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AI-Driven Automation Can Become the Foundation of Next-Era Science of Science Research

(/pdf?id=u0FB996GIH)

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Keywords: Automated Scientific Discovery, AI for Science, Science of Science
TL;DR: AI-driven automated scientific discovery marks the future trajectory of Science of Science research.

Abstract:
The Science of Science (SoS) explores the mechanisms underlying scientific discovery, and offers valuable insights for enhancing scientific efficiency and fostering innovation. Traditional approaches often rely on simplistic assumptions and basic statistical tools, such as linear regression and rule-based simulations, which struggle to capture the complexity and scale of modern research ecosystems. The advent of artificial intelligence (AI) presents a transformative opportunity for the next generation of SoS, enabling the automation of large-scale pattern discovery and uncovering insights previously unattainable. This paper offers a forward-looking perspective on the integration of Science of Science with AI for automated research pattern discovery and highlights key open challenges that could greatly benefit from AI. We outline the advantages of AI over traditional methods, discuss potential limitations, and propose pathways to overcome them. Additionally, we present a preliminary multi-agent system as an illustrative example to simulate research societies, showcasing AI's ability to replicate real-world research patterns and accelerate progress in Science of Science research.

Submission Number: 110

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Paper Decision

Decision by Program Chairs 25 Sept 2025, 20:51 (modified: 17 Oct 2025, 12:38) Everyone
Revisions (/revisions?id=yVRtPbNEWA)

Decision: Reject

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Meta Review of Submission110 by Area Chair jB3Q

Meta Review by Area Chair jB3Q 09 Sept 2025, 07:40 (modified: 28 Oct 2025, 23:09) Everyone
Revisions (/revisions?id=oTlQBkUn0v)

Ethics:
No ethical violations or concerns.

Strengths:
The paper explores the intersection of AI and scientific research. Reviewers consider it to be of high quality and note the strong relevance of the topic. They also highlight positively that it combines theoretical and empirical support, incorporating simulations as well as references to real-world data, thereby presenting a compelling case.

Weaknesses:
The length of the paper and the scope of the discussions and experiments is criticised, e.g., one reviewer mentions that "experimental validation seems quite preliminary and limited in its scope" or that the paper "does not discuss scientific research that requires physical experiments". Similarity to some existing perspective articles about the topic is also mentioned.

Questions:
Reviewers ask for some more detailed discussion about the risks and negative sides of the vision presented in the paper.

Agreement: 4: agree
Rating: 8: Strong Accept: The paper presents a strong argument about an important issue that ought to be discussed and is of importance to a sub-area within the NeurIPS community.
Confidence: 3: You are fairly confident in your assessment. It is possible that you did not understand some parts of the submission or that you are unfamiliar with some pieces of related work.
Thoroughness: 3: You read the paper carefully but did not check all of the details.
Code Of Conduct Acknowledgement: Yes

Add: **Official Comment**

Official Review of Submission110 by Reviewer 3VY2

Official Review by Reviewer 3VY2 07 Aug 2025, 02:50 (modified: 28 Oct 2025, 23:03) Everyone
Revisions (/revisions?id=57eh9aM2dX)

Ethics: NO or VERY MINOR ethics concerns only
Position: Yes, the paper argues for or against a position related to machine learning.
Summary:
This paper offers a forward-looking perspective on the integration of Science of Science with AI for automated research pattern discovery and highlights key open challenges that could greatly benefit from AI. The authors discussed the forecasting trends in technology and innovation, and analyzed the evolution of research communities. It is a forward-looking paper

Author Identification: No.

Support: 4: excellent
Significance: 3: good
Presentation: 3: good
Context: 2: fair
Discussion: 3: possibly
Alternative Position: Yes, and alternative positions are trivial straw-man arguments
Strengths:
The authors has well described the flow chart of the Human-Driven research process and the AI-Driven research process in Figure 1, which well illustrates that AI has the potential to revolutionize SoS. And the authors defines AI for Science and AI for Science of Science very well in Table 1.

Weaknesses:
1. The author does not discuss scientific research that requires physical experiments, such as biology, chemistry, and other scenarios that require hands-on experiments, and discusses the role of Embodied AI and robots in Science of Science Research.
2. In section 2.2, Automation Degree in AI4SoS is somewhat similar to some existing perspective articles. The author needs to discuss their similarities and differences in the article: "Transforming science labs into automated factories of discovery", "Scaling Laws in Scientific Discovery with AI and Robot Scientists", "Empowering biomedical discovery with AI agents".

Questions:
Similar to the question in Weaknesses, the author did not discuss AI and robots conducting autonomous experiments in the physical world. I wonder what role and function robots will play in SoS?

Agreement: 4: agree
Rating: 8: Strong Accept: The paper presents a strong argument about an important issue that ought to be discussed and is of importance to a sub-area within the NeurIPS community.
Confidence: 5: You are absolutely certain about your assessment. You are very familiar with the related work.
Thoroughness: 5: You read the paper and appendices rigorously and checked all of the details carefully, including references and proofs (if present).
Code Of Conduct Acknowledgement: Yes

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Official Review of Submission110 by Reviewer URur

Official Review by Reviewer URur 23 Jul 2025, 10:43 (modified: 28 Oct 2025, 23:03) Everyone
Revisions (/revisions?id=b4vBAwxUnz)

Ethics: Major Concern: Discrimination, bias, and fairness
Details Of Ethics Concerns:
The paper dives deep into the issue of bias in AI systems, highlighting the uneven distribution of data across various fields and how this can amplify existing inequalities in scientific research. While the authors do recognize these challenges and suggest ways to address them, the core issue of AI systems potentially reinforcing biases in scientific discovery really calls for an ethics review. Additionally, the simulation of research communities brings up further concerns about how well diverse scientific groups are represented.

Position: Yes, the paper argues for or against a position related to machine learning.
Summary:
This paper makes a strong case for using AI-driven automation as the cornerstone of next-generation Science of Science (SoS) research. The authors contend that the traditional SoS methods, which rely on basic statistical tools, just don't cut it anymore given the complexities of modern research. They introduce AI4SoS as a unique field, outline a 5-level hierarchy of automation that ranges from no automation to fully automated discovery, and share some initial

findings from a multi-agent system that simulates scientific collaboration. The main takeaway is that AI has the potential to revolutionize SoS by uncovering patterns automatically, leading to insights that manual methods simply can't achieve.

Author Identification: No.
Support: 2: fair
Significance: 3: good
Presentation: 2: fair
Context: 3: good
Discussion: 3: possibly
Alternative Position: Yes, and alternative positions are well-considered and named but not addressed
Strengths:
The paper dives into a crucial intersection between AI and scientific research. It introduces a 5-level hierarchy that serves as a helpful framework for grasping how AI automation fits into the Science of Science. The authors clearly differentiate between AI4S and AI4SoS, which is well explained. Their extensive literature review reflects a deep understanding of the field. Additionally, the initial multi-agent simulation indicates that they've thoughtfully considered the practical aspects of their proposed approach. They also recognize the significant challenges ahead, such as bias, evaluation hurdles, and the complexity of systems.

Weaknesses:
The paper feels a bit too lengthy and technical for what's meant to be a position paper that sparks wide-ranging community discussion. The experimental validation seems quite preliminary and limited in its scope. It doesn't really tackle the essential questions about whether fully automated scientific discovery is something we actually want or if it's even possible. Plus, the exploration of alternative viewpoints is pushed off to an appendix instead of being woven into the main argument. Some of the claims regarding AI's transformative potential don't seem to have enough empirical backing. Also, the emphasis on the Science of Science might be a bit too narrow for the diverse NeurIPS audience.

Questions:
How do the authors tackle the worries that fully automated scientific discovery could diminish human insight and the happy accidents that often lead to significant breakthroughs?

What specific measures are in place to ensure that AI4SoS systems don't reinforce or worsen existing biases in scientific publishing and collaboration?

How would the suggested framework deal with fields that have limited data or research methods that can't be easily quantified?

Is there any evidence that the 5-level hierarchy truly reflects the natural evolution of AI automation in scientific research?

Agreement: 3: neither agree nor disagree
Rating: 6: Weak Accept: The paper presents a solid argument about an issue of moderate importance to at least one sub-area of theNeurIPScommunity.
Confidence: 4: You are confident in your assessment, but not absolutely certain. It is unlikely, but not impossible, that you did not understand some parts of the submission or that you are unfamiliar with some pieces of related work.
Thoroughness: 4: You read the paper and appendices and checked most of the details, including references..
Code Of Conduct Acknowledgement: Yes

Add: **Official Comment**

Official Review of Submission110 by Reviewer FFXE

Official Review by Reviewer FFXE (Vivek Kumar Mishra (/profile?id=~Vivek_Kumar_Mishra1))
08 Jul 2025, 21:21 (modified: 28 Oct 2025, 23:03) Everyone Revisions (/revisions?id=V7IgtIU30v)

Ethics: NO or VERY MINOR ethics concerns only
Position: Yes, the paper argues for or against a position related to machine learning.

Summary:
This paper puts forward a timely and ambitious perspective on how artificial intelligence particularly large language models and multi-agent systems can reshape the Science of Science (SoS) field. It introduces a structured framework called AI4SoS, outlining five levels of automation in studying scientific progress, from fully manual analysis to fully autonomous discovery. The authors argue that AI can go beyond supporting individual tasks to simulating entire research ecosystems, enabling better understanding of research trends, collaboration patterns, and innovation triggers.

To support this, the paper presents a proof-of-concept multi-agent simulation that models a research society and evaluates how factors like diversity and institutional ranking relate to citation outcomes. While still in early stages, the results show promising alignment with real-world patterns. The paper also discusses key challenges such as data bias, system evaluation, and explainability and proposes thoughtful strategies to address them. Overall, it makes a strong case for why AI could play a foundational role in the next generation of SoS research.

Author Identification: No.
Support: 4: excellent
Significance: 4: excellent
Presentation: 3: good
Context: 4: excellent
Discussion: 4: very likely
Alternative Position: Yes, and alternative positions are well-considered and addressed by the argument
Strengths:
Offers both theoretical and empirical support, including simulations and references to real-world data Introduces a compelling case for why AI can revolutionize how scientific collaboration and innovation are understood.

Weaknesses:
The paper is dense in parts, especially where it explains the technical systems and hierarchy levels. A bit more clarity or simplification in those sections would help more readers engage with the ideas. Finally, while ethical risks like bias and fairness are mentioned, the paper could say more about how we ensure humans stay involved when these AI systems get really powerful.

Questions:
How can we make sure these AI systems don't just reinforce the current winners in science—like elite institutions or already famous researchers—while missing out on new or underrepresented voices?

As AI takes over more parts of the research cycle, how can we make sure it's still helping people discover new things rather than just optimizing for what already works?

Agreement: 4: agree
Rating: 8: Strong Accept: The paper presents a strong argument about an important issue that ought to be discussed and is of importance to a sub-area within the NeurIPS community.
Confidence: 4: You are confident in your assessment, but not absolutely certain. It is unlikely, but not impossible, that you did not understand some parts of the submission or that you are unfamiliar with some pieces of related work.
Thoroughness: 5: You read the paper and appendices rigorously and checked all of the details carefully, including references and proofs (if present).
Code Of Conduct Acknowledgement: Yes