

Review on Compositional Generalization on LLMs, LLMs for Organization Modelling and Agent-Based Modelling

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Abstract

This document presents a literature review exploring Compositional Generalization (CG) in Large Language Models (LLM), The application of LLMs on Organization Modelling (OM), and finally Agent-Based Modeling (ABM). It aims to explore how CG enhances LLMs' problem-solving capabilities, how LLMs can be applied to Organization Modelling and finally how ABM's can be enriched by embedding LLMs to provide agents with advanced, human-like decision-making skills. The document reviews the problems solved by the articles, summarizes all of them, and concludes with a synthesis of the collective advancements and challenges identified across the studies, emphasizing the potential of combining LLMs and ABM for Compositional Generation to push the boundaries of digital transformation.

1 Introduction

This document embarks on a cross-sector literature review aimed to assess the convergence of two pivotal technological spheres and their leasing: Compositional Generalization (CG) in Large Language Models (LLMs) and the application of LLMs for Organization Modelling (OM). Following these, the review explores Agent-Based Modeling (ABM) technique, as base for Modelling Organizations using LLMs and not only for Modelling, but also for Digitalization.

Compositional Generalization is and advanced LLM technique focused on several aspects of LLMs, but one in concrete is solving complex problems. The application of LLMs for OM is opening new trends on the field. By the other side ABM could serve as framework for Organization Modelling and their well-known software frameworks support for these applications. And at the heart of this leap is the empowerment of agents of AMB, providing them

“intelligence” and “skills” by introducing LLM at their core, allowing them to solve complex operations, make sophisticated dialogues, and informed decisions as humans does.

2 Literature review method

This section outlines the methodology employed for making the literature review.

Scope	Compositional Generalization on LLMs. LLMs for Organization modelling and simulation. Agent-Based Modeling and Simulation.
Sources	Google Scholar.
Search phrases	Compositional Generalization. LLMs for Organization Modelling and Simulation. Agent-Based Modelling and Simulation
Screening	Only free access articles selected. Books discarded. Title analysis used to discard.
Research Questions	General Problem. Summary. Compare and contrast. Future work.

3 General Problems

This point extracts and highlights the key problems analyzed in each article, presented in three blocks, Compositional Generalization in LLMs, LLMs for Organization Modeling and Agent-Based Modeling. The discussion aims to outline the current research landscape.

3.1 Compositional Generalization.

The review covers the challenge of Compositional Generalization within LLMs. Below we outline what the papers try to solve.

A novel method for creating realistic benchmarks to address the lack of compositional generalization in ML, particularly in NLU, is proposed in (Daniel Keysers, 2020).

Meta seq2seq learning, introduced in (Lake, 2019), enhances compositional generalization in seq2seq neural networks by learning from a series of tasks.

R&R, a data augmentation method discussed in (Ekin Akyürek, 2021) improves Compositional Generalization by recombining training examples and resampling.

A formal study to establish conditions for successful Compositional Generalization is proposed in (Thaddäus Wiedemer, 2023).

Lastly, the introduction of COGS, a dataset that challenges language models' Compositional Generalization testing their ability to parse and generate novel expressions from known components, is detailed in (Najoung Kim, 2020).

In summary, the articles encapsulate the progress in refining LLMs to better align with human behavior taking several work lines always in the scope of Compositional Generalization.

3.2 LLMs and Organization Modelling.

Now we try to try to search for application of LLMs on Organization Modelling in another set of articles.

The study from (Mohammad Asfour, 2023) focuses on the simulation and understanding of human responses to social engineering attacks, specifically phishing attacks, through the lens of LLMs like OpenAI's GPT-4. By examining how personality traits influenced by the Big Five personality model affect susceptibility to these attacks, the research aims to provide organizations and policymakers with insights to improve cybersecurity measures against social engineering threats effectively.

The article from (Giabbanelli, 2023) addresses the integration of large-scale pre-trained LLMs, such as

GPT-4 and ChatGPT, into scientific simulations. The goal is to enhance the engagement, comprehension, and accessibility of these simulations by leveraging LLMs for tasks ranging from explaining conceptual models to summarizing outputs and elucidating errors. This paper underscores the potential of LLMs to revolutionize the field of scientific modeling and simulation by improving its usability and reach.

In (Yuan Li, 2023), the paper explores the capacity of LLMs to coordinate within task-oriented social contexts, with a particular focus on a simulated job fair environment. It introduces collaborative generative agents designed to display human-like social behavior and collaboration skills, aiming to bridge the gap in understanding LLMs' potential for complex coordination tasks. This research endeavors to augment LLM-based agents with advanced reasoning and specialized skills, thereby enhancing their applicability in real-world scenarios requiring nuanced social interactions.

Lastly, (Mingyu Jin, 2024) jumps into the speculative domain of simulating interactions between human and extraterrestrial civilizations through LLMs, inspired by concerns raised by Stephen Hawking. The study introduces "Cosmo Agent," an AI framework designed to explore the dynamics of inter-civilizational relations across diverse ethical and moral landscapes. By observing the feasibility of peaceful coexistence among civilizations with vastly different worldviews, the research seeks to expand our comprehension of cosmic diversity and devise strategies for averting interstellar conflicts.

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Theme	Article	General Problems
CG	(Daniel Keysers, 2020)	• Challenge of Compositional Generalization in LLMs. • Proposed novel method for realistic benchmarks in ML, especially NLU.
	(Lake, 2019)	• Introduced meta seq2seq learning to enhance Compositional Generalization in neural networks.
	(Ekin Akyürek, 2021)	• Discussed R&R, a data augmentation method, to improve Generalization by recombining and resampling training examples.
	(Thaddäus Wiedemer, 2023)	• Proposed a study to establish conditions for successful Compositional Generalization.
	(Najoung Kim, 2020)	• Introduced COGS dataset to challenge and assess language models' Compositional Generalization.
LLM OM	(Mohammad Asfour, 2023)	• Focused on simulating human responses to social engineering attacks using LLMs like GPT-4.
	(Giabbanelli, 2023)	• Addressed the integration of LLMs into scientific simulations to enhance engagement, comprehension, and accessibility.
	(Yuan Li, 2023)	• Explored LLMs' capacity for coordination within task-oriented social contexts.
	(Mingyu Jin, 2024)	• Ventured into simulating interactions between human and extraterrestrial civilizations through LLMs.
ABM	(Christopher W. Weimer, 2016)	• Provided a foundational introduction to ABM, emphasizing its flexible, bottom-up simulation technique.
	(Singh, 2019)	• Discussed ABM's benefits over EBM, particularly for understanding dynamic interactions within systems.
	(Osgood, 2023)	• Addressed the challenge of comprehending complex systems' behavior through agent interactions and the environment.

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Table 1: General Problems Summary

3.3 Agent Based Modelling.

Finally, we intend to provide an overview on ABM in order to use as support framework for the two previous points reviewed.

The article referenced as (Christopher W. Weimer, 2016) provides a foundational introduction to ABM, scoping it as a bottom-up simulation technique that emphasizes the autonomous interactions of agents within an environment. It contrasts with traditional top-down modeling strategies, presenting ABM as a more flexible and intuitive method for analyzing systems where direct experimentation is impractical or unethical.

The article listed as (Singh, 2019) discusses the escalating interest among researchers in utilizing ABM to conceptualize and analyze complex systems. It outlines the benefits of ABM over Equation-Based Modeling (EBM), particularly for understanding dynamic interactions within systems.

Further delving into the intricacies of ABM, the text by G. Wade McDonald and Nathaniel D. Osgood, mentioned in (Osgood, 2023), specifically addresses the challenge of comprehending the behavior of complex systems through the lens of agent interactions and the environment. The article articulates why traditional compartmental models are often inadequate for representing the heterogeneity of agents, the complexity of their networks and spatial contexts, and the significance of individual histories within these systems.

4 Concise Summaries

This point presents the concise summaries extracted from the articles under review. Again, we follow the previous structure of three main points: Compositional Generalization in LLMs, their application in organization modeling, and Agent-based modeling.

4.1 Compositional Generalization

The Article from (Daniel Keysers, 2020), presents Cutting-edge machine learning techniques struggle with limited compositional generalization. Additionally, there is a lack of benchmarks that thoroughly assess this capability, making it difficult to identify and evaluate enhancements. The solution provided addresses this challenge by introducing a novel method that systematically constructs such benchmarks. This is achieved by maximizing compound divergence while ensuring minimal atom divergence between train and test sets. When compared quantitatively against alternative approaches for creating compositional generalization benchmarks, the effectiveness of this method is showcased. Furthermore, a substantial and practical natural language question answering dataset crafted in accordance with this methodology is unveiled. Analyzing the compositional generalization prowess of three machine learning architectures using this dataset,

their failure to generalize compositionally is uncovered. Intriguingly, a significant negative correlation between compound divergence and accuracy is observed. Additionally, it is illustrated how this method extends to creating fresh compositionality benchmarks based on the existing SCAN dataset, reaffirming the discoveries.

The work of (Lake, 2019) focus on while humans can intuitively apply new concepts in a compositional manner, sequence-to-sequence (seq2seq) neural networks often falter in integrating new with known concepts. The paper introduces a novel approach using memory-augmented neural networks trained via meta seq2seq learning to enhance compositional skills in these models. By training on a series of seq2seq problems, the models develop the ability to navigate new compositional challenges, showing promise in several SCAN tests for compositional learning. This advancement in leveraging meta-learning techniques could lead to neural networks with improved compositional generalization, impacting the development of AI systems capable of more complex and adaptable compositional task performance.

The 2021 article by (Ekin Akyürek, 2021) highlights that while neural sequence models outperform traditional grammar- and automaton-based methods in many tasks, they struggle with compositional generalization, particularly with rare or new subsequences. It introduces "R&R," a novel data augmentation method that enhances compositional generalization without depending on symbolic structures. R&R recombines training data through a prototype-based model and resamples to encourage extrapolation. When applied to language tasks like the SCAN instruction following and SIGMORPHON 2018's morphological analysis, R&R significantly improves a neural model's ability to generalize, even learning new constructions from minimal examples, demonstrating its potential to advance compositional generalization in neural sequence models.

(Thaddäus Wiedemer, 2023) presents another approach: Harnessing the inherent compositional structure of the environment to accelerate learning and foster generalization represents a fundamental aspect of human cognition. However, achieving compositional generalization in machine learning has remained a challenging objective, even for models explicitly designed with compositional priors. In proposed approach a bottom-up perspective is adopted: drawing inspiration from identifiable representation learning, compositionality is explored as a characteristic of the underlying data-generating process rather than the data itself. This reframing allows to establish mild conditions solely based on the support of the training distribution and the model architecture, which prove adequate for enabling compositional generalization. Moreover, this

illustrates how the proposed theoretical framework can be applied to real-world scenarios and validate our findings through empirical analysis. These results lay the groundwork for a systematic and principled theoretical examination of compositional generalization in machine learning.

The article from (Najoung Kim, 2020) deeps in the fact that, the essence of natural language lies in compositionality, wherein the meaning of a complex expression emerges from the meanings of its individual components. To enable a thorough assessment of language processing architectures' compositional abilities, the paper presents COGS, a semantic parsing dataset derived from a subset of English. The evaluation segment of COGS incorporates numerous deliberate gaps that demand compositional generalization, such as novel combinations of familiar syntactic structures or novel combinations of known words and structures. The experimentation with COGS experiments involving Transformers and LSTMs revealed that while in-distribution accuracy on the COGS test set approached perfection (96-99%), generalization accuracy markedly declined (16-35%) and exhibited considerable sensitivity to random seed variations ($\pm 6-8\%$). These outcomes underscore the limited compositional generalization capacity of contemporary standard NLP models, positioning COGS as a valuable tool for gauging progress in this domain.

4.2 LLMs and Organization Modelling

The study by Asfour and Murillo (Mohammad Asfour, 2023) investigates the use of large language models (LLMs) like OpenAI's GPT-4 for simulating human responses to social engineering attacks, specifically phishing, based on the Big Five personality traits. It highlights the potential of LLMs to provide realistic simulations that help in understanding human vulnerabilities to these attacks. The research is motivated by the need to explore the susceptibility of different personality traits to manipulation, aiming to enhance cybersecurity strategies and training.

The methodology involved creating simulated personas with distinct personality traits and subjecting them to phishing attack simulations. The study found that personas with high agreeableness (naivety), low conscientiousness (carelessness), and high neuroticism (impulsiveness) were more susceptible to phishing attacks. In contrast, traits associated with openness to experience, and extraversion showed resilience against these attacks.

This research contributes to the field by demonstrating that individual personality traits can significantly influence the success rate of social engineering attacks. It suggests that cybersecurity strategies and awareness campaigns should be personalized to address the vulnerabilities associated

with specific personality traits. Additionally, it proposes the potential for organizations to use such simulations for risk assessment and the development of targeted protective measures. However, the study acknowledges limitations, such as the inability of simulated personas to fully capture the complexity of human behavior and the generalizability of findings to other forms of social engineering attacks. Further research involving real-world subjects is recommended to validate and expand upon these findings, underlining the importance of a human-centric approach in cybersecurity.

This paper from (Giabbanelli, 2023) explores the integration of Natural Language Generation (NLG) with LLMs like GPT in the context of Modeling & Simulation. Initially, it outlines the evolution and capabilities of LLMs, mentioning their significance in tasks ranging from academic writing to coding, and highlights both opportunities and challenges, including errors like "hallucination." The focus then shifts to the potential for LLMs to play central roles in Modelling and Simulation tasks, suggesting a move beyond traditional uses towards more specific applications within the M&S domain. The paper proceeds to discuss the utility of NLG in explaining the structure of simulation models, emphasizing the importance of clear communication within interdisciplinary teams, and proposing NLG as a means to generate accessible textual narratives of models. It addresses the challenge of explaining model structures and dynamics through text, detailing the methodology of converting model schemas to linearized text for LLM processing. Further, it covers the use of NLG for comparing outcomes from predictive simulations, aiming to enhance transparency and engagement by summarizing key differences across simulation scenarios. The paper also explores emerging capabilities like transforming simulation visualizations into text, enhancing accessibility for individuals with visual impairments, and suggests this as a compliance strategy for legal requirements. Additionally, the paper considers the frontier of using LLMs to explain and correct simulation errors, highlighting the current gaps and potential future developments in automating feedback for modelers.

In conclusion, the paper emphasizes the burgeoning role of LLMs in Modelling and Simulation, from explaining model structures and dynamics to improving accessibility and automating error feedback. It points to ongoing and future research needed to fully harness LLMs' capabilities, suggesting a promising avenue for further integration of NLG and LLMs in Modelling and Simulation, thereby preparing the research community for these technological shifts.

The study conducted by Yuan Li, Yixuan Zhang, and Lichao Sun (Yuan Li, 2023) explores the development and application of "METAAGENTS," which are collaborative generative agents powered by Large

Language Models (LLMs) such as GPT-4. These agents are designed to simulate human-like behaviors and capabilities, particularly focusing on task-solving abilities and coordination within a job fair context. This simulation allows the agents to engage in complex social interactions, including interviewing, recruiting, and coordinating, to form teams for specific projects. The core innovation of this study lies in its attempt to bridge the gap in current LLM applications, which have largely focused on individual task-solving capabilities, by introducing the capacity for dynamic and collaborative coordination among agents.

The researchers developed a comprehensive framework for METAAGENTS that incorporates four key modules: perception, memory, reasoning, and execution. These modules collectively enable the agents to receive and process information from their environment, recall past interactions, make informed decisions based on this information, and execute actions that align with their goals. This multi-module framework allows the agents to not only imitate human-like behaviors more accurately but also to showcase progressively enhanced abilities in handling complex tasks through collaboration.

In their evaluation, the authors situated METAAGENTS within a simulated job fair environment, serving as a testbed to scrutinize their coordination skills. This environment was chosen due to its potential to demonstrate a broad range of human-like behaviors and the necessity for effective communication and collaboration among participants. Through this simulation, the study aimed to assess whether these generative agents could effectively form cohesive teams to complete specific tasks and dynamically create customized workflows that utilize the individual expertise of each team member.

The results of the study reveal that METAAGENTS exhibit a promising level of performance in terms of information retrieval and coordination capabilities. However, the study also uncovers limitations that affect the agents' effectiveness in more complex coordination tasks. These challenges are primarily attributed to the misalignment of LLMs' objectives or intentions with the tasks at hand, highlighting a critical area for future improvement.

This research contributes valuable insights into the role and evolution of LLMs in task-oriented social simulations, emphasizing the potential of collaborative generative agents in mimicking complex human interactions. By introducing an advanced form of generative agents capable of meaningful interaction and collaboration, the study opens up new avenues for exploring the application of LLMs in simulating and understanding human social behaviors.

Looking forward, the authors suggest several areas for further research and development, including enhancing the utility of the framework, scaling up the simulations to involve more agents and longer time spans, increasing the complexity of the tasks and interactions, and enriching the evaluation methods to provide deeper insights into the agents' performance. These future directions hold significant promise for advancing the field of artificial intelligence and its applications in simulating human social behavior and collaborative work.

The study by Mingyu Jin et al (Mingyu Jin, 2024) introduces "Cosmo Agent," a novel AI framework that employs Large Language Models (LLMs) to simulate interactions between human and extraterrestrial civilizations. Highlighting Stephen Hawking's warnings about the dangers of haphazardly broadcasting signals into space, the research aims to assess the possibility of peaceful coexistence among civilizations while identifying potential threats to benevolent societies. Using mathematical models and state transition matrices, the study quantitatively evaluates the developmental trajectories of civilizations, providing critical insights for decision-making during expansion and peak phases.

The researchers acknowledge the diversity in potential living conditions across the universe, which could lead to civilizations developing unique cosmologies, ethical codes, and worldviews. This approach offers a new perspective on understanding complex inter-civilizational dynamics and proposes novel strategies for conflict resolution, which are crucial for preventing interstellar conflicts.

Cosmo Agent's framework uses a Multi-Agent System (MAS) where civilizations can choose between hiding, fighting, or collaborating based on their characteristics and decision-making processes. This dynamic environment facilitates the exploration of potential civilizational alliances or rivalries, adherence to specific rules or agreements, and the development of novel cultures or technologies. By situating the study within the broader discourse on the existence, communication, conflict, and cooperation of various civilizations in the universe, the research opens new avenues for investigating these mysteries.

The study's significant implications span computational social science, astronomy, and philosophy, introducing innovative methods for using AI to mimic complex social phenomena. It provides a fresh perspective for astronomy in exploring and understanding civilizations beyond Earth and creates a new platform for philosophical exploration regarding the existence, communication, conflicts, and collaborations among civilizations with different moral standards.

Despite its groundbreaking approach, the study faces limitations such as an Earth-centric bias in LLMs, simplification of inter-civilizational interactions through mathematical models, and speculative predictions due to the absence of real-world extraterrestrial data. Future work aims to address these challenges by enhancing

LLMs to cover more ethical paradigms, investigating unforeseen technological advances, and fostering interdisciplinary collaborations. By deepening the understanding of complex inter-civilizational dynamics, future research can contribute to developing strategies for peaceful and mutually beneficial extraterrestrial interactions. This extended analysis showcases the distinct contributions of LLMs and ABMs to the digital transformation landscape and their potential synergistic application in agent-based digitalization. By leveraging the strengths of both methodologies, researchers and practitioners can push the boundaries of simulation, behavioral analysis, and complex system modeling, paving the way for innovative solutions to intricate problems across various domains.

4.3 Agent-Based Modelling

Christopher W. Weimer's 2016 article (Christopher W. Weimer, 2016) discusses agent-based models (ABMs) as frameworks allowing agents to interact within environments, enabling the development of complex, bottom-up models that mimic individual behaviors. ABMs are highlighted for their adaptability and intuitive approach to modeling, proving particularly valuable in fields like social sciences. The article positions ABMs as versatile tools for a range of applications, from social simulations to supply chain management, and offers a tutorial for beginners, illustrated with a war-gaming scenario.

Singh's 2019 (Singh, 2019) article highlights the increasing use of agent-based modeling (ABM) in tackling complex problems across various fields. ABM is praised for its ability to simulate individual agents' behaviors and interactions, offering insights into complex systems' dynamics that are not easily captured by traditional equation-based modeling (EBM). Unlike EBM, which focuses on system-level behaviors through equations, ABM excels in modeling individual decision-making processes and their emergent macro-level phenomena. The article points out ABM's advantages, such as accommodating spatial aspects and individual-level intricacies, making it ideal for social systems modeling. It also reviews the range of tools available for ABM, from the accessible NetLogo to advanced suites like GAMA and Repast, showcasing its application through practical examples like forest fire spread simulations. Concluding, Singh emphasizes ABM's role in creating precise models that deepen our understanding of complex phenomena, facilitate hypothesis testing, and explore interventions, underscoring its significance in advancing scientific research and addressing real-world issues.

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Osgood's 2023 article (Osgood, 2023) introduces Agent-based Modeling (ABM) as a computational approach for studying complex systems by simulating the interactions of autonomous agents. ABMs stand out for their ability to model dynamic interactions and individual histories, surpassing simpler compartmental models in representing system complexity. These models operate from the bottom up, where individual agent behaviors lead to emergent system-wide patterns. ABMs are adaptable, allowing for simulations in various temporal and spatial settings and enabling the exploration of "what-if" scenarios through interventions. This approach provides a rich framework for understanding the nuances of complex systems and their potential responses to changes.

5 Compare and Contrast

In this section we delve into an examination of how the featured studies align and diverge in their approaches to the three themes reviewed. To that we review Methodologies, Key Findings, Contributions, and Limitation and Challenges. Table 2 improves this comparison.

In Compositional Generalization, diverse methodologies emerge from creating benchmarks and datasets (Daniel Keysers, 2020) and (Najoung Kim, 2020) to leveraging memory-augmented neural networks (Lake, 2019) and data augmentation techniques (Ekin Akyürek, 2021). These efforts highlight both the struggle for machine learning models to generalize compositionally and the innovative approaches to mitigate these challenges.

The integration of LLMs with Organization Modelling explores applications ranging from cybersecurity strategies against phishing attacks (Mohammad Asfour, 2023) to scientific simulations (Giabbanelli, 2023) and coordination in task-oriented contexts (Yuan Li, 2023). This includes speculative simulations involving human and extraterrestrial civilizations (Mingyu Jin, 2024) showcasing the depth of LLMs' application in modeling complex systems and interactions.

ABM is portrayed as a flexible modeling technique, for its detailed representation of individual agents and dynamic interactions (Christopher W. Weimer, 2016); (Singh, 2019); (Osgood, 2023) It's underscored for its broad applicability and potential as a virtual laboratory, especially in fields where direct experimentation is challenging.

Finally, the following table provides a comprehensive compare and contrast analysis of the articles under review, focusing on their methodologies, key findings, contributions, and limitations.

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Category	Compositional Generalization on LLMs	LLMs for Organization Modelling and Simulation	Agent-Based Modelling
Methodologies	<ul style="list-style-type: none"> - (Daniel Keysers, 2020): Benchmarks for compositional generalization. - (Lake, 2019): Memory-augmented neural networks. - (Ekin Akyürek, 2021): Data augmentation technique R&R. - (Thaddäus Wiedemer, 2023) Bottom-up approach to compositional generalization. - (Najoung Kim, 2020): COGS dataset for language processing architectures. 	<ul style="list-style-type: none"> - (Mohammad Asfour, 2023): Simulated personas for cybersecurity. - (Giabbanelli, 2023): Integration of NLG with LLMs. - (Yuan Li, 2023)METAAGENTS for task-oriented coordination. - (Mingyu Jin, 2024)Simulating interstellar interactions. 	<ul style="list-style-type: none"> - (Christopher W. Weimer, 2016)Intro to ABM as a flexible tool. - (Singh, 2019)ABM vs EBM. - (Osgood, 2023)ABM's advantages over compartmental models.
Key Findings	<ul style="list-style-type: none"> - (Daniel Keysers, 2020) & (Najoung Kim, 2020): Machine learning architectures struggle with compositional generalization. - (Lake, 2019)& (Ekin Akyürek, 2021)Innovative solutions for enhancing model performance. 	<ul style="list-style-type: none"> - (Mohammad Asfour, 2023) Insights into personalized cybersecurity strategies. - Enhanced accessibility of scientific simulations. - METAAGENTS exhibit human-like coordination. - (Mingyu Jin, 2024) Developmental trajectories of civilizations. 	<ul style="list-style-type: none"> - (Christopher W. Weimer, 2016)ABM's broad applicability. - (Singh, 2019)& (Osgood, 2023) Unique advantages of ABM in modelling complex systems.
Contributions	<ul style="list-style-type: none"> - Practical solutions for neural network training. - Evaluation tools like datasets and benchmarks. - Theoretical frameworks for understanding compositional generalization. 	<ul style="list-style-type: none"> - (Mohammad Asfour, 2023): - Applications of LLMs in diverse domains. - Improved communication in scientific models. - (Mingyu Jin, 2024) Speculative simulations of interstellar relations. 	<ul style="list-style-type: none"> - (Christopher W. Weimer, 2016)Guide for aspiring modelers. - (Singh, 2019) Comparative analysis of ABM and EBM. - (Osgood, 2023)Detailed discussion on ABM's advantages.
Limitations and Challenges	<ul style="list-style-type: none"> - (Daniel Keysers, 2020) Existing architectures' limitations in achieving compositional generalization. - Scalability and applicability challenges. 	<ul style="list-style-type: none"> - (Mohammad Asfour, 2023) Complexity in simulating human behaviour. - (Mingyu Jin, 2024) "Hallucination" errors and speculative nature of models. 	<ul style="list-style-type: none"> - Computational demands and the complexity of accurately modelling agent behaviours.

Table 2: Compare and contrast.

Despite these advancements, challenges remain, such as the scalability of approaches, the complexity of accurately modeling human behavior, and the ethical considerations in LLM applications. These findings illustrate the progress and ongoing efforts in these areas, underscoring the need for continued research to refine these technologies and their integration for complex problem solving. At the end, we can see a open scope in Compositional Generalization for LLMs, while we see that LLMs for Organization Modelling articles use ABM as modelling framework. **This indicates that our approach would be correct as all three domains could be highly related.** Finally, Table 2 presents a summary for this point.

6 Future Work

In the landscape of Compositional Generalization, LLMs and ABM research, the quest for advancing technology and expanding our understanding of complex systems has led to a set of interesting future investigations. **Together, they represent a roadmap for researchers seeking to push the boundaries of knowledge in fields such as artificial intelligence, agent-based modeling, cybersecurity, natural language processing, and beyond.** The Future work is presented in the Table 3 below. The table presents a structured overview of future research directions across three themes: Compositional Generalization, Large Language Models for Organization Modelling and Agent-Based Modeling. In the domain of Compositional Generalization, future work includes applying unsupervised pre-training and targeted learning approaches (Daniel Keysers, 2020)extending methodologies to broader domains (Lake, 2019); (Ekin Akyürek, 2021) developing advanced memory mechanisms, and integrating unsupervised learning to tackle scalability issues. There is also an emphasis on exploring prototype identification models and extending frameworks to cover complex compositions (Thaddäus Wiedemer, 2023); (Najoung Kim, 2020) for LLMs and ABM, proposed future directions involve enhancing natural language generation (NLG) integration for simulation analysis and customizing LLMs for specific domains (Asfour, 2023), validating cybersecurity strategies through empirical studies, and refining LLMs for cybersecurity applications (Giabbanelli, 2023). Additionally, there's a focus on developing sophisticated agent behaviors (Yuan Li, 2023) and enhancing LLMs to cover ethical paradigms and simulate interstellar communication delays (Jin, 2024). In Agent-Based Modeling, future work aims at applying ABM to new

areas such as healthcare and urban planning, developing tools for easier access, and integrating ABMs with real-world data streams for scalability and realism (Christopher W. Weimer, 2016); (Singh, 2019); (Osgood, 2023)). Researchers are encouraged to compare ABM with traditional equation-based modeling (EBM), expand ABM toolsets with artificial intelligence (AI), and conduct empirical studies to validate models against real-world data, underscoring a broad and ambitious roadmap for advancing these fields.

Theme	Article	Future Work
Compositional Generation	(Daniel Keysers, 2020)	<ul style="list-style-type: none"> • Apply unsupervised pre-training and targeted learning approaches. • Extend the DBCA methodology to more domains and languages.
	(Lake, 2019)	<ul style="list-style-type: none"> • Tackle scalability in seq2seq problems. • Develop advanced memory mechanisms. • Integrate unsupervised learning.
	(Ekin Akyürek, 2021)	<ul style="list-style-type: none"> • Explore models identifying prototype groups with posterior constraints for rare tags.
	(Thaddäus Wiedemer, 2023)	<ul style="list-style-type: none"> • Broaden the framework to cover new types of generalization and complex compositions.
	(Najoung Kim, 2020)	<ul style="list-style-type: none"> • Develop models for high accuracy on the COGS dataset. • Explore tree-structured neural networks.
LLMs and OM	(Mohammad Asfour, 2023)	<ul style="list-style-type: none"> • Enhance NLG integration for simulation analysis. • Customize LLMs for specific domains.
	(Giabbanelli, 2023)	<ul style="list-style-type: none"> • Validate cybersecurity strategies through real-world studies. • Refine LLMs for cybersecurity applications.
	(Yuan Li, 2023)	<ul style="list-style-type: none"> • Develop sophisticated agent behaviors and decision-making processes. • Focus on scalability and validation methodologies.
	(Mingyu Jin, 2024)	<ul style="list-style-type: none"> • Enhance LLM capabilities to cover broader ethical paradigms. • Explore simulations of interstellar communication delays.
	(Christopher W. Weimer, 2016)	<ul style="list-style-type: none"> • Explore ABM in domains like healthcare, urban planning. • Develop sophisticated tools for easier ABM access.
Agent Based Modelling	(Singh, 2019)	<ul style="list-style-type: none"> • Compare ABM with EBM; expand ABM toolsets with AI. • Conduct empirical studies for real-world data validation.
	(Osgood, 2023)	<ul style="list-style-type: none"> • Address scalability challenges; integrate ABM with real-world data streams. • Capture and incorporate individual histories.

Table 3: Future Work

Table 3 highlights the emphasis on reinforcing work in Compositional Generalization, the confirmation that LLMs apply for Organization Modelling, and the fact the Agent Based Modelling powered by LLMs are interesting subjects of research combined.

References

- Christopher W. Weimer, J. O. (2016). Agent Based Modelling: An Introduction. *Proceedings of the 2016 Winter Simulation Conference*.
- Daniel Keysers, N. S. (2020). Measuring Compositional Generalization: A Comprehensive Method on Realistic Data. *arxiv > Computer Science > Machine Learning*.
- Ekin Akyürek, A. F. (2021). Learning to Recombine and Resample Data for Compositional Generalization. *arxiv > Computer Science > Computation and Language*.
- Giabbanelli, P. J. (2023). GPT-Based Models Meet Simulation: How to Efficiently Use Large-Scale Pre-Trained Language Models Across Simulation Tasks. *Arxiv > Computer Science > Human-Computer Interaction*.
- Lake, B. M. (2019). Compositional generalization through meta sequence-to-sequence learning. <https://proceedings.neurips.cc/>.
- Mingyu Jin, B. W. (2024). What if LLMs Have Different World Views: Simulating Alien Civilizations with LLM-based Agents. *Arxiv > Computer Science > Computation and Language*.
- Mohammad Asfour, J. C. (2023). Harnessing Large Language Models to Simulate Realistic Human Responses to Social Engineering Attacks: A Case Study. *International Journal of Cybersecurity Intelligence & Cybercrime*.
- Najoung Kim, T. L. (2020). COGS: A Compositional Generalization Challenge Based on Semantic Interpretation. *Arxiv > Computer Science > Computation and Language*.
- Osgood, G. W. (2023). Agent-Based Modeling and its Tradeoffs: An Introduction & Examples. *Arxiv > Computer Science > Multiagent Systems*.
- Singh, K. (2019). *Introduction to Agent-Based Modeling*. Obtenido de <https://dzone.com/articles/introduction-to-agent-based-modelling>
- Thaddäus Wiedemer, P. M. (2023). Compositional Generalization from First Principles. *Advances in Neural Information Processing Systems* 36.
- Yuan Li, Y. Z. (2023). MetaAgents: Simulating Interactions of Human Behaviors for LLM-based Task-oriented Coordination via Collaborative Generative Agents. *Arxiv > Computer Science > Artificial Intelligence*.