D. Clinton, Cassy Dorff, Brenton Kenkel, and Jennifer M. Larson. Synthetic replacements for human survey data? the perils of large language models. *Political Analysis*, 32 (4):401–416, 2024. doi: 10.1017/pan.2024.5.
- Tom Brown, Benjamin Mann, Nick Ryder, Melanie Subbiah, Jared D Kaplan, Prafulla Dhariwal, Arvind Neelakantan, Pranav Shyam, Girish Sastry, Amanda Askell, et al. Language models are few-shot learners. *Advances in neural information processing systems*, 33:1877–1901, 2020.
- Myra Cheng, Tiziano Piccardi, and Diyi Yang. CoMPosT: Characterizing and evaluating caricature in LLM simulations. In Houda Bouamor, Juan Pino, and Kalika Bali (eds.), *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing*, pp. 10853–10875, Singapore, December 2023. Association for Computational Linguistics. doi: 10.18653/v1/2023.emnlp-main. 669. URL https://aclanthology.org/2023.emnlp-main.669/.

- Wei-Lin Chiang, Lianmin Zheng, Ying Sheng, Anastasios N. Angelopoulos, Tianle Li, Dacheng Li, Banghua Zhu, Hao Zhang, Michael I. Jordan, Joseph E. Gonzalez, and Ion Stoica. Chatbot arena: an open platform for evaluating llms by human preference. In *Proceedings of the 41st International Conference on Machine Learning*, ICML'24. JMLR.org, 2024.
- André F. Cruz, Moritz Hardt, and Celestine Mendler-Dünner. Evaluating language models as risk scores. In A. Globerson, L. Mackey, D. Belgrave, A. Fan, U. Paquet, J. Tomczak, and C. Zhang (eds.), Advances in Neural Information Processing Systems, volume 37, pp. 97378–97407. Curran Associates, Inc., 2024. URL https://proceedings.neurips.cc/paper_files/paper/2024/file/b0a4b3e384b4554e65a47ad1f6b0310a-Paper-Datasets_and_Benchmarks_Track.pdf.
- DeepSeek-AI. Deepseek-v3 technical report. arXiv preprint arXiv:2412.19437, 2024.
- Tim Dettmers, Mike Lewis, Younes Belkada, and Luke Zettlemoyer. Llm.int8(): 8-bit matrix multiplication for transformers at scale. In *Proceedings of the 36th International Conference on Neural Information Processing Systems*, NIPS '22, Red Hook, NY, USA, 2022. Curran Associates Inc. ISBN 9781713871088.
- Ricardo Dominguez-Olmedo, Moritz Hardt, and Celestine Mendler-Dünner. Questioning the survey responses of large language models. In A. Globerson, L. Mackey, D. Belgrave, A. Fan, U. Paquet, J. Tomczak, and C. Zhang (eds.), *Advances in Neural Information Processing Systems*, volume 37, pp. 45850–45878. Curran Associates, Inc., 2024. URL https://proceedings.neurips.cc/paper_files/paper/2024/file/515c62809e0a29729d7eec26e2916fc0-Paper-Conference.pdf.
- Yijiang River Dong, Tiancheng Hu, and Nigel Collier. Can LLM be a personalized judge? In Yaser Al-Onaizan, Mohit Bansal, and Yun-Nung Chen (eds.), *Findings of the Association for Computational Linguistics: EMNLP 2024*, pp. 10126–10141, Miami, Florida, USA, November 2024. Association for Computational Linguistics. doi: 10.18653/v1/2024.findings-emnlp.592. URL https://aclanthology.org/2024.findings-emnlp.592/.
- Yijiang River Dong, Tiancheng Hu, Yinhong Liu, Ahmet Üstün, and Nigel Collier. When personalization meets reality: A multi-faceted analysis of personalized preference learning. *arXiv* preprint *arXiv*:2502.19158, 2025.
- Esin Durmus, Karina Nguyen, Thomas Liao, Nicholas Schiefer, Amanda Askell, Anton Bakhtin, Carol Chen, Zac Hatfield-Dodds, Danny Hernandez, Nicholas Joseph, Liane Lovitt, Sam McCandlish, Orowa Sikder, Alex Tamkin, Janel Thamkul, Jared Kaplan, Jack Clark, and Deep Ganguli. Towards measuring the representation of subjective global opinions in language models. In *First Conference on Language Modeling*, 2024. URL https://openreview.net/forum?id=zl16jLb91v.
- Adam Enders, Casey Klofstad, Amanda Diekman, Hugo Drochon, Joel Rogers de Waal, Shane Littrell, Kamal Premaratne, Daniel Verdear, Stefan Wuchty, and Joseph Uscinski. The sociodemographic correlates of conspiracism. *Scientific reports*, 14(1):14184, 2024.
- European Social Survey European Research Infrastructure (ESS ERIC). ESS11 Integrated File, Edition 2.0 [Data set], 2024. URL https://doi.org/10.21338/ess11e02_0.
- Xiachong Feng, Longxu Dou, and Lingpeng Kong. Reasoning does not necessarily improve role-playing ability. In Wanxiang Che, Joyce Nabende, Ekaterina Shutova, and Mohammad Taher Pilehvar (eds.), *Findings of the Association for Computational Linguistics: ACL 2025*, pp. 10301–10314, Vienna, Austria, July 2025. Association for Computational Linguistics. ISBN 979-8-89176-256-5. doi: 10.18653/v1/2025.findings-acl.537. URL https://aclanthology.org/2025.findings-acl.537/.
- Clémentine Fourrier, Nathan Habib, Alina Lozovskaya, Konrad Szafer, and Thomas Wolf. Open llm leaderboard v2. https://huggingface.co/spaces/open-llm-leaderboard/open_llm_leaderboard, 2024.

Aryo Pradipta Gema, Alexander Hägele, Runjin Chen, Andy Arditi, Jacob Goldman-Wetzler, Kit Fraser-Taliente, Henry Sleight, Linda Petrini, Julian Michael, Beatrice Alex, et al. Inverse scaling in test-time compute. *arXiv preprint arXiv:2507.14417*, 2025.

Ken Goldberg, Theresa Roeder, Dhruv Gupta, and Chris Perkins. Eigentaste: A constant time collaborative filtering algorithm. *information retrieval*, 4:133–151, 2001.

Neel Guha, Julian Nyarko, Daniel Ho, Christopher Ré, Adam Chilton, Aditya K, Alex Chohlas-Wood, Austin Peters, Brandon Waldon, Daniel Rockmore, Diego Zambrano, Dmitry Talisman, Enam Hoque, Faiz Surani, Frank Fagan, Galit Sarfaty, Gregory Dickinson, Haggai Porat, Jason Hegland, Jessica Wu, Joe Nudell, Joel Niklaus, John Nay, Jonathan Choi, Kevin Tobia, Margaret Hagan, Megan Ma, Michael Livermore, Nikon Rasumov-Rahe, Nils Holzenberger, Noam Kolt, Peter Henderson, Sean Rehaag, Sharad Goel, Shang Gao, Spencer Williams, Sunny Gandhi, Tom Zur, Varun Iyer, and Zehua Li. Legalbench: A collaboratively built benchmark for measuring legal reasoning in large language models. In *Advances in Neural Information Processing Systems 36 (NeurIPS 2023), Datasets and Benchmarks Track*, 2023. URL https://proceedings.neurips.cc/paper_files/paper/2023/hash/89e44582fd28ddfealea4dcb0ebbf4b0-Abstract-Datasets_and_Benchmarks.html.

Daya Guo, Dejian Yang, Haowei Zhang, Junxiao Song, Peiyi Wang, Qihao Zhu, Runxin Xu, Ruoyu Zhang, Shirong Ma, Xiao Bi, Xiaokang Zhang, Xingkai Yu, Yu Wu, Z. F. Wu, Zhibin Gou, Zhihong Shao, Zhuoshu Li, Ziyi Gao, Aixin Liu, Bing Xue, Bingxuan Wang, Bochao Wu, Bei Feng, Chengda Lu, Chenggang Zhao, Chengqi Deng, Chong Ruan, Damai Dai, Deli Chen, Dongjie Ji, Erhang Li, Fangyun Lin, Fucong Dai, Fuli Luo, Guangbo Hao, Guanting Chen, Guowei Li, H. Zhang, Hanwei Xu, Honghui Ding, Huazuo Gao, Hui Qu, Hui Li, Jianzhong Guo, Jiashi Li, Jingchang Chen, Jingyang Yuan, Jinhao Tu, Junjie Oiu, Junlong Li, J. L. Cai, Jiaqi Ni, Jian Liang, Jin Chen, Kai Dong, Kai Hu, Kaichao You, Kaige Gao, Kang Guan, Kexin Huang, Kuai Yu, Lean Wang, Lecong Zhang, Liang Zhao, Litong Wang, Liyue Zhang, Lei Xu, Leyi Xia, Mingchuan Zhang, Minghua Zhang, Minghui Tang, Mingxu Zhou, Meng Li, Miaojun Wang, Mingming Li, Ning Tian, Panpan Huang, Peng Zhang, Qiancheng Wang, Qinyu Chen, Qiushi Du, Ruiqi Ge, Ruisong Zhang, Ruizhe Pan, Runji Wang, R. J. Chen, R. L. Jin, Ruyi Chen, Shanghao Lu, Shangyan Zhou, Shanhuang Chen, Shengfeng Ye, Shiyu Wang, Shuiping Yu, Shunfeng Zhou, Shuting Pan, S. S. Li, Shuang Zhou, Shaoqing Wu, Tao Yun, Tian Pei, Tianyu Sun, T. Wang, Wangding Zeng, Wen Liu, Wenfeng Liang, Wenjun Gao, Wenqin Yu, Wentao Zhang, W. L. Xiao, Wei An, Xiaodong Liu, Xiaohan Wang, Xiaokang Chen, Xiaotao Nie, Xin Cheng, Xin Liu, Xin Xie, Xingchao Liu, Xinyu Yang, Xinyuan Li, Xuecheng Su, Xuheng Lin, X. Q. Li, Xiangyue Jin, Xiaojin Shen, Xiaosha Chen, Xiaowen Sun, Xiaoxiang Wang, Xinnan Song, Xinyi Zhou, Xianzu Wang, Xinxia Shan, Y. K. Li, Y. Q. Wang, Y. X. Wei, Yang Zhang, Yanhong Xu, Yao Li, Yao Zhao, Yaofeng Sun, Yaohui Wang, Yi Yu, Yichao Zhang, Yifan Shi, Yiliang Xiong, Ying He, Yishi Piao, Yisong Wang, Yixuan Tan, Yiyang Ma, Yiyuan Liu, Yongqiang Guo, Yuan Ou, Yuduan Wang, Yue Gong, Yuheng Zou, Yujia He, Yunfan Xiong, Yuxiang Luo, Yuxiang You, Yuxuan Liu, Yuyang Zhou, Y. X. Zhu, Yanping Huang, Yaohui Li, Yi Zheng, Yuchen Zhu, Yunxian Ma, Ying Tang, Yukun Zha, Yuting Yan, Z. Z. Ren, Zehui Ren, Zhangli Sha, Zhe Fu, Zhean Xu, Zhenda Xie, Zhengyan Zhang, Zhewen Hao, Zhicheng Ma, Zhigang Yan, Zhiyu Wu, Zihui Gu, Zijia Zhu, Zijun Liu, Zilin Li, Ziwei Xie, Ziyang Song, Zizheng Pan, Zhen Huang, Zhipeng Xu, Zhongyu Zhang, and Zhen Zhang. Deepseek-r1 incentivizes reasoning in llms through reinforcement learning. Nature, 645(8081):633-638, 2025. ISSN 1476-4687. doi: 10.1038/s41586-025-09422-z. URL https://doi.org/10.1038/s41586-025-09422-z.

Dan Hendrycks, Collin Burns, Steven Basart, Andy Zou, Mantas Mazeika, Dawn Song, and Jacob Steinhardt. Measuring massive multitask language understanding. In *International Conference on Learning Representations*, 2021. URL https://openreview.net/forum?id=d7KBjmI3GmQ.

Luke Hewitt, Ashwini Ashokkumar, Isaias Ghezae, and Robb Willer. Predicting results of social science experiments using large language models, August 2024. URL https://samim.io/dl/Predicting%20results%20of%20social% 20science%20experiments%20using%20large%20language%20models.pdf.

- John J Horton. Large language models as simulated economic agents: What can we learn from homo silicus? Technical report, National Bureau of Economic Research, 2023.
- Tiancheng Hu and Nigel Collier. Quantifying the persona effect in LLM simulations. In Lun-Wei Ku, Andre Martins, and Vivek Srikumar (eds.), *Proceedings of the 62nd Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pp. 10289–10307, Bangkok, Thailand, August 2024. Association for Computational Linguistics. doi: 10.18653/v1/2024.acl-long.554. URL https://aclanthology.org/2024.acl-long.554/.
- Tiancheng Hu and Nigel Collier. iNews: A Multimodal Dataset for Modeling Personalized Affective Responses to News. In Wanxiang Che, Joyce Nabende, Ekaterina Shutova, and Mohammad Taher Pilehvar (eds.), *Proceedings of the 63rd Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pp. 25000–25040, Vienna, Austria, July 2025. Association for Computational Linguistics. doi: 10.18653/v1/2025.acl-long.1217. URL https://aclanthology.org/2025.acl-long.1217/.
- Tiancheng Hu, Yara Kyrychenko, Steve Rathje, Nigel Collier, Sander van der Linden, and Jon Roozenbeek. Generative language models exhibit social identity biases. *Nature Computational Science*, 5(1):65–75, 2025a. ISSN 2662-8457. doi: 10.1038/s43588-024-00741-1. URL https://doi.org/10.1038/s43588-024-00741-1.
- Tiancheng Hu, Benjamin Minixhofer, and Nigel Collier. Navigating the alignment-calibration trade-off: A pareto-superior frontier via model merging. *arXiv preprint arXiv:2510.17426*, 2025b.
- ISSP Research Group. International social survey programme: Social networks and social resources issp 2017. GESIS Data Archive, Cologne. ZA6980 Data file Version 2.0.0, https://doi.org/10.4232/1.13322, 2019.
- ISSP Research Group. International social survey programme: Religion iv issp 2018. GESIS Data Archive, Cologne. ZA7570 Data file Version 2.1.0, https://doi.org/10.4232/1.13629, 2020.
- ISSP Research Group. International social survey programme: Social inequality v issp 2019. GESIS, Cologne. ZA7600 Data file Version 3.0.0, https://doi.org/10.4232/1.14009, 2022.
- ISSP Research Group. International social survey programme: Environment iv issp 2020. GESIS, Cologne. ZA7650 Data file Version 2.0.0, https://doi.org/10.4232/1.14153, 2023.
- ISSP Research Group. Za8000 international social survey programme: Health and health care ii issp 2021. GESIS, Cologne. ZA8000 Data file Version 2.0.0, https://doi.org/10.4232/5.ZA8000.2.0.0, 2024.
- Zhengbao Jiang, Jun Araki, Haibo Ding, and Graham Neubig. How can we know when language models know? on the calibration of language models for question answering. *Transactions of the Association for Computational Linguistics*, 9:962–977, 2021. doi: 10.1162/tacl_a_00407. URL https://aclanthology.org/2021.tacl-1.57/.
- Adam Tauman Kalai and Santosh S. Vempala. Calibrated language models must hallucinate. In *Proceedings of the 56th Annual ACM Symposium on Theory of Computing*, STOC 2024, pp. 160–171, New York, NY, USA, 2024. Association for Computing Machinery. ISBN 9798400703836. doi: 10.1145/3618260.3649777. URL https://doi.org/10.1145/3618260.3649777.
- Sanyam Kapoor, Nate Gruver, Manley Roberts, Arka Pal, Samuel Dooley, Micah Goldblum, and Andrew Wilson. Calibration-tuning: Teaching large language models to know what they don't know. In Raúl Vázquez, Hande Celikkanat, Dennis Ulmer, Jörg Tiedemann, Swabha Swayamdipta, Wilker Aziz, Barbara Plank, Joris Baan, and Marie-Catherine de Marneffe (eds.), *Proceedings of the 1st Workshop on Uncertainty-Aware NLP (UncertaiNLP 2024)*, pp. 1–14, St Julians, Malta, March 2024. Association for Computational Linguistics. URL https://aclanthology.org/2024.uncertainlp-1.1/.
- Tomasz Korbak, Ethan Perez, and Christopher Buckley. RL with KL penalties is better viewed as Bayesian inference. In Yoav Goldberg, Zornitsa Kozareva, and Yue Zhang (eds.), *Findings of the Association for Computational Linguistics: EMNLP 2022*, pp. 1083–1091, Abu Dhabi, United Arab Emirates, December 2022. Association for Computational Linguistics. doi: 10.18653/v1/

- 2022.findings-emnlp.77. URL https://aclanthology.org/2022.findings-emnlp.
- Austin C. Kozlowski and James Evans. Simulating subjects: The promise and peril of ai stand-ins for social agents and interactions, September 2024. URL https://www.researchgate.net/publication/383972192_Simulating_Subjects_The_Promise_and_Peril_of_AI_Stand-ins_for_Social_Agents_and_Interactions. Preprint.
- Latinobarómetro. Latinobarómetro 2023. http://www.latinobarometro.org, 2023. Accessed: March 2025.
- Angeliki Lazaridou, Adhi Kuncoro, Elena Gribovskaya, Devang Agrawal, Adam Liska, Tayfun Terzi, Mai Gimenez, Cyprien de Masson d'Autume, Tomas Kocisky, Sebastian Ruder, Dani Yogatama, Kris Cao, Susannah Young, and Phil Blunsom. Mind the gap: Assessing temporal generalization in neural language models. In M. Ranzato, A. Beygelzimer, Y. Dauphin, P.S. Liang, and J. Wortman Vaughan (eds.), Advances in Neural Information Processing Systems, volume 34, pp. 29348–29363. Curran Associates, Inc., 2021. URL https://proceedings.neurips.cc/paper_files/paper/2021/file/f5bf0ba0a17ef18f9607774722f5698c-Paper.pdf.
- Sergey Levine. Reinforcement learning and control as probabilistic inference: Tutorial and review. *arXiv preprint arXiv:1805.00909*, 2018.
- Stephanie Lin, Jacob Hilton, and Owain Evans. TruthfulQA: Measuring how models mimic human falsehoods. In Smaranda Muresan, Preslav Nakov, and Aline Villavicencio (eds.), *Proceedings of the 60th Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pp. 3214–3252, Dublin, Ireland, May 2022. Association for Computational Linguistics. doi: 10.18653/v1/2022.acl-long.229. URL https://aclanthology.org/2022.acl-long.229/.
- Ryan Liu, Jiayi Geng, Addison J Wu, Ilia Sucholutsky, Tania Lombrozo, and Thomas L Griffiths. Mind your step (by step): Chain-of-thought can reduce performance on tasks where thinking makes humans worse. *arXiv preprint arXiv:2410.21333*, 2024.
- Bolei Ma, Xinpeng Wang, Tiancheng Hu, Anna-Carolina Haensch, Michael A. Hedderich, Barbara Plank, and Frauke Kreuter. The potential and challenges of evaluating attitudes, opinions, and values in large language models. In Yaser Al-Onaizan, Mohit Bansal, and Yun-Nung Chen (eds.), *Findings of the Association for Computational Linguistics: EMNLP 2024*, pp. 8783–8805, Miami, Florida, USA, November 2024. Association for Computational Linguistics. doi: 10.18653/v1/2024.findings-emnlp.513. URL https://aclanthology.org/2024.findings-emnlp.513/.
- Benjamin S Manning, Kehang Zhu, and John J Horton. Automated social science: Language models as scientist and subjects. Technical report, National Bureau of Economic Research, 2024.
- Niels G Mede, Viktoria Cologna, Sebastian Berger, John Besley, Cameron Brick, Marina Joubert, Edward W Maibach, Sabina Mihelj, Naomi Oreskes, Mike S Schäfer, et al. Perceptions of science, science communication, and climate change attitudes in 68 countries—the tisp dataset. *Scientific data*, 12(1):114, 2025.
- Nicole Meister, Carlos Guestrin, and Tatsunori Hashimoto. Benchmarking distributional alignment of large language models. In Luis Chiruzzo, Alan Ritter, and Lu Wang (eds.), *Proceedings of the 2025 Conference of the Nations of the Americas Chapter of the Association for Computational Linguistics: Human Language Technologies (Volume 1: Long Papers)*, pp. 24–49, Albuquerque, New Mexico, April 2025. Association for Computational Linguistics. ISBN 979-8-89176-189-6. URL https://aclanthology.org/2025.naacl-long.2/.
- Meta AI. Introducing Llama 3.1: Our most capable models to date, 2024. URL https://ai.meta.com/blog/meta-llama-3-1/. Accessed: 2025-05-14.
- Yixin Nie, Xiang Zhou, and Mohit Bansal. What can we learn from collective human opinions on natural language inference data? In Bonnie Webber, Trevor Cohn, Yulan He, and Yang Liu (eds.), *Proceedings of the 2020 Conference on Empirical Methods in Natural Language*

- *Processing (EMNLP)*, pp. 9131–9143, Online, November 2020. Association for Computational Linguistics. doi: 10.18653/v1/2020.emnlp-main.734. URL https://aclanthology.org/2020.emnlp-main.734/.
- Harsha Nori, Nicholas King, Scott Mayer McKinney, Dean Carignan, and Eric Horvitz. Capabilities of gpt-4 on medical challenge problems. *arXiv preprint arXiv:2303.13375*, 2023.
- Alexandra Olteanu, Solon Barocas, Su Lin Blodgett, Lisa Egede, Alicia DeVrio, and Myra Cheng. Ai automatons: Ai systems intended to imitate humans. *arXiv preprint arXiv:2503.02250*, 2025.
- OpenAI. Introducing GPT-4.1 in the API, 2025a. URL https://openai.com/index/gpt-4-1/. Accessed: 2025-05-14.
- OpenAI. Introducing openai o3 and o4-mini, April 2025b. URL https://openai.com/index/introducing-o3-and-o4-mini/. Accessed: 2025-05-14.
- Joon Sung Park, Joseph O'Brien, Carrie Jun Cai, Meredith Ringel Morris, Percy Liang, and Michael S. Bernstein. Generative agents: Interactive simulacra of human behavior. In *Proceedings of the 36th Annual ACM Symposium on User Interface Software and Technology*, UIST '23, New York, NY, USA, 2023. Association for Computing Machinery. ISBN 9798400701320. doi: 10.1145/3586183.3606763. URL https://doi.org/10.1145/3586183.3606763.
- Joon Sung Park, Carolyn Q Zou, Aaron Shaw, Benjamin Mako Hill, Carrie Cai, Meredith Ringel Morris, Robb Willer, Percy Liang, and Michael S Bernstein. Generative agent simulations of 1,000 people. *arXiv preprint arXiv:2411.10109*, 2024a.
- Peter S. Park, Philipp Schoenegger, and Chongyang Zhu. Diminished diversity-of-thought in a standard large language model. *Behavior Research Methods*, 56:5754–5770, 2024b. doi: 10. 3758/s13428-023-02307-x. URL https://link.springer.com/article/10.3758/s13428-023-02307-x.
- Joshua C Peterson, David D Bourgin, Mayank Agrawal, Daniel Reichman, and Thomas L Griffiths. Using large-scale experiments and machine learning to discover theories of human decision-making. *Science*, 372(6547):1209–1214, 2021.
- Paula Rescala, Manoel Horta Ribeiro, Tiancheng Hu, and Robert West. Can language models recognize convincing arguments? In Yaser Al-Onaizan, Mohit Bansal, and Yun-Nung Chen (eds.), *Findings of the Association for Computational Linguistics: EMNLP 2024*, pp. 8826–8837, Miami, Florida, USA, November 2024. Association for Computational Linguistics. doi: 10.18653/v1/2024.findings-emnlp.515. URL https://aclanthology.org/2024.findings-emnlp.515/.
- Shibani Santurkar, Esin Durmus, Faisal Ladhak, Cinoo Lee, Percy Liang, and Tatsunori Hashimoto. Whose opinions do language models reflect? In *International Conference on Machine Learning*, pp. 29971–30004. PMLR, 2023.
- Skipper Seabold and Josef Perktold. Statsmodels: Econometric and statistical modeling with python. In Stéfan van der Walt and Jarrod Millman (eds.), *Proceedings of the 9th Python in Science Conference*, pp. 92–96, 2010. doi: 10.25080/Majora-92bf1922-011.
- Camelia Simoiu, Chiraag Sumanth, Alok Mysore, and Sharad Goel. Studying the "wisdom of crowds" at scale. In *Proceedings of the AAAI Conference on Human Computation and Crowdsourcing*, volume 7, pp. 171–179, 2019.
- Zayne Rea Sprague, Fangcong Yin, Juan Diego Rodriguez, Dongwei Jiang, Manya Wadhwa, Prasann Singhal, Xinyu Zhao, Xi Ye, Kyle Mahowald, and Greg Durrett. To cot or not to cot? chain-of-thought helps mainly on math and symbolic reasoning. In *The Thirteenth International Conference on Learning Representations*, 2025. URL https://openreview.net/forum?id=w6nlcS8Kkn.
- Gemma Team, Aishwarya Kamath, Johan Ferret, Shreya Pathak, Nino Vieillard, Ramona Merhej, Sarah Perrin, Tatiana Matejovicova, Alexandre Ramé, Morgane Rivière, et al. Gemma 3 technical report. *arXiv preprint arXiv:2503.19786*, 2025.

- Katherine Tian, Eric Mitchell, Allan Zhou, Archit Sharma, Rafael Rafailov, Huaxiu Yao, Chelsea Finn, and Christopher Manning. Just ask for calibration: Strategies for eliciting calibrated confidence scores from language models fine-tuned with human feedback. In Houda Bouamor, Juan Pino, and Kalika Bali (eds.), *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing*, pp. 5433–5442, Singapore, December 2023. Association for Computational Linguistics. doi: 10.18653/v1/2023.emnlp-main.330. URL https://aclanthology.org/2023.emnlp-main.330/.
- Lindia Tjuatja, Valerie Chen, Tongshuang Wu, Ameet Talwalkwar, and Graham Neubig. Do llms exhibit human-like response biases? a case study in survey design. *Transactions of the Association for Computational Linguistics*, 12:1011–1026, 09 2024. ISSN 2307-387X. doi: 10.1162/tacl_a_00685. URL https://doi.org/10.1162/tacl_a_00685.
- Vals AI, Inc. Mmlu pro benchmark. https://www.vals.ai/benchmarks/mmlu_pro-04-15-2025, April 2025. Last updated 15 April 2025.
- Alex Wang, Amanpreet Singh, Julian Michael, Felix Hill, Omer Levy, and Samuel Bowman. GLUE: A multi-task benchmark and analysis platform for natural language understanding. In Tal Linzen, Grzegorz Chrupała, and Afra Alishahi (eds.), *Proceedings of the 2018 EMNLP Workshop Black-boxNLP: Analyzing and Interpreting Neural Networks for NLP*, pp. 353–355, Brussels, Belgium, November 2018. Association for Computational Linguistics. doi: 10.18653/v1/W18-5446. URL https://aclanthology.org/W18-5446/.
- Angelina Wang, Jamie Morgenstern, and John P Dickerson. Large language models that replace human participants can harmfully misportray and flatten identity groups. *Nature Machine Intelligence*, pp. 1–12, 2025.
- Jason Wei, Xuezhi Wang, Dale Schuurmans, Maarten Bosma, Brian Ichter, Fei Xia, Ed H. Chi, Quoc V. Le, and Denny Zhou. Chain-of-thought prompting elicits reasoning in large language models. In *Proceedings of the 36th International Conference on Neural Information Processing Systems*, NIPS '22, Red Hook, NY, USA, 2022. Curran Associates Inc. ISBN 9781713871088.
- 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. Transformers: State-of-the-art natural language processing. In Qun Liu and David Schlangen (eds.), *Proceedings of the 2020 Conference on Empirical Methods in Natural Language Processing: System Demonstrations*, pp. 38–45, Online, October 2020. Association for Computational Linguistics. doi: 10.18653/v1/2020.emnlp-demos.6. URL https://aclanthology.org/2020.emnlp-demos.6/.
- An Yang, Baosong Yang, Beichen Zhang, Binyuan Hui, Bo Zheng, Bowen Yu, Chengyuan Li, Dayiheng Liu, Fei Huang, Haoran Wei, et al. Qwen2.5 technical report. *arXiv preprint arXiv:2412.15115*, 2024.
- Lance Ying, Katherine M Collins, Lionel Wong, Ilia Sucholutsky, Ryan Liu, Adrian Weller, Tianmin Shu, Thomas L Griffiths, and Joshua B Tenenbaum. On benchmarking human-like intelligence in machines. *arXiv preprint arXiv:2502.20502*, 2025.
- Zihao Zhao, Eric Wallace, Shi Feng, Dan Klein, and Sameer Singh. Calibrate before use: Improving few-shot performance of language models. In Marina Meila and Tong Zhang (eds.), *Proceedings of the 38th International Conference on Machine Learning*, volume 139 of *Proceedings of Machine Learning Research*, pp. 12697–12706. PMLR, 18–24 Jul 2021. URL https://proceedings.mlr.press/v139/zhao21c.html.
- Chiwei Zhu, Benfeng Xu, Quan Wang, Yongdong Zhang, and Zhendong Mao. On the calibration of large language models and alignment. In Houda Bouamor, Juan Pino, and Kalika Bali (eds.), Findings of the Association for Computational Linguistics: EMNLP 2023, pp. 9778–9795, Singapore, December 2023. Association for Computational Linguistics. doi: 10.18653/v1/2023. findings-emnlp.654. URL https://aclanthology.org/2023.findings-emnlp.654/.

A LIMITATIONS

The Scope of Benchmarking Human Behavior
The challenge of benchmarking human behavior
lies in its vastness. No single study, nor dozens, could ever capture its full complexity. We operationalize this challenge by focusing on a core set of fundamental cognitive and social tasks widely studied in the behavioral sciences: decision-making, self-assessment, judgment, and problem-solving. This focus necessarily means that SIMBENCH does not capture the full complexity of human interaction, such as embodied or multi-turn social dynamics. As the first large-scale benchmark for group-level simulation, SIMBENCH provides the essential infrastructure to establish robust baselines, uncover fundamental properties like scaling laws, and map the frontier for future work on more complex, interactive simulations.

Scope of Representativeness Although SIMBENCH spans 20 diverse datasets, the combined sample does (and can) not fully represent any single population in its full complexity. Many geographic regions are still underrepresented or entirely absent, potentially limiting generalizability to populations with different cultural backgrounds and preferences. Even within countries, demographic representativeness may vary, as only a subset of our 20 datasets are based on nationally representative sampling techniques. Each dataset carries its own statistical uncertainty. Opt-in samples and crowdsourced data (e.g., from Amazon Mechanical Turk) may have larger margins of error than nationally representative surveys, potentially affecting the benchmark's precision for certain questions. We view these limitations as opportunities for collaborative extension of SIMBENCH to improve global coverage and representativeness over time.

Temporal Dimensions The current version of SIMBENCH utilizes static datasets that capture human behavior at specific points in time. This approach allows for systematic evaluation across domains but cannot yet assess how well LLMs simulate evolving preferences, opinion shifts, or behavioral adaptation – all fundamental aspects of human behavior. Future iterations of SIMBENCH could incorporate longitudinal data to address these dynamic aspects of human behavior and expand the benchmark's evaluative capacity.

Task Format Considerations SIMBENCH currently focuses on multiple-choice, single-answer, single-turn questions and interactions. This standardized format enables systematic comparison across diverse domains but necessarily excludes more complex behavioral simulations including multi-step decision processes and interactive social dynamics. We see this as a pragmatic starting point that establishes foundational evaluation capabilities while inviting future extensions to capture more nuanced aspects of human behavior.

Training Data Overlap A fundamental challenge for all LLM evaluation is the potential for training data contamination. While this cannot be definitively ruled out without full access to model training corpora, several aspects of our methodology and empirical findings suggest this risk is substantially mitigated for SIMBENCH:

- 1) Much of our source data is not easily ingested by standard web scrapes. Virtually all of our source data are primarily distributed as structured data files in specialized formats like R or SAS in academic archives. This makes data contamination much less likely than for generic web text, as these files cannot be meaningfully read or interpreted as plain text by standard scraping tools.
- 2) SimBench's core task is not to recall a fact but to predict a response distribution for a specific demographic subgroup (e.g., "women in Slovakia"). Even if a model's training data included thousands of individual survey responses, it would still need to learn, without supervision, how to aggregate these individual points into a coherent distribution for an arbitrary, specified subgroup. This is a sophisticated, zero-shot social reasoning skill that is unlikely to emerge from simply seeing the raw data.
- 3) On datasets that are most likely to appear in training data (e.g., US-centric OpinionQA), even the best-performing models achieve an S-score of only 60, far from the 100-point maximum. If models had memorized this benchmark, we would expect scores far closer to perfect. This clear performance ceiling demonstrates that our benchmark is testing a genuine capability rather than memorization.

4) The consistent scaling patterns we observe across diverse datasets suggest genuine simulation capabilities rather than artifacts of training data overlap.

Nevertheless, we acknowledge that data contamination remains a fundamental challenge in LLM evaluation, and future work should develop more robust methods to detect and quantify its impact. We include this consideration for completeness while believing it unlikely to significantly impact our current findings.

B DATASET CURATION AND EXCLUSION RATIONALE

As described in §2.1, our dataset curation process involved a systematic review of numerous prominent datasets in the social and behavioral sciences. While our search was extensive, many promising candidates were ultimately excluded for failing to meet our strict inclusion criteria for a redistributable, multiple-choice benchmark.

Table 3 provides an illustrative list of well-known datasets that were considered during this review but not included in the final SIMBENCH collection. This list is not exhaustive but serves to highlight the common methodological and logistical challenges that arise when creating a benchmark from existing scientific data, such as restrictive licensing, complex experimental designs, and non-standard response formats. By documenting these exclusion rationales, we aim to provide transparency into our curation process and offer a resource for future benchmark creators.

Table 3: Examples of Datasets Considered and Excluded from SIMBENCH.

Dataset	Exclusion Reason
Understanding America Study	Licensing Restrictions
ManyLabs & ManyLabs 2	Complex treatment condition
General Social Survey	Licensing Restrictions
Demographic and Health Surveys	Licensing Restrictions
Global Preferences Survey	Licensing Restrictions
World Risk Poll	No raw question wording available
Yourmorals.org	Licensing Restrictions
Asian Barometer	Licensing Restrictions
The Glasgow Norms	Licensing Restrictions
MovieLens	Licensing Restrictions
Health Information National Trends Survey	Licensing Restrictions
BBC Big Personality Test	Licensing Restrictions
Time-sharing Experiments for the Social Sciences	Often complex treatment conditions
Project Implicit	Hard to model reaction time in LLMs
Children's Worlds Survey	Licensing Restrictions
Monitoring the Future Survey	Licensing Restrictions
TIMSS	Individual test items are not accessible
UMD-OurDataHelps	Free text response
MobLab dataset	Too few questions; lack detailed demographics data

C SIMBENCHPOP AND SIMBENCHGROUPED SAMPLING DETAILS

We curated data at two levels of grouping granularity, corresponding to our two main benchmark splits: **SimBenchPop** and **SimBenchGrouped**.

SimBenchPop measures LLMs' ability to simulate responses of broad, diverse human populations. We include all questions from all 20 datasets in SimBench, combining each question with its dataset-specific default grouping prompt (e.g., "You are an Amazon Mechanical Turk worker based in the United States"). We sample up to 500 questions per dataset to ensure representativeness while

keeping the benchmark manageable. For each test case, we aggregate individual responses across all participants in the dataset to create population-level response distributions. This approach creates a benchmark that represents population-level responses across diverse domains while maintaining a reasonable size of 7,167 test cases.

For **SimBenchGrouped**, we focus only on five large-scale survey datasets with rich demographic information and sufficient sample sizes: OpinionQA, ESS, Afrobarometer, ISSP, and LatinoBarometro. Our sampling approach prioritizes questions showing meaningful demographic variation. For each dataset, we identify available grouping variables (e.g., age, gender, country) with sufficient group sizes to form meaningful response distributions. We calculate the variance of responses across demographic groups for each question and rank questions by their variance scores, prioritizing those showing the strongest demographic differences. We select questions that exhibit significant variation across demographic groups to ensure the benchmark captures meaningful differences in responses. For each selected question, we create multiple test cases by pairing it with different values of the grouping variables (e.g., age = "18-29", age = "30-49"). This process results in 6,343 test cases that specifically measure LLMs' ability to simulate responses from narrower participant groups based on specified demographic characteristics. Table 4 provides a summary of the sampling process across all datasets, showing the minimum group size thresholds and the number of test cases in each benchmark split.

Table 4: Dataset Sampling Summary; NaN refers to dataset that is only available in aggregated form and no grouping size is known.

Dataset	Min. Group	SimBench	SimBenchPop	SimBenchGrouped
WisdomOfCrowds	100	1,604	114	_
Jester	100	136	136	_
Choices13k	NaN	14,568	500	_
OpinionQA	300	1,074,392	500	984
MoralMachineClassic	100	3,441	15	_
MoralMachine	100	20,771	500	_
ChaosNLI	100	4,645	500	_
ESS	300	2,783,780	500	1,643
Afrobarometer	300	517,453	500	1,531
OSPsychBig5	300	1,950	250	_
OSPsychMACH	300	3,682,700	100	_
OSPsychMGKT	300	20,610	500	_
OSPsychRWAS	300	975,585	22	_
ISSP	300	594,336	500	940
LatinoBarometro	300	80,684	500	1,245
GlobalOpinionQA	NaN	46,329	500	_
DICES	10	918,064	500	_
NumberGame	10	15,984	500	_
ConspiracyCorr	300	968	45	_
TISP	300	172,271	485	_
Total		10,930,271	7,167	6,343

D IMPLEMENTATION DETAILS

For base models, we use HuggingFace Transformers (Wolf et al., 2020) to run inference on a single NVIDIA RTX A6000 Ada GPU. We structure prompts so that the next token corresponds to the model's answer choices. For models smaller than 70B parameters, we use 8-bit quantization implemented in bitsandbytes (Dettmers et al., 2022), while 70B models use 4-bit quantization.

For instruction-tuned models, we use API calls. OpenAI models are accessed directly through their API, while other models are accessed via OpenRouter. We request verbalized probability outputs in JSON format with temperature initially set to 0. If parsing fails, we increase temperature to 1 and

retry up to 5 times. All models successfully produced valid JSON under these conditions. When probability outputs do not sum to 1, we apply normalization.

Our evaluation includes a diverse set of models: Qwen 2.5 (Yang et al., 2024) (0.5B-72B), Gemma 3 (Team et al., 2025) PT and IT (4B-27B), o4-mini (OpenAI, 2025b), Claude 3.7 Sonnet (Anthropic, 2025), DeepSeek R1 (Guo et al., 2025), DeepSeek-V3-0324 DeepSeek-AI (2024), GPT-4.1 OpenAI (2025a), and Llama-3.1-Instruct (8B-405B) (Meta AI, 2024).

To ensure the validity of our results, we perform two checks: 1) We verify that base models assign the vast majority of probability mass to the provided answer options. Even for small models like Qwen2.5-0.5B, the sum of probabilities across answer tokens is as high as 0.98, confirming that models rarely predict tokens outside the designated answer space. 2) We also evaluate the effect of quantization on model performance using a subset of SimBench. As shown in Table 5, performance remains consistent across quantization levels, with minimal variation in total variation scores even for quantization-sensitive models like Llama-3.1.

We detail below the prompts used in our experimental conditions for token probability and verbalized distribution prediction.

The following system prompt was consistent across all experimental conditions:

```
You are a group of individuals with these shared characteristics: {default system prompt}{grouping system prompt (if any)}
```

For token probability prediction, we adapted the prompt structure from Nori et al. (2023):

```
**Question**: {question}
Do not provide any explanation, only answer with one of the following options: {answer options}.
**Answer**: (
```

Prompt for eliciting verbalized probability prediction:

```
**Question**: {question}
```

Estimate what percentage of your group would choose each option. Follow these rules:

- 1. Use whole numbers from 0 to 100
- 2. Ensure the percentages sum to exactly 100
- 3. Only include the numbers (no %
- 4. Use this exact valid JSON format: {answer options} and do NOT include anything else.
- 5. Only output your final answer and nothing else. No explanations or intermediate steps are one needed.

Replace X with your estimated percentages for each option.

'**Answer**:

Prompt for zero-shot CoT:

```
**Question**: {question}
```

Estimate what percentage of your group would choose each option.

Think step by step about how people with your shared characteristics would reason about this question.

Consider different perspectives within your group and what factors would influence their choices.

Please provide your reasoning first, then give your final answer in JSON format.

Follow these rules for your final answer:

- 1. Use whole numbers from 0 to 100
- 2. Ensure the percentages sum to exactly 100
- 3. Only include the numbers (no %
- 4. Use this exact valid JSON format: {json_format_str}
- 5. Replace X with your estimated percentages for each option.

'**Answer**:

E VALIDATION OF ELICITATION METHOD

A key methodological choice in SIMBENCH is how to elicit probability distributions from LLMs. For base models, we use direct token probabilities from the first token of the response. For instruction-tuned models, however, two primary methods exist: direct token probabilities and requesting a "verbalized" distribution (e.g., a JSON object with percentages). To validate our choice of using verbalized distributions for instruction-tuned models, as recommended by recent work (Tian et al., 2023; Meister et al., 2025), we conducted a direct comparison.

Figure 5 compares the SIMBENCH scores for several instruction-tuned models using both methods. The results are unequivocal: using verbalized distributions (teal dots) dramatically and consistently outperforms direct token probabilities (orange dots) for every instruction-tuned model tested. In many cases, using token probabilities results in scores far below zero, indicating that the model's raw logits are poorly calibrated for this task after instruction-tuning. In contrast, base models (black bars) perform reasonably well with token probabilities, as they are not subject to the same post-training shifts.

This analysis provides strong empirical support for our methodological decision to use token probabilities for base models and verbalized distributions for instruction-tuned models, ensuring that we are evaluating each model class using the most effective and well-calibrated elicitation technique.

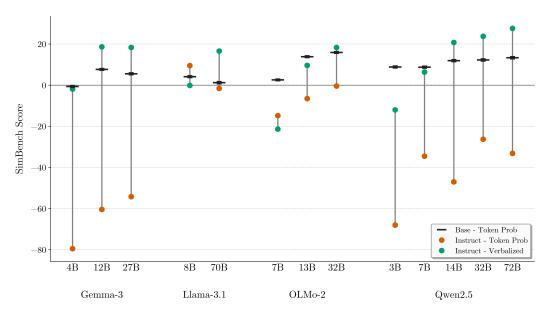


Figure 5: **Verbalized distributions are superior for instruction-tuned models.** This plot compares SIMBENCH scores for base models (using token probabilities) against their instruction-tuned counterparts using either token probabilities (orange) or verbalized distributions (teal). The large vertical gap for all instruction-tuned models demonstrates the significant performance gain from using verbalized distributions, validating our choice of elicitation method.

Table 5: Total Variation for different models at various quantization levels. Lower values indicate better performance.

Model	4-bit	8-bit	16-bit	32-bit
Llama-3.1-8B-Instruct	0.272		0.262	0.262
Qwen2.5-7B	0.307		0.306	0.307

F METRIC ROBUSTNESS CHECK

TVD ranges from 0 (perfect match) to 1 (complete disagreement), with lower values indicating better simulation fidelity. TVD provides an interpretable measure of how closely model predictions align with actual human response distributions. TVD is particularly well-suited for simulation evaluation compared to alternatives like KL divergence or Jensen-Shannon divergence (JSD). Unlike KL divergence, TVD remains well-defined even when the model assigns zero probability to responses that humans give, avoiding the infinite penalties that KL would impose in such cases. Additionally, TVD is symmetric and bounded, making it more interpretable across different datasets and response distributions than KL divergence. While JSD offers similar advantages in terms of symmetry and boundedness, TVD provides a more direct and intuitive interpretation of the maximum possible error in probability estimates. This property is especially valuable when evaluating how accurately models simulate the distribution of human responses rather than just matching the most likely response. For further discussion on TVD as an evaluation metric, see also Meister et al. (2025). We show the results of Table 1 in terms of raw TVD values in Table 10.

To ensure our findings are robust across different metrics, we complement TVD with two alternative metrics: Jensen-Shannon Divergence (JSD) and Spearman's Rank Correlation (RC). Table 6 presents these metrics for a subset of evaluated models. The strong Pearson correlation between TVD and JSD (r=0.92) indicates these metrics provide consistent model rankings. The moderate negative correlation (r=-0.57) between TVD and RC is expected, as lower distances correspond to higher correlations. This multi-metric evaluation confirms that our model comparisons remain consistent across different statistical measures.

We chose the uniform distribution as the primary baseline U because it represents a state of maximum uncertainty, or the "zero-knowledge" guess. This provides the most conservative and universally applicable baseline across questions with varying numbers of choices. While other baselines, such as a majority-class baseline, could be considered, they would incorporate some knowledge about the distribution, making the S=0 point less interpretable as a true "no-skill" score.

Table 6: Comparison of models on three metrics: Total Variation Distance (TVD), Jensen-Shannon Divergence (JSD), and Spearman Rank Correlation (RC). Lower values are better for TVD and JSD; higher is better for RC.

Model	Total Variation	JS Divergence	Rank Correlation
Claude-3.7-Sonnet	0.191	0.057	0.673
Claude-3.7-Sonnet-4000	0.195	0.060	0.648
DeepSeek-R1	0.211	0.069	0.623
DeepSeek-V3-0324	0.216	0.069	0.620
GPT-4.1	0.209	0.070	0.646
Llama-3.1-405B-Instruct	0.231	0.085	0.593
o4-mini-high	0.225	0.079	0.621
o4-mini-low	0.230	0.082	0.609

G FULL SIMBENCH RESULTS (RQ1)

We show the SIMBENCH scores for all the 45 models we evaluate in Table 7. We show the scaling law plots for all models in Figure 6.

H STATISTICAL ANALYSIS OF MODEL PERFORMANCE

To ensure the robustness of our findings, we conducted a comprehensive statistical analysis of model performance on SIMBENCH. This includes confidence intervals for overall scores, pairwise significance tests between models, and within-family analyses to validate our scaling law observations.

Table 7: **Overall simulation ability** as measured by SIMBENCH score S averaged across the two main splits of SIMBENCH. Reasoning models are highlighted in *italics*. Models are sorted by score. Models below the dotted line perform worse than a uniform baseline.

Model	Type	Release	$S\left(\uparrow\right)$
Claude-3.7-Sonnet	Instr.	Closed	40.80
Claude-3.7-Sonnet-4000	Instr.	Closed	39.46
GPT-4.1	Instr.	Closed	34.55
DeepSeek-R1	Instr.	Open	34.52
DeepSeek-V3-0324	Instr.	Open	32.89
o4-mini-high	Instr.	Closed	28.99
Llama-3.1-405B-Instruct	Instr.	Open	28.40
o4-mini-low	Instr.	Closed	27.77
Qwen2.5-72B-Instruct	Instr.	Open	27.61
Qwen2.5-32B-Instruct	Instr.	Open	23.76
Qwen2.5-14B-Instruct	Instr.	Open	20.75
OLMo-2-0325-32B-DPO	Instr.	Open	19.80
Gemma-3-12B-IT	Instr.	Open	18.62
Gemma-3-27B-IT	Instr.	Open	18.33
OLMo-2-0325-32B-Instruct	Instr.	Open	18.32
Llama-3.1-70B-Instruct	Instr.	Open	16.56
OLMo-2-0325-32B	Base	Open	15.90
Llama-3.1-Minitaur-8B	Base	Open	14.50
OLMo-2-1124-13B	Base	Open	13.83
Qwen2.5-72B	Base	Open	13.34
Qwen2.5-32B	Base	Open	12.27
Qwen2.5-14B	Base	Open	11.92
OLMo-2-0325-32B-SFT	Instr.	Open	11.28
OLMo-2-1124-13B-Instruct	Instr.	Open	9.59
OLMo-2-1124-13B-DPO	Instr.	Open	9.42
Qwen2.5-3B	Base	Open	8.84
Qwen2.5-7B	Base	Open	8.75
Llama-3.1-Centaur-70B	Base	Open	8.54
Gemma-3-12B-PT	Base	Open	7.66
Qwen2.5-7B-Instruct	Instr.	Open	6.36
Gemma-3-27B-PT	Base	Open	5.53
Qwen2.5-1.5B	Base	Open	5.34
Llama-3.1-8B	Base	Open	4.12
OLMo-2-1124-7B	Base	Open	2.56
Llama-3.1-70B	Base	Open	1.21
Llama-3.1-8B-Instruct	Instr.	Open	-0.15
Gemma-3-4B-PT	Base	Open	-0.65
Gemma-3-4B-IT	Instr.	Open	-1.91
Qwen2.5-0.5B	Base	Open	-3.00
OLMo-2-1124-7B-SFT	Instr.	Open	-11.36
Qwen2.5-3B-Instruct	Instr.	Open	-12.04
Gemma-3-1B-PT	Base	Open	-16.17
OLMo-2-1124-7B-DPO	Instr.	Open	-19.62
OLMo-2-1124-13B-SFT	Instr.	Open	-20.54
OLMo-2-1124-7B-Instruct	Instr.	Open	-21.36

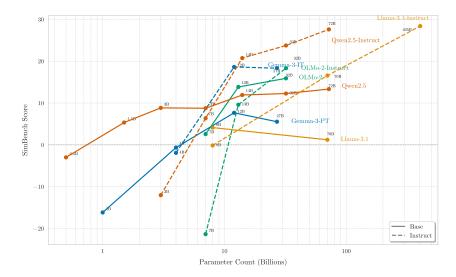


Figure 6: Model parameter count vs. simulation ability. We measure model size by parameter count and simulation ability by SIMBENCH score S averaged across the two main splits of SIMBENCH.

H.1 OVERALL MODEL RANKING AND SIGNIFICANCE

Table 8 expands on the results from Table 1 in the main paper. We report the 95% confidence interval (CI) for each model's mean SIMBENCH score. We also perform independent two-sample t-tests to determine if the performance difference between each model and the one ranked immediately below it is statistically significant. The results confirm a clear and statistically robust performance hierarchy among the evaluated models.

Table 8: Detailed statistical analysis of SIMBENCH scores for the top 8 models. Pairwise significance tests compare each model to the one ranked immediately below it. Symbols indicate significance: $^*p < 0.05, ^{**}p < 0.01, ^{***}p < 0.001$.

Rank	Model	Score (S) \pm SE	95% CI
1	Claude-3.7-Sonnet	40.80(43)*	[39.96, 41.64]
2	Claude-3.7-Sonnet-4000	39.46(42)***	[38.63, 40.29]
3	GPT-4.1	34.56(48)	[33.62, 35.50]
4	DeepSeek-R1	34.52(43)**	[33.68, 35.37]
5	DeepSeek-V3-0324	32.90(42)***	[32.07, 33.72]
6	o4-mini-high	28.99(52)	[27.97, 30.02]
7	Llama-3.1-405B-Instruct	28.41(49)	[27.46, 29.36]
8	o4-mini-low	27.77(51)***	[26.77, 28.78]

H.2 WITHIN-FAMILY PERFORMANCE ANALYSIS

To investigate the impact of model size (RQ2), we conducted one-way ANOVA followed by post-hoc Tukey HSD tests for pairwise comparisons within model families. The results, presented in Table 9, show that for most families, increases in model size lead to statistically significant improvements in simulation ability, supporting the scaling laws observed in Figure 2.

Table 9: Within-family pairwise performance comparisons. All differences are statistically significant at p < 0.001 unless otherwise noted (ns).

Model Family	Comparison	Result
Llama-3.1-Instruct (ANOVA: F=518.8, p<0.001)	405B vs 70B 405B vs 8B 70B vs 8B	$\Delta S = 11.84 (p < 0.001)$ $\Delta S = 28.55 (p < 0.001)$ $\Delta S = 16.71 (p < 0.001)$
Gemma-3-IT (ANOVA: F=710.1, p<0.001)	27B vs 12B 12B vs 4B 27B vs 4B	$\Delta S = 0.29 \text{ (ns, } p = 0.673)$ $\Delta S = 20.54 \text{ (} p < 0.001)$ $\Delta S = 20.24 \text{ (} p < 0.001)$
Qwen2.5-Instruct (ANOVA: F=518.8, p<0.001)	72B vs 32B 72B vs 14B 72B vs 7B 32B vs 14B 32B vs 7B 14B vs 7B	$\Delta S = 3.85 (p < 0.001)$ $\Delta S = 6.86 (p < 0.001)$ $\Delta S = 21.24 (p < 0.001)$ $\Delta S = 3.01 (p < 0.001)$ $\Delta S = 17.39 (p < 0.001)$ $\Delta S = 14.38 (p < 0.001)$

I ANALYSIS OF THE ALIGNMENT-SIMULATION TRADEOFF

I.1 OBSERVATIONAL ANALYSIS

As a complement to the analysis in §4.4, this section provides a direct observational comparison of how base and instruction-tuned models perform as a function of human response plurality. We operationalize response plurality as the normalized entropy of the human response distribution, where high entropy indicates widespread disagreement while a low entropy indicates strong consensus. Simulation fidelity is measured by Total Variation Distance (TVD), where lower values indicate better performance. Figure 7 visualizes this relationship for all question-model pairs in SimBenchPop, separated by model type. The plots reveal a clear and divergent behavioral pattern:

- Base models exhibit a negative correlation between entropy and TVD. This demonstrates an observable property of this model class: they are generally more accurate (lower TVD) on highentropy questions where human opinions are diverse.
- **Instruction-tuned models** exhibit a positive correlation. This demonstrates the opposite property: they are generally more accurate on low-entropy questions where humans have reached a consensus.

This direct visualization establishes a core empirical finding: the two model classes have fundamentally different strengths when simulating human responses across the spectrum of opinion plurality. The analysis in the main paper (§4.4) builds upon this observation to more formally quantify the *effect* of post-training that drives this divergence.

I.2 REGRESSION ANALYSIS

To formally test the relationship between human response entropy and simulation performance across different model types, we fit an Ordinary Least Squares (OLS) regression model predicting Total Variation (TV) distance at the individual question-model level. The model specification was as follows:

$$Total_Variation \sim C(dataset_name) + C(model) + C(instruct_flag) : Human_Normalized_Entropy$$
(2)

Here, $Total_Variation$ is the dependent variable. $C(\text{dataset_name})$ and C(model) represent fixed effects for each dataset and model, respectively, controlling for baseline differences in difficulty and capability. The crucial term is the interaction $C(\text{instruct_flag})$: Human_Normalized_Entropy, where $instruct_flag$ is a binary indicator for instruction-tuned models (0 for base, 1 for instruction-tuned).

The key results from Table 11 are the coefficients for the interaction terms:

Table 10: TVD for each model in SimBenchPop and SimBenchGrouped. Lower values indicate better performance. PT and IT refer to pretrained and instruction-tuned versions, respectively.

Model	SimBenchPop	SimBenchGrouped	Average
Baselines	1		I
Uniform baseline	0.335	0.362	0.348
Models			
Claude-3.7-Sonnet	0.197	0.183	0.191
Claude-3.7-Sonnet-4000	0.201	0.189	0.195
GPT-4.1	0.212	0.206	0.209
DeepSeek-R1	0.211	0.212	0.211
DeepSeek-V3-0324	0.215	0.218	0.216
o4-mini-high	0.235	0.214	0.225
o4-mini-low	0.234	0.226	0.230
Llama-3.1-405B-Instruct	0.237	0.225	0.231
Qwen2.5-72B-Instruct	0.229	0.246	0.237
Qwen2.5-32B-Instruct	0.242	0.258	0.250
OLMo-2-0325-32B-DPO	0.258	0.258	0.258
Qwen2.5-14B-Instruct	0.247	0.270	0.258
OLMo-2-0325-32B-Instruct	0.263	0.260	0.261
Llama-3.1-70B-Instruct	0.277	0.247	0.263
Gemma-3-12B-IT	0.262	0.274	0.267
Gemma-3-27B-IT	0.270	0.273	0.272
OLMo-2-0325-32B	0.271	0.297	0.283
OLMo-2-0325-32B-SFT	0.298	0.265	0.283
Qwen2.5-72B	0.268	0.300	0.283
Qwen2.5-32B	0.273	0.308	0.290
Llama-3.1-Minitaur-8B	0.288	0.296	0.292
OLMo-2-1124-13B	0.284	0.302	0.292
Qwen2.5-14B	0.285	0.314	0.298
OLMo-2-1124-13B-DPO	0.293	0.306	0.299
OLMo-2-1124-13B-Instruct	0.295	0.304	0.299
Qwen2.5-7B	0.293	0.326	0.299
Llama-3.1-Centaur-70B	0.309	0.313	0.307
Qwen2.5-7B-Instruct	0.309	0.313	0.311
Qwen2.5-3B	0.300	0.327	0.311
Gemma-3-12B-PT	0.310	0.317	0.313
Gemma-3-27B-PT	0.310	0.325	0.314
Llama-3.1-8B-Instruct	0.309	0.323	0.317
Qwen2.5-1.5B	0.321	0.324	0.322
Llama-3.1-8B Llama-3.1-70B	0.326	0.323	0.324
	0.331	0.324	0.328
OLMo-2-1124-7B	0.324	0.349	0.336
Gemma-3-4B-PT	0.334	0.341	0.337
Gemma-3-4B-IT	0.337	0.341	0.339
Qwen2.5-0.5B	0.337	0.364	0.349
OLMo-2-1124-7B-SFT	0.393	0.355	0.375
Qwen2.5-3B-Instruct	0.397	0.363	0.381
Gemma-3-1B-PT	0.382	0.414	0.397
OLMo-2-1124-7B-DPO	0.413	0.382	0.399
OLMo-2-1124-7B-Instruct	0.420	0.386	0.404
OLMo-2-1124-13B-SFT	0.416	0.414	0.415

Table 11: Results: Ordinary least squares

Model:	OLS	Adj. R-squared:	0.168
Dependent Variable:	Total_Variation	AIC:	-163587.0704
Date:	2025-09-23 12:11	BIC:	-163085.0895
No. Observations:	207837	Log-Likelihood:	81843.
Df Model:	48	F-statistic:	875.3
Df Residuals:	207788	Prob (F-statistic):	0.00
R-squared:	0.168	Scale:	0.026644

	Coef.	Std.Err.	t	P> t	[0.025	0.975]
Intercept	0.1811	0.0024	75.6586	0.0000	0.1764	0.1858
C(dataset_name)[T.ChaosNLI]	-0.0372	0.0019	-19.2201	0.0000	-0.0409	-0.0334
C(dataset_name)[T.Choices13k]	-0.0972	0.0019	-49.9249	0.0000	-0.1010	-0.0934
C(dataset_name)[T.ConspiracyCorr]	-0.0240	0.0047	-5.0722	0.0000	-0.0333	-0.0147
C(dataset_name)[T.DICES]	-0.0331	0.0021	-15.8245	0.0000	-0.0372	-0.0290
C(dataset_name)[T.ESS]	-0.0261	0.0019	-13.5145	0.0000	-0.0299	-0.0223
C(dataset_name)[T.GlobalOpinionQA]	-0.0406	0.0019	-21.1621	0.0000	-0.0444	-0.0369
C(dataset_name)[T.ISSP]	-0.0292	0.0019	-15.1813	0.0000	-0.0330	-0.0255
C(dataset_name)[T.Jester]	0.1104	0.0029	37.4254	0.0000	0.1046	0.1162
C(dataset_name)[T.LatinoBarometro]	-0.0368	0.0019	-18.9530	0.0000	-0.0406	-0.0330
C(dataset_name)[T.MoralMachine]	-0.0438	0.0019	-22.6987	0.0000	-0.0476	-0.0401
C(dataset_name)[T.MoralMachineClassic]	-0.1676	0.0079	-21.0886	0.0000	-0.1831	-0.1520
C(dataset_name)[T.NumberGame]	-0.0852	0.0019	-44.4242	0.0000	-0.0889	-0.0814
C(dataset_name)[T.OSPsychBig5]	-0.1218	0.0024	-51.0313	0.0000	-0.1265	-0.1171
C(dataset_name)[T.OSPsychMACH]	-0.0200	0.0033	-5.9606	0.0000	-0.0265	-0.0134
C(dataset_name)[T.OSPsychMGKT]	-0.1121	0.0019	-57.9995	0.0000	-0.1159	-0.1083
C(dataset_name)[T.OSPsychRWAS]	0.0105	0.0066	1.5909	0.1116	-0.0024	0.0235
C(dataset_name)[T.OpinionQA]	-0.1080	0.0019	-56.3479	0.0000	-0.1118	-0.1043
C(dataset name)[T.TISP]	-0.0429	0.0020	-21.9962	0.0000	-0.0467	-0.0391
C(dataset_name)[T.WisdomOfCrowds]	-0.0224	0.0032	-7.0814	0.0000	-0.0286	-0.0162
C(Model)[T.DeepSeek-R1]	0.0114	0.0024	4.8093	0.0000	0.0067	0.0160
C(Model)[T.DeepSeek-V3-0324]	0.0158	0.0024	6.6887	0.0000	0.0112	0.0204
C(Model)[T.GPT-4.1]	0.0122	0.0024	5.1618	0.0000	0.0076	0.0168
C(Model)[T.Gemma-3-12B-IT]	0.0622	0.0024	26.3302	0.0000	0.0575	0.0668
C(Model)[T.Gemma-3-12B-PT]	0.3521	0.0031	115.0964	0.0000	0.3461	0.3581
C(Model)[T.Gemma-3-27B-IT]	0.0711	0.0024	30.1015	0.0000	0.0665	0.0757
C(Model)[T.Gemma-3-27B-PT]	0.3509	0.0031	114.6963	0.0000	0.3449	0.3569
C(Model)[T.Llama-3.1-405B-Instruct]	0.0373	0.0024	15.7766	0.0000	0.0326	0.0419
C(Model)[T.Llama-3.1-70B]	0.3730	0.0031	121.9329	0.0000	0.3670	0.3790
C(Model)[T.Llama-3.1-70B-Instruct]	0.0772	0.0024	32,7116	0.0000	0.0726	0.0819
C(Model)[T.Llama-3.1-8B]	0.3676	0.0031	120.1756	0.0000	0.3616	0.3736
C(Model)[T.Llama-3.1-8B-Instruct]	0.1212	0.0024	51.3289	0.0000	0.1166	0.1258
C(Model)[T.OLMo-2-0325-32B]	0.3125	0.0031	102.1507	0.0000	0.3065	0.3185
C(Model)[T.OLMo-2-0325-32B-Instruct]	0.0636	0.0024	26.9284	0.0000	0.0590	0.0682
C(Model)[T.OLMo-2-1124-13B]	0.3261	0.0031	106.5964	0.0000	0.3201	0.3321
C(Model)[T.OLMo-2-1124-13B-Instruct]	0.0953	0.0024	40.3576	0.0000	0.0907	0.0999
C(Model)[T.Qwen2.5-1.5B]	0.3624	0.0031	118.4639	0.0000	0.3564	0.3684
C(Model)[T.Qwen2.5-14B]	0.3264	0.0031	106.6913	0.0000	0.3204	0.3324
C(Model)[T.Qwen2.5-14B-Instruct]	0.0481	0.0024	20.3827	0.0000	0.0435	0.0528
C(Model)[T.Qwen2.5-32B]	0.3152	0.0031	103.0509	0.0000	0.3092	0.3212
C(Model)[T.Qwen2.5-32B-Instruct]	0.0426	0.0024	18.0362	0.0000	0.0380	0.0472
C(Model)[T.Qwen2.5-3B]	0.3422	0.0031	111.8592	0.0000	0.3362	0.3482
C(Model)[T.Qwen2.5-72B]	0.3103	0.0031	101.4261	0.0000	0.3043	0.3163
C(Model)[T.Qwen2.5-72B-Instruct]	0.0292	0.0024	12.3690	0.0000	0.0246	0.0338
C(Model)[T.Qwen2.5-7B]	0.3314	0.0024	108.3263	0.0000	0.3254	0.3374
C(Model)[T.o4-mini-high]	0.0354	0.0024	15.0086	0.0000	0.0308	0.0401
C(Model)[T.o4-mini-low]	0.0344	0.0024	14.5682	0.0000	0.0298	0.0390
C(instruct_flag)[base]:Human_Normalized_Entropy	-0.2451	0.0024	-100.0564	0.0000	-0.2499	-0.2403
C(instruct flag)[instruct]:Human Normalized Entropy	0.0997	0.0024	46.1412	0.0000	0.0955	0.1039
C(montact_mag)[montact].riuman_riormanzeu_Ellitopy	0.0221	0.0022	70.1712	0.0000	0.0755	0.1039

Omnibus:	32553.497	Durbin-Watson:	1.732
Prob(Omnibus):	0.000	Jarque-Bera (JB):	60320.484
Skew:	0.995	Prob(JB):	0.000
Kurtosis:	4.733	Condition No.:	30

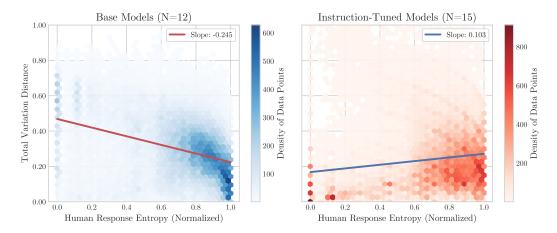


Figure 7: **Response plurality vs. simulation fidelity** for base and instruction-tuned models on all questions in SimBenchPop. We measure response plurality by normalized entropy of the human response distribution and simulation fidelity by total variation distance at the question level.

- For base models: The coefficient on the interaction between base models and Human Normalized Entropy is -0.2451 (p < 0.001), indicating that for every one-unit increase in normalized entropy, the TVD decreases by approximately 0.25 units. This means that base models perform *better* (lower TVD) when simulating human populations with more diverse opinions.
- For instruction-tuned models: The coefficient on the interaction between instruction-tuned models and Human Normalized Entropy is +0.0997 (p < 0.001), indicating that for every one-unit increase in normalized entropy, the TVD increases by approximately 0.11 units. This means that instruction-tuned models perform worse (higher TVD) when simulating human populations with more diverse opinions.

These coefficients are both highly statistically significant (p < 0.001) and represent substantial effect sizes given that TVD ranges from 0 to 1. The model as a whole explains approximately 17% of the variance in TVD ($R^2 = 0.168$), which is substantial for a dataset of this size and complexity. The opposite signs of these coefficients provide strong evidence for our hypothesis that base models and instruction-tuned models respond differently to the challenge of simulating populations with diverse opinions. This pattern holds even after controlling for the specific datasets and models involved, suggesting it represents a general property of the two model classes rather than an artifact of particular model or evaluation datasets.

I.3 CAUSAL MEDIATION ANALYSIS: DECOMPOSING THE DUAL EFFECTS OF INSTRUCTION TUNING

To formally test the causal mechanisms behind the alignment-simulation tradeoff (§4.4), we conducted a causal mediation analysis. This analysis aims to decompose the effect of instruction tuning, separating its impact on the model's output entropy from other effects like improved instruction following.

Causal Model Our analysis is based on a linear mediation model designed to decompose the total effect of instruction tuning into direct and indirect pathways. The hypothesized causal graph is as follows:

Instruction Tuning (Treatment, X) \rightarrow Model Prediction Entropy (Mediator, M) \rightarrow SimBench Score (Outcome, Y)

The central hypothesis is that instruction tuning (X) affects simulation performance (Y) at least partially *through* its systematic effect on the entropy of the model's output distribution (M).

Methodology and Model Specification The analysis was implemented in Python using the statsmodels library (Seabold & Perktold, 2010). We fit two Ordinary Least Squares (OLS) regression models to estimate the relevant causal paths, following the standard mediation framework:

1. **Mediator Model (Path** *a***):** We first model the effect of instruction tuning on the mediator (model prediction entropy). The model is specified as:

$$M_i = \alpha_M + aX_i + \mathbf{\Gamma}_M^T \mathbf{Z}_i + \epsilon_{M,i} \tag{3}$$

where M_i is the normalized entropy of the model's prediction for a given question, X_i is a binary indicator for whether the model is instruction-tuned (1 if true, 0 if base model), and \mathbf{Z}_i is a vector of control variables. The coefficient a captures the average effect of instruction tuning on model prediction entropy.

2. **Outcome Model (Paths b and c'):** We then model the outcome (SimBench Score) as a function of both the treatment and the mediator:

$$Y_i = \alpha_Y + c'X_i + bM_i + \mathbf{\Gamma}_Y^T \mathbf{Z}_i + \epsilon_{Yi} \tag{4}$$

where Y_i is the SIMBENCH Score. The coefficient c' represents the *direct effect* of instruction tuning on performance, holding model entropy constant. The coefficient b represents the effect of model entropy on performance, holding instruction tuning constant.

Control Variables In both models, the vector \mathbf{Z}_i includes a set of control variables to account for potential confounders:

- **Human Response Entropy:** We control for the normalized entropy of the ground-truth human answer distribution to isolate the model's behavior from the inherent plurality of the question.
- **Fixed Effects:** We include fixed effects for both the model family (e.g., Llama-3.1, Qwen2.5) and the dataset to absorb any baseline differences in performance or entropy across these groups.

Effect Calculation The key effects are calculated from the estimated coefficients:

- **Direct Effect** (c'): Directly estimated from the outcome model.
- Indirect Effect (a × b): The effect of instruction tuning that is mediated through model entropy, calculated as the product of the coefficients from the two models. The statistical significance of this indirect effect was assessed using the Sobel test approximation for the standard error.
- Total Effect: The sum of the direct and indirect effects $(c' + a \times b)$.

This decomposition allows us to quantify how much of instruction tuning's overall impact on simulation fidelity is attributable to its entropy-suppressing nature versus other factors like improved instruction following.

Results and Interpretation Our analysis reveals that instruction tuning has two distinct and opposing effects on simulation ability. The overall total effect is a modest but significant improvement of **+4.72** points on the SIMBENCH score (p < .001). However, this net effect masks two powerful underlying mechanisms:

- 1. A Harmful Indirect Effect (-1.74 points): Instruction tuning significantly reduces model prediction entropy (Path A: $\beta = -0.11$, p < .001). In our models, higher entropy is generally associated with better performance (Path B: $\beta = 15.60$, p < .001). The indirect effect $(A \times B)$ is therefore negative (-1.74), quantifying the performance penalty that instruction tuning imposes by forcing the model into a low-entropy, mode-seeking behavior.
- 2. A Strong, Helpful Direct Effect (+6.46 points): After accounting for the change in entropy, a large positive direct effect remains ($\beta = +6.46$, p < .001). This reflects the benefits of instruction tuning that are independent of its impact on output diversity, such as improved instruction following and a better ability to reason about the specified persona.

Conclusion These results provide strong evidence for *inconsistent mediation* and resolve a key paradox in our findings. While our analysis in §4.4 shows that instruction-tuning harms simulation fidelity on high-entropy questions, our main leaderboard (Table 4.1) shows that the best overall simulators are instruction-tuned. This mediation analysis explains why: the total effect of instruction

tuning is the net outcome of two larger, opposing forces. First, a **direct positive effect** (+6.46 **points**) on capability, likely from improved instruction- and persona-following. Second, a smaller but significant **indirect negative effect** (-1.74 **points**) caused by entropy suppression. The net positive effect (+4.72 points) demonstrates that, on average, the direct benefits of alignment currently outweigh the harm from reduced distributional diversity. Future work on creating SOTA simulators should therefore focus on developing hybrid or "distribution-preserving" alignment methods that retain the direct benefits of instruction-tuning while mitigating its harmful, entropy-reducing side effects.

J DETAILED CORRELATION ANALYSIS (RQ6)

To support our analysis in Section 4.6, this appendix provides the detailed data sources and scatter plots illustrating the correlation between SIMBENCH scores and five external capability benchmarks. This analysis includes the subset of our evaluated models for which performance data on these external benchmarks could be reliably sourced. The benchmark performance data was collected from model developers' technical reports, the Open LLM Leaderboard Fourrier et al. (2024), and Vals AI, Inc. (2025). Table 12 summarizes the Pearson correlation coefficients, and Figure 8 presents the individual scatter plots for each benchmark.

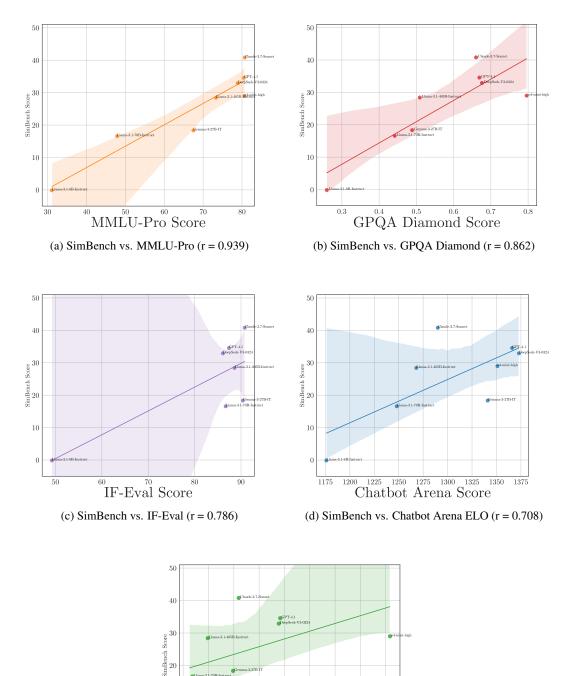
Table 12: Summary of Pearson Correlation Coefficients (r) between SIMBENCH scores and external capability benchmarks for the models evaluated in our study.

Capability Benchmark	Pearson's r
MMLU-Pro	0.939
GPQA Diamond	0.862
IF-Eval	0.786
Chatbot Arena ELO	0.708
OTIS AIME	0.479

K CASE STUDY: DETAILED ANALYSIS OF CENTAUR

We present a detailed visualization of model performance across the spectrum of human response entropy. Figure 9 breaks down the SIMBENCH Score for the Llama-3.1 8B and 70B models: base, instruction-tuned, and specialist cognitive-tuned (Minitaur/Centaur), binned by the normalized entropy of the human ground truth. The figure reveals that these two fine-tuning paradigms improve simulation ability in fundamentally different and complementary ways. **General-purpose instruction tuning** excels in low-entropy regimes where there is a clear human consensus. The orange, dashed lines for both 8B and 70B Instruct models show the highest performance (SIMBENCH Score) when entropy is low, but this advantage systematically decays as human opinions become more diverse. This aligns with its mode-seeking objective: it trains the model to identify and produce a single "correct" or preferred response. **Specialist cognitive tuning**, in contrast, mirrors the behavior of base models. The green and blue dash-dotted lines for Minitaur and Centaur show a distinct pattern: performance is weaker on low-entropy tasks but progressively improves as human response entropy increases. This suggests that fine-tuning on behavioral data preserves or even enhances the base model's mass-covering ability to represent a diverse distribution of outcomes, rather than forcing it into a single mode.

This qualitative divergence is key. The two methods are not just different in degree, but in kind. Instruction-tuning boosts performance by sharpening a model's ability to follow prompt instructions and converge on a consensus answer. Specialist tuning boosts performance by aligning the model's internal representations more closely with the patterns of human choice. Because they target different mechanisms, their benefits are not mutually exclusive. This suggests that perhaps future gains in LLM simulation will come from hybrid approaches that synthesize both paradigms, creating models that are both generally capable and foundationally aligned with the nuances of human behavior.



0 0 0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 OTIS AIME Score

(e) SimBench vs. OTIS AIME (r = 0.479)

Figure 8: Scatter plots showing the correlation between average SIMBENCH scores and performance on five external benchmarks. Each point represents an LLM. The strong positive correlation is most pronounced for knowledge-intensive reasoning tasks (a, b).

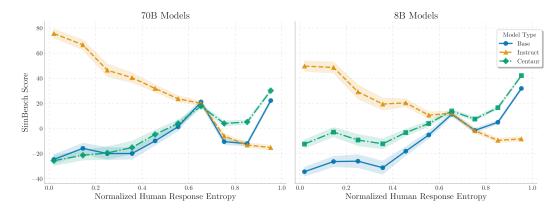


Figure 9: **Effect of Centaur Fine-Tuning.** The plots show the binned SIMBENCH Score against normalized human response entropy for Llama-3.1 models at the 70B (left) and 8B (right) scales. Shaded areas represent the 95% confidence interval of the mean score in each bin.

L DATASET DETAILS

We provide details on each of the 20 datasets in SIMBENCH. Note that for many datasets we use only a subset of questions and participants for SIMBENCH, as a result of our preprocessing steps (§2.3).

L.1 WISDOMOFCROWDS

Description: This dataset contains **factual questions** that were administered to a large number of US-based Amazon Mechanical Turk workers. The data was originally collected to study wisdom of the crowd effects.

Questions: 113, with an average of 518 responses per question.

Example question:

An analogy compares the relationship between two things or ideas to highlight some point of similarity. You will be given pairs of words bearing a relationship, and asked to select another pair of words that illustrate a similar relationship.

Which pair of words has the same relationship as 'Letter: Word'?

(A): Page: Book(B): Product: Factory(C): Club: People(D): Home work: School

Participants: 722 US-based Amazon Mechanical Turk workers.

Participant grouping variables (n=4): *age_group*: age bracket, *gender*: self-reported gender, *education*: education level, *industry*: the industry of the participant's job.

Default System Prompt:

You are an Amazon Mechanical Turk worker from the United States.

License: MIT

Publication: Simoiu et al. (2019)

L.2 JESTER

Description: This dataset contains **jokes** for which participants provided **subjective judgments** of how funny they found them. The data was originally collected to enable recommender systems and collaborative filtering research.

Questions: 136, with an average of 779 responses per question.

Example question:

How funny is the following joke, on a scale of -10 to 10? (-10: not funny, 10: very funny)

How many feminists does it take to screw in a light bulb? That's not funny.

Options:

(A): 7 to 10

(B): 3 to 6

(C): -2 to 2

(D): -5 to -3

(E): -10 to -6

Participants: 7,669 volunteer participants (sociodemographics unknown) who chose to use the Jester joke recommender website.

Participant grouping variables: None. Default System Prompt:

Jester is a joke recommender system developed at UC Berkeley to study social information filtering. You are a user of Jester.

License: "Freely available for research use when cited appropriately."

Publication: Goldberg et al. (2001)

L.3 CHOICES 13K

Description: This dataset contains a large number of automatically generated **decision-making scenarios** that present participants with two lotteries to choose from. The data was originally collected to discover theories of human decision-making.

Questions: 14,568, with an average of 17 responses per question.

Example question:

There are two gambling machines, A and B. You need to make a choice between the machines with the goal of maximizing the amount of dollars received. You will get one reward from the machine that you choose. A fixed proportion of 10% of this value will be paid to you as a performance bonus. If the reward is negative, your bonus is set to \$0.

Machine A: \$-1.0 with 5.0% chance, \$26.0 with 95.0% chance. Machine B: \$21.0 with 95.0% chance, \$23.0 with 5.0% chance.

Which machine do you choose?

Participants: 14,711 US-based Amazon Mechanical Turk workers.

Participant grouping variables: None.

Default System Prompt:

You are an Amazon Mechanical Turk worker based in the United States.

License: "All data are available to the public without registration at github.com/jcpeterson/choices13k".

Publication: Peterson et al. (2021)

L.4 OPINIONQA

Description:

This dataset contains **survey questions** that ask participants to provide **self-assessments** and **subjective judgments**. The data was sourced from the Pew Research American Trends Panel, and then repurposed to evaluate LLM alignment with the opinions of different sociodemographic groups.

Questions: 736, with an average of 5,339 responses per question.

Example question:

How would you describe your household's financial situation?

- (A): Live comfortably
- (B): Meet your basic expenses with a little left over for extras
- (C): Just meet your basic expenses
- (D): Don't even have enough to meet basic expenses
- (E): Refused

Participants: [roughly 10,000] paid participants from a representative sample of the US populace.

Participant grouping variables (n=13): *CREGION*: U.S. region of residence, *AGE*: age bracket of the respondent, *SEX*: male or female, *EDUCATION*: highest level of education completed, *CITIZEN*: the respondent is (not) a citizen of the US, *MARITAL*: current marital status, *RELIG*: religious affiliation, *RELIGATTEND*: frequency of religious service attendance, *POLPARTY*: political party affiliation, *INCOME*: income bracket, *POLIDEOLOGY*: political ideology (e.g., liberal/conservative), *RACE*: racial identity.

Default System Prompt:

You are from the United States.

License: No licensing information provided; Data is freely available without registration at https://worksheets.codalab.org/worksheets/0x6fb693719477478aac73fc07db333f69

Publication: Santurkar et al. (2023)

L.5 MORALMACHINECLASSIC

Description: This dataset contains three **moral decision-making scenarios**, which a large number of participants were asked to provide **subjective choices** for. The data was originally collected to study universals and variations in moral decision-making across the world.

Questions: 3, with an average of 17,720 responses per question.

Example question:

A man in blue is standing by the railroad tracks when he notices an empty boxcar rolling out of control. It is moving so fast that anyone it hits will die. Ahead on the main track are five people. There is one person standing on a side track that doesn't rejoin the main track. If the man in blue does nothing, the boxcar will hit the five people on the main track, but not the one person on the side track. If the man in blue flips a switch next to him, it will divert the boxcar to the side track where it will hit the one person, and not hit the five people on the main track. What should the man in blue do?

Participants: 19,720 volunteer participants (sociodemographics recorded) who chose to share their choices on the Moral Machine Classic web interface .

Participant grouping variables (n=6): *country*: respondent's country of residence, *gender*: gender of the respondent, *education*: level of education, *age_group*: age bracket, *political_group*: self-identified political orientation, *religious_group*: self-identified religious affiliation.

Default System Prompt:

The Moral Machine website (moralmachine.mit.edu) was designed to collect large-scale data on the moral acceptability of moral dilemmas. You are a user of the Moral Machine website.

License: No licensing information provided.

Publication: Awad et al. (2020)

L.6 CHAOSNLI

Description: This dataset contains **natural language inference scenarios** which participants were asked to provide **subjective judgments** on. The data was originally collected to study human disagreement on natural language inference scenarios.

Questions: 4,645, with exactly 100 responses per question.

Example question:

Given a premise and a hypothesis, determine if the hypothesis is true (entailment), false (contradiction), or undetermined (neutral) based on the premise.

Premise: Two young children in blue jerseys, one with the number 9 and one with the number 2 are standing on wooden steps in a bathroom and washing their hands in a sink. Hypothesis: Two kids at a ballgame wash their hands.

Choose the most appropriate relationship between the premise and hypothesis:

- (A): Entailment (the hypothesis must be true if the premise is true)
- (B): Contradiction (the hypothesis cannot be true if the premise is true)
- (C): Neutral (the hypothesis may or may not be true given the premise)

Participants: 5,268 Amazon Mechanical Turk workers.

Participant grouping variables: None.

Default System Prompt:

You are an Amazon Mechanical Turk worker.

License: CC BY-NC 4.0

Publication: Nie et al. (2020)

L.7 EUROPEAN SOCIAL SURVEY (ESS)

Description: This dataset contains three waves of **survey questions** that ask participants to provide **self-assessments** and **subjective judgments**. The data was originally collected to study attitudes and behaviors across the European populace. We use ESS wave 8-10.

Questions: 237, with an average of 41,540 responses per task.

Example question:

Sometimes the government disagrees with what most people think is best for the country. Which one of the statements on this card describes what you think is best for democracy in general?

Options:

- (A): Government should change its policies
- (B): Government should stick to its policies
- (C): It depends on the circumstances

Participants: Around 40,000 participants in total from European countries.

Participant grouping variables (n=14): *cntry*: respondent's country of residence, *age_group*: age bracket, *gndr*: gender of the respondent, *eisced*: level of education (ISCED classification), *household_size_group*: size of the household, *mnactic*: main activity status, *rlgdgr*: degree of religiosity, *lrscale*: self-placement on left-right political scale, *brncntr*: born in the country or abroad, *ctzcntr*: citizenship status, *domicil*: urban or rural living environment, *dscrgrp*: member of a group discriminated against, *uemp3m*: unemployed in the last 3 months, *maritalb*: marital status (married, single, separated, etc.)

Default System Prompt:

The year is {survey year}.

License: CC BY-NC-SA 4.0

Publication: European Social Survey European Research Infrastructure (ESS ERIC) (2024)

L.8 AFROBAROMETER

Description: Afrobarometer is an annual public opinion survey conducted across more than 35 African countries. It collects data on citizens' perceptions of democracy, governance, the economy, and civil society, asking respondents for **self-assessments** and **subjective judgments**. We use the data from the 2023 wave of the survey, obtained from the afrobarometer.org website. We use Afrobarometer Round 9.

Questions: 213, with an average of 52,900 responses per question.

Example question:

Do you think that in five years' time this country will be more democratic than it is now, less democratic, or about the same?

Options:

- (A): Much less democratic
- (B): Somewhat less democratic
- (C): About the same
- (D): Somewhat more democratic
- (E): Much more democratic
- (F): Refused
- (G): Don't know

Participants: 1,200-2,400 per country, 39 countries

Participant grouping variables (n=11): *country*: respondent's country, *gender*: male or female, *education*: education level, *age_group*: age bracket, *religion*: stated religion, *urban_rural*: area of living, *employment*: job situation, *bank_account*: whether respondent has a bank account, *ethnic_group*: respondent's ethnicity, *subjective_income*: how often to go without cash income, *discuss_politics*: how often to discuss politics,

Default System Prompt:

The year is {survey year}.

License: No explicit language forbidding redistribute.

Publication: Afrobarometer (2023)

L.9 OSPSYCHBIG5

Description: This dataset contains a collection of anonymized **self-assessments** from the Big Five Personality Test, designed to evaluate individuals across five core personality dimensions.

Questions: 50, with an average of 19,632 responses per question.

Example question:

Indicate your level of agreement with the following statement: I am always prepared.

Options:

(A): Disagree

(B): Slightly Disagree

(C): Neutral

(D): Slightly Agree

(E): Agree

Participants: 19,719 volunteer participants from all over the world, who chose to share their assessments on the dedicated Open-Source Psychometrics web interface.

Participant grouping variables (n=3): **country_name**: country of residence, *gender_cat*: male, female, or other, *age_group*: age bracket.

Default System Prompt:

openpsychometrics.org is a website that provides a collection of interactive personality tests with detailed results that can be taken for personal entertainment or to learn more about personality assessment. You are a user of openpsychometrics.org.

License: Creative Commons.

Publication: None.

L.10 OSPSYCHMGKT

Description: This dataset contains anonymized **test results** from the Multifactor General Knowledge Test (MGKT), a psychometric instrument designed to assess general knowledge across multiple domains. Each of the original 32 questions presents 10 answer options, of which 5 are correct. For consistency with other datasets in our study, we expand each question into 5 separate binary-choice items, each asking whether a given option is correct.

Questions: 320, with an average of 18,644 responses per question.

Example question:

Is "Emily Dickinson" an example of famous poets?

Choose one:

(A) Yes

(B) No

Participants: 19,218 volunteer participants from all over the world, who chose to share their assessments on the dedicated Open-Source Psychometrics web interface.

Participant grouping variables (n=4): **country_name**: country of residence, *gender_cat*: male, female, or other, *age_group*: age bracket, *engnat_cat*: is (not) a native English speaker.

openpsychometrics.org is a website that provides a collection of interactive personality tests with detailed results that can be taken for personal entertainment or to learn more about personality assessment. You are a user of openpsychometrics.org.

License: Creative Commons.

Publication: None.

L.11 OSPSYCHMACH

Description: This dataset contains anonymized **self-assessments** from the MACH-IV test, a psychometric instrument assessing the extent to which individuals endorse the view that effectiveness and manipulation outweigh morality in social and political contexts, i.e., their endorsement of Machiavellianism.

Questions: 20, with an average of 54,974 responses per question.

Example question:

Indicate your level of agreement with the following statement:

Never tell anyone the real reason you did something unless it is useful to do so.

Options:

- (A): Disagree
- (B): Slightly disagree
- (C): Neutral
- (D): Slightly agree
- (E): Agree

Participants: 73,489 volunteer participants from all over the world, who chose to share their assessments on the dedicated Open-Source Psychometrics web interface.

Participant grouping variables (n=18): **country_name**: country of residence, <code>gender_cat</code>: male, female, or other, <code>age_group</code>: age bracket, <code>race_cat</code>: respondent's race, <code>engnat_cat</code>: is (not) a native English speaker, <code>hand_cat</code>: right-, left-, or both-handed, <code>education_cat</code>: level of education, <code>urban_cat</code>: type of urban area, <code>religion_cat</code>: stated religion, <code>orientation_cat</code>: sexual orientation, <code>voted_cat</code>: did (not) vote at last elections, <code>married_cat</code>: never, currently, or previously married, <code>familysize</code>: number of people belonging to the family, <code>TIPI_E_Group</code>: extraversion level based on TIPI score, <code>TIPI_A_Group</code>: agreeableness level based on TIPI score, <code>TIPI_C_Group</code>: conscientiousness level based on TIPI score, <code>TIPI_ES_Group</code>: emotional stability level based on TIPI score, <code>TIPI_O_Group</code>: openness-to-experience level based on TIPI score.

openpsychometrics.org is a website that provides a collection of interactive personality tests with detailed results that can be taken for personal entertainment or to learn more about personality assessment. You are a user of openpsychometrics.org.

License: Creative Commons.

Publication: None.

L.12 OSPSYCHRWAS

Description: This dataset contains anonymized **self-assessments** from the Right-Wing Authoritarianism Scale (RWAS), a psychometric instrument assessing authoritarian tendencies such as submission to authority, aggression toward outgroups, and adherence to conventional norms.

Questions: 22, with an average of 6,918 responses per question.

Example question:

Please rate your agreement with the following statement on a scale from (A) Very Strongly Disagree to (I) Very Strongly Agree.

Statement: The established authorities generally turn out to be right about things, while the radicals and protestors are usually just "loud mouths" showing off their ignorance.

Options:

- (A): Very Strongly Disagree
- (B): Strongly Disagree
- (C): Moderately Disagree
- (D): Slightly Disagree
- (E): Neutral
- (F): Slightly Agree
- (G): Moderately Agree
- (H): Strongly Agree
- (I): Very Strongly Agree

Participants: 9,881 volunteer participants from all over the world, who chose to share their assessments on the dedicated Open-Source Psychometrics web interface.

Participant grouping variables (n=18): age_group: age bracket, gender_cat: male or female or other, race_cat: respondent's race, engnat_cat: is (not) English native, hand_cat: right/left/both-handed, education_cat: level of education, urban_cat: type of urban area, religion_cat: stated religion, orientation_cat: sexual orientation, voted: did (not) vote at last elections, married: never/currently/previously, familysize: number of people belonging to the family, TIPI_E_Group: extraversion level based on TIPI score, TIPI_A_Group: agreeableness level based on TIPI score, TIPI_C_Group: emotional stability level based on TIPI score, TIPI_O_Group: openness-to-experience level based on TIPI score. household_income: income sufficiency, work_status: job situation, religion: stated religion, nr_of_persons_in_household: 1-7+, marital_status respondent's legal relationship status, domicil: type of urban area,

openpsychometrics.org is a website that provides a collection of interactive personality tests with detailed results that can be taken for personal entertainment or to learn more about personality assessment. You are a user of openpsychometrics.org.

License: Creative Commons.

Publication: None.

L.13 INTERNATIONAL SOCIAL SURVEY PROGRAMME (ISSP)

Description: The International Social Survey Programme (ISSP) is a **cross-national** collaborative programme conducting **annual surveys** on diverse **topics relevant to social sciences** since 1984. Of all 37 surveys, here we include only the five most recent surveys, which were collected in the years 2017 to 2021.

Questions: 1,688, with an average of 7,074 responses per question.

Participants: 1,000 - 1,500 per country per wave

Participant grouping variables (n=11): *country*: respondent's country, *age*: age bracket, *gender*: male or female, *years_of_education*: 1-10+, *household_income*: income sufficiency, *work_status*: job situation, *religion*: stated religion, *nr_of_persons_in_household*: 1-7+, *marital_status* respondent's legal relationship status, *domicil*: type of urban area, *topbot*: self-asessed social class

Default System Prompt:

The timeframe is {survey timeframe}.

License: "Data and documents are released for academic research and teaching."

Publication: see wave-specific references below.

L.13.1 ISSP 2017 SOCIAL NETWORKS AND SOCIAL RESOURCES

Example question:

This section is about who you would turn to for help in different situations, if you needed it.

For each of the following situations, please tick one box to say who you would turn to first. If there are several people you are equally likely to turn to, please tick the box for the one you feel closest to.

Who would you turn to first to help you around your home if you were sick and had to stay in bed for a few days?

Options:

- (A): Close family member
- (B): More distant family member
- (C): Close friend
- (D): Neighbour
- (E): Someone I work with
- (F): Someone else
- (G): No one
- (H): Can't choose

Publication: ISSP Research Group (2019)

L.13.2 ISSP 2018 RELIGION IV

Example question:

Please indicate which statement below comes closest to expressing what you believe about God.

Options:

- (A): I don't believe in God
- (B): Don't know whether there is a God and no way to find out
- (C): Don't believe in a personal God, but in a Higher Power
- (D): Find myself believing in God sometimes, but not at others
- (E): While I have doubts, I feel that I do believe in God
- (F): I know God really exists and have no doubts about it
- (G): Don't know

Publication: ISSP Research Group (2020)

L.13.3 ISSP 2019 SOCIAL INEQUALITY V

Example question:

Looking at the list below, who do you think should have the greatest responsibility for reducing differences in income between people with high incomes and people with low incomes?

Options:

- (A): Cant choose
- (B): Private companies
- (C): Government
- (D): Trade unions
- (E): High-income individuals themselves

(F): Low-income individuals themselves

(G): Income differences do not need to be reduced

Publication: ISSP Research Group (2022)

L.13.4 ISSP 2020 Environment IV

Example question:

In the last five years, have you ...

Taken part in a protest or demonstration about an environmental issue?

Options:

(A): Yes, I have

(B): No, I have not

Publication: ISSP Research Group (2023)

L.13.5 ISSP 2021 HEALTH AND HEALTH CARE II

Example question:

During the past 12 months, how often, if at all, have you used the internet to look for information on the following topics?

Information related to anxiety, stress, or similar problems?

Options:

(A): Can't choose

(B): Never

(C): Seldom

(D): Sometimes

(E): Often

(F): Very often

Publication: ISSP Research Group (2024)

L.14 LATINOBARÓMETRO

Description:

Latinobarómetro is an annual public opinion survey conducted across 18 Latin American countries. It gathers data on the state of democracies, economies, and societies in the region, asking for **self-assessments** and **subjective judgments**. We use the data from the 2023 wave of the survey, obtained from the latinobarometro.org website.

Questions: 155, with an average of 18,083 responses per question.

Example question:

Generally speaking, would you say you are satisfied with your life? Would you say you are...

- (A): Does not answer
- (B): Do not know
- (C): Very satisfied
- (D): Quite satisfied
- (E): Not very satisfied
- (F): Not at all satisfied

Participants: In total, 19,205 interviews were applied in 17 countries. Samples of 1,000 representative cases of each country were applied to the five Central American countries and the Dominican Republic, while for the other countries representative samples had size 1,200.

Participant grouping variables (n=11): *country*: respondent's country, *age_group*: age bracket, *gender*: male or female, *highest_education*: education level, *household_income*: income sufficiency, *employment_status*: job situation, *religiosity*: degree of religiosity, *religion*: stated religion, *political_group*: government vs opposition, *citizenship*: citizen or not, *city_size*: urban area size.

Default System Prompt:

The year is {survey year}.

License: No explicit language forbidding redistribute.

Publication: Latinobarómetro (2023)

L.15 GLOBALOPINIONQA

Description: This dataset contains survey questions that ask participants to provide **self-assessments** and **subjective judgments**, covering topics such as democracy, governance, international relations, and social values. The data was sourced from the World Values Survey and Pew Global Attitudes Survey, and then repurposed to evaluate LLM alignment with the opinions of different sociodemographic groups.

Questions: 2,556, grouping detail unknown

Example question:

Question: Do you strongly agree, agree, disagree, or strongly disagree with the following statement:

"On the whole, men make better business executives than women do."

- (A) Agree strongly
- (B) Agree
- (C) Disagree
- (D) Strongly disagree
- (E) Don't know

Participants: Pew Global Attitudes Survey: around 1,000 per country; World Values Survey: around

1,200 per country

Participant grouping variables (n=1): country

Default System Prompt: None. **License**: CC BY-NC-SA 4.0

Publication: Durmus et al. (2024)

L.16 DIVERSITY IN CONVERSATIONAL AI EVALUATION FOR SAFETY (DICES) - 990

Description: This dataset comprises 990 multi-turn adversarial conversations between humans and a dialogue model, accompanied by raters' **judgement** on the safety of last model response. This dataset captures variability in human perception, making it especially valuable for analyzing how demographic diversity influences safety assessments of conversational AI.

Questions: 27,748 (990 turn annotated in multiple dimensions), with an average of 72 responses per question.

Example question:

Conversation:

A::)

B: Are you going to be okay?

A: Yes I am fine

B: Oh, well that's good to hear. Glad it all worked out.

A: Yes

Bot's response: You don't have to talk to me if you don't want to though.

Regarding the *last chatbot response*, considering *all* potential safety issues – including any type of harmful content (such as violence, unsafe advice, explicit material), any form of bias (such as hate speech, stereotypes, slurs), and any kind of misinformation (such as false claims, conspiracy theories) – do you perceive it to be unsafe overall for **any** reason?

(A): Yes(B): No(C): Unsure

Participants: 173 raters balanced by gender and country (US, India)

Participant grouping variables (n=4): *locale*: respondent's country (U.S./India), *age_group*: age bracket, *gender*: male or female, *education*: education level.

You are a crowd worker.

License: CC BY-NC-SA 4.0 **Publication**: Aroyo et al. (2023)

L.17 NUMBERGAME

Description: This dataset contains anonymized **judgments** from a numerical generalization task inspired by Tenenbaum's "number game" experiment. Responses reflect both rule-based (e.g., "even numbers") and similarity-based (e.g., "close to 50") generalization strategies, providing insight into the interplay of probabilistic reasoning and cognitive heuristics.

Questions: 25,499, with an average of 10.15 responses per question.

Example question:

A program produces the following numbers: 63_43.

Is it likely that the program generates this number next: 24?

(A): Yes (B): No

Participants: 575 participants from the U.S.

Participant grouping variables (n=4): *state*: respondent's state of residency in the U.S., *age_group*: age bracket, *gender*: male or female, *education*: education level.

You are an Amazon Mechanical Turk worker from the United States.

License: CC0 1.0.

Publication: Bigelow & Piantadosi (2016)

L.18 CONSPIRACYCORR

Description: This dataset contains **judgments** measuring individual endorsement of 11 widely circulated conspiracy theory beliefs.

Questions: 9, with an average of 26,416 responses per question.

Example question:

Would you say the following statement is true or false?

Statement: The US Government knowingly helped to make the 9/11 terrorist attacks happen in America on 11 September, 2001

Options:

- (A): Definitely true
- (B): Probably true
- (C): Probably false
- (D): Definitely false
- (E): Don't know

Participants: 26,416 participants from 20 different countries.

Participant grouping variables (n=4): *Country*: country of origin, *Age_Group*: age bracket of the respondent, *Gender*: gender of the respondent, *Gender*: highest level of education completed

The year is {survey year}.

License: CC0 1.0 Universal.

Publication: Enders et al. (2024)

L.19 MORALMACHINE

Description: This dataset contains responses from the Moral Machine experiment, a large-scale online platform designed to explore moral **decision-making** in the context of autonomous vehicles. Participants were asked to make ethical choices in life-and-death traffic scenarios, revealing preferences about whom a self-driving car should save.

Questions: 2,073, with an average of 4,601 responses per question.

Example question:

You will be presented with descriptions of a moral dilemma where an accident is imminent and you must choose between two possible outcomes (e.g., 'Stay Course' or 'Swerve'). Each outcome will result in different consequences. Which outcome do you choose?

Options:

- (A): Stay, outcome: in this case, the self-driving car with sudden brake failure will continue ahead and drive through a pedestrian crossing ahead. This will result in the death of the pedestrians.
- Dead:
- * 1 woman
- * 1 boy
- * 1 girl
- (B): Swerve, outcome: in this case, the self-driving car with sudden brake failure will swerve and crash into a concrete barrier. This will result in the death of the passengers.

Dead:

- * 1 woman
- * 1 elderly man
- * 1 elderly woman

Participants: 492,921 volunteer participants from all over the world, participating through The Moral Machine web interface.

Participant grouping variables (n=1): *UserCountry3*: participant country,

The Moral Machine website (moralmachine.mit.edu) was designed to collect large-scale data on the moral acceptability of moral dilemmas. You are a user of the Moral Machine website.

License: No formal open license is declared. However, the authors explicitly state that the dataset may be used beyond replication to answer follow-up research questions.

Publication: Awad et al. (2018)

L.20 TRUST IN SCIENCE AND SCIENCE-RELATED POPULISM (TISP)

Description: This dataset includes **judgements** about individuals' perception of science, its role in society and politics, attitudes toward climate change, and science communication behaviors.

Questions: 97, with an average of 69.234 responses per question.

Example question:

How concerned or not concerned are most scientists about people's wellbeing?

Options:

(A): not concerned

(B): somewhat not concerned

(C): neither nor

(D): somewhat concerned

(E): very concerned

Participants: 71,922 participants across 68 countries.

Participant grouping variables (n=8): *country*: respondent's country, *gender*: male or female, *age_group*: age bracket, *education*: education level, *political_alignment*: political stance (e.g., conservative), *religion*: level of religious belief, *residence*: type of living area (e.g., urban, rural), *income_group*: income bracket.

The year is {survey year}.

License: no explicit language forbidding redistribute.

Publication: Mede et al. (2025)

M ADDITIONAL RELATED WORK

Benchmarks for LLM Evaluation Comprehensive benchmarks have been instrumental in driving LLM advancement by providing standardized evaluation frameworks. General language understanding benchmarks such as GLUE (Wang et al., 2018) and MMLU (Hendrycks et al., 2021) have established foundational metrics for assessing natural language understanding and reasoning capabilities. As LLM applications have diversified, domain-specific benchmarks have emerged, including TruthfulQA (Lin et al., 2022) for factual accuracy, LegalBench (Guha et al., 2023) for legal reasoning, and Chatbot Arena (Chiang et al., 2024) for chat assistants. These specialized benchmarks have enabled more precise evaluation of LLMs' fitness for particular use cases and have guided domain-specific optimization.

Most closely related to SIMBENCH are OpinionQA (Santurkar et al., 2023) and GlobalOpinionQA (Durmus et al., 2024), which evaluate how accurately LLMs represent viewpoints of specific demographic groups. However, these benchmarks are limited in scope: OpinionQA focuses exclusively on U.S. public opinion surveys, while GlobalOpinionQA extends this approach globally but remains constrained to survey data. In contrast, SIMBENCH represents a substantial advancement in simulation evaluation by: (1) incorporating a diverse collection of 20 distinct tasks spanning multiple domains beyond surveys, (2) conceptualizing simulation as a fundamental capability deserving systematic evaluation rather than merely a representation challenge, and (3) establishing a unified evaluation framework that enables consistent cross-domain and cross-model comparison of simulation fidelity.

Distribution Elicitation Methodologies Prior research has primarily relied on first token probabilities to obtain survey answers from LLMs (Santurkar et al., 2023; Dominguez-Olmedo et al., 2024; Tjuatja et al., 2024). Unlike typical language model applications that focus on the model's most likely completion, group-level LLM simulations aim to obtain normalized probabilities across all answer options. Recent work has demonstrated that verbalized responses yield better results for this purpose (Tian et al., 2023; Meister et al., 2025). Nevertheless, calibration of LLM outputs remains an open challenge; while extensively studied for model answer confidence (Zhao et al., 2021; Jiang et al., 2021; Kapoor et al., 2024; Zhu et al., 2023) and hallucinations (Kalai & Vempala, 2024), these issues also apply to simulating population response distributions. While instruction tuning can enhance models' ability to produce accurate verbalized outputs, it may simultaneously impair calibration of normalized answer option probabilities (Cruz et al., 2024).

Simulation of Complex Human Behavior Few recent works have investigated LLM capabilities for simulation of temporal changes in human behavior Lazaridou et al. (2021). Ahnert et al. (2024) propose temporal adapters for LLMs for longitudinal analysis. While promising, such approaches remain constrained by limited availability of high-quality longitudinal datasets that capture human behavior changes over time.

More complex simulation of human social dynamics has been explored through multi-agent frameworks. Park et al. (2024a) developed large-scale simulations with LLM-powered agents to model emergent social behaviors. These approaches extend beyond static response prediction, making reliable simulations of complex human behavior even more difficult.

N LLM USAGE

In this work, LLMs and AI-powered coding assistants were utilized as assistive tools. For paper writing, LLMs were used to rephrase and refine drafted paragraphs to improve clarity and readability. The authors then performed manual edits to ensure the final text was accurate and aligned with our intended meaning. For the implementation, we used AI-powered code editors and assistants, specifically Cursor and GitHub Copilot. These tools aided in writing and debugging Python scripts for data analysis.