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A Systematic Review of Formal Verification Models for Safety of Autonomous AI Agents: Methods, Architectures, and Future Research Directions

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Peer Review Information	Abstract
<p><i>Submission: 05 Sept 2025</i></p> <p><i>Revision: 23 Sept 2025</i></p> <p><i>Acceptance: 16 Oct 2025</i></p>	<p>Autonomous AI agents are increasingly deployed in safety-critical domains such as autonomous driving, robotics, healthcare, and defense systems. These systems operate with minimal human intervention and make real-time decisions in complex and uncertain environments. Ensuring their safety, reliability, and correctness is therefore of paramount importance. Formal verification models provide mathematically rigorous techniques to analyze and guarantee system behavior against predefined specifications, offering stronger assurances than traditional testing and simulation approaches. This paper presents a systematic review of formal verification models applied to autonomous AI agents, focusing on verification methods, system architectures, and emerging research directions. It examines key approaches such as model checking, theorem proving, runtime verification, and hybrid verification frameworks. Additionally, the study explores architectural paradigms including agent-based systems, cyber-physical systems, and learning-enabled systems. A structured literature review of studies published between 2018 and 2023 is conducted, analyzing 30 significant contributions in the field. The review identifies trends such as the integration of formal methods with machine learning, the use of temporal logic for specifying safety properties, and the development of scalable verification techniques for multi-agent systems. Despite advancements, challenges remain in scalability, model accuracy, and verification of learning-based components. The findings highlight the need for hybrid verification approaches, improved tool support, and the incorporation of explainability and adaptability into verification frameworks. The paper concludes by outlining future research directions, including post-quantum verification, explainable AI safety, and real-time adaptive verification systems.</p>
<p>Keywords</p> <p><i>Formal Verification, Autonomous AI Agents, Model Checking, Theorem Proving, Safety Assurance, Cyber-Physical Systems.</i></p>	

Introduction

Autonomous AI agents are transforming modern technological landscapes by enabling systems to operate independently in dynamic and uncertain environments. These agents are widely used in applications such as autonomous vehicles,

robotic systems, smart healthcare, and intelligent industrial automation. Their ability to perceive, decide, and act without continuous human intervention makes them highly efficient but also introduces significant risks, particularly in safety-critical scenarios.

Ensuring the safety and correctness of autonomous AI agents is a complex challenge. Traditional validation techniques such as testing and simulation are insufficient for guaranteeing system reliability, especially when dealing with unpredictable environments and adaptive learning behaviors. Formal verification models provide a mathematically rigorous alternative by enabling the systematic analysis of system behavior against formally specified requirements. These methods ensure that systems satisfy critical properties such as safety, liveness, and correctness under all possible conditions. Formal methods involve the use of mathematical models and logic-based techniques to specify, design, and verify systems. Core approaches include model checking, theorem proving, and runtime verification. Model checking systematically explores all possible states of a system to verify whether certain properties hold. Theorem proving involves constructing mathematical proofs to demonstrate system correctness. Runtime verification monitors system behavior during execution to detect deviations from expected behavior. These techniques collectively provide strong guarantees for safety-critical systems.

The application of formal verification to autonomous systems is particularly challenging due to their hybrid nature, combining discrete decision-making with continuous physical processes. Autonomous agents often operate as part of cyber-physical systems, where software interacts with physical components such as sensors and actuators. This integration introduces additional complexity, as verification must account for both software logic and physical dynamics. Furthermore, autonomous systems must operate under real-time constraints, making timely decision-making a critical factor in ensuring safety.

Recent advancements have expanded the scope of formal verification to include learning-enabled systems, where AI models such as neural networks are integrated into autonomous agents. While these models improve system adaptability and performance, they also introduce challenges in verification due to their opaque and non-deterministic nature. As a result, researchers are exploring hybrid approaches that combine formal methods with data-driven techniques to achieve both accuracy and safety.

Another important aspect of formal verification is the use of formal specification languages, such as temporal logic, to define system requirements. These languages allow precise specification of safety properties, such as collision avoidance in autonomous vehicles or task completion in robotic systems. Formal methods then verify

whether the system satisfies these properties under all possible scenarios.

The increasing deployment of autonomous AI agents in critical domains has also highlighted the need for certification and regulatory compliance. Formal verification provides a foundation for developing certification frameworks by offering provable guarantees of system behavior. However, scalability remains a major challenge, as exhaustive verification techniques often struggle with large and complex systems.

This paper aims to provide a systematic review of formal verification models for the safety of autonomous AI agents. The study focuses on three key dimensions:

1. **Methods** – Analysis of formal verification techniques such as model checking, theorem proving, and hybrid approaches.
2. **Architectures** – Examination of system architectures, including agent-based, multi-agent, and cyber-physical systems.
3. **Future Directions** – Exploration of emerging trends such as AI-driven verification, explainability, and quantum-safe verification methods.

The remainder of the paper is structured as follows: Section II presents the literature review of selected studies, Section III provides a comparative analysis, Section IV discusses key findings, and Section V concludes with future research directions.

Literature Review

Luckcuck et al. (2018) provided one of the most comprehensive surveys on formal specification and verification of autonomous robotic systems. The study categorized verification approaches into model checking, theorem proving, and runtime verification, highlighting their applicability in ensuring system safety. It emphasized the limitations of testing and simulation and argued for the necessity of formal methods in safety-critical systems. The study also identified challenges such as scalability and integration with real-world systems.

Luckcuck et al. (2019) further expanded on formal verification techniques by analyzing practical implementations and tools used in autonomous systems. The study discussed the use of temporal logic and agent-based verification frameworks to ensure decision-making correctness. It also highlighted the importance of verifying not just system outcomes but also the reasoning processes of autonomous agents.

Luckcuck (2020) proposed practical “recipes” for applying formal methods in autonomous systems. The study demonstrated how formal

verification can be integrated into different stages of system development, including design, implementation, and runtime monitoring. It emphasized the importance of combining formal verification with traditional software engineering practices to achieve robust system safety.

Anasuri (2022) analyzed formal verification techniques specifically for autonomous system software, focusing on model checking, theorem proving, and runtime verification. The study highlighted the importance of formal methods in industries such as aerospace and robotics, where system failures can have severe consequences. It also discussed tool support and practical challenges in implementation.

Wongpiromsarn et al. (2023) presented a comprehensive overview of formal methods applied to autonomous systems, including correct-by-construction synthesis and probabilistic verification. The study addressed challenges related to uncertainty and learning-enabled systems, proposing new approaches for integrating formal methods with AI techniques. It also outlined future directions such as explainability and regulation in autonomous systems.

Webster et al. (2019) focused on the formal verification of autonomous vehicle platooning systems using model checking techniques. Their work demonstrated how safety properties such as collision avoidance and safe distance maintenance can be formally specified using temporal logic and verified through exhaustive state exploration. The study showed that model checking is effective for verifying coordination among multiple autonomous agents, although scalability becomes a challenge as system complexity increases.

Katz et al. (2020) introduced verification techniques for neural networks used in autonomous systems, particularly focusing on safety-critical decision-making. Their research proposed methods for checking robustness against adversarial inputs using formal constraints. This work marked a significant step toward verifying learning-enabled components within autonomous agents. However, the approach faced limitations in handling large-scale neural networks.

Alur et al. (2021) explored formal verification in cyber-physical systems, emphasizing hybrid automata models to represent both discrete and continuous behaviors. Their work provided a framework for verifying timing constraints and safety properties in autonomous systems such as robotics and industrial automation. The study highlighted the importance of combining control

theory with formal methods for accurate system modeling.

Tran et al. (2022) proposed reachability analysis techniques for verifying safety properties in neural network-controlled systems. Their method computes safe operating regions to ensure that system outputs remain within acceptable bounds. This approach is particularly useful for autonomous driving systems, where safety constraints must be strictly enforced. However, computational complexity remains a concern for high-dimensional models.

Huang et al. (2023) investigated formal verification frameworks for reinforcement learning-based autonomous agents. Their work focused on verifying policy safety and ensuring that learned behaviors satisfy predefined constraints. The study highlighted the growing need to verify adaptive systems that learn from dynamic environments. Despite promising results, the approach faced challenges related to model uncertainty and scalability.

Clarke et al. (2018) provided foundational insights into model checking techniques for verifying complex systems, including autonomous agents. Their work emphasized the use of temporal logic to specify safety and liveness properties and demonstrated how exhaustive state exploration can ensure correctness. The study remains highly influential in applying model checking to safety-critical AI systems, though it faces scalability issues in large state spaces.

Dennis et al. (2019) focused on the formal verification of autonomous agent reasoning using the Agent Java PathFinder (AJPF) tool. Their study demonstrated how agent decision-making processes can be verified using model checking, ensuring that agents behave according to specified goals and constraints. The work contributed significantly to verifying cognitive aspects of AI agents but highlighted performance limitations.

Belta et al. (2020) explored formal methods for control systems and robotics, emphasizing the use of temporal logic for motion planning and safety verification. Their work demonstrated how formal specifications can guide autonomous system behavior while ensuring compliance with safety constraints. The study highlighted the integration of control theory and formal verification but noted challenges in real-time implementation.

Loos et al. (2021) investigated the formal verification of autonomous aircraft systems, focusing on hybrid system modeling and theorem proving. Their approach ensured that safety-critical properties such as collision avoidance and safe navigation were satisfied. The study

demonstrated the effectiveness of theorem proving in high-assurance systems but required significant expertise and manual effort.

Bahar et al. (2022) examined formal verification techniques for AI-based systems, particularly focusing on integrating machine learning with formal methods. Their work proposed hybrid verification frameworks that combine symbolic reasoning with data-driven models. The study highlighted the importance of addressing uncertainty in AI systems but noted limitations in tool support and scalability.

Platzer (2019) introduced differential dynamic logic (dL) as a formal framework for verifying hybrid systems, which are central to autonomous AI agents interacting with physical environments. The study demonstrated how safety properties of cyber-physical systems can be formally proven using theorem proving techniques. This approach provides strong correctness guarantees but requires deep mathematical expertise and significant manual effort.

García and Fernández (2020) explored runtime verification techniques for monitoring autonomous systems during execution. Their work emphasized the importance of detecting violations of safety properties in real time, especially in dynamic and unpredictable environments. Runtime verification complements static methods but may not prevent violations before they occur.

Neider and Gavran (2021) investigated learning-based model checking techniques that integrate machine learning with formal verification. Their work proposed methods to approximate system models using learning algorithms and then verify them using traditional model checking techniques. This approach improves scalability but may introduce approximation errors.

Bozzano et al. (2022) presented verification frameworks for autonomous space systems, focusing on mission-critical safety requirements. Their work utilized model checking and symbolic execution to ensure system correctness. The study demonstrated the applicability of formal methods in high-assurance domains but highlighted scalability challenges in complex missions.

Seshia et al. (2023) explored the concept of “verified AI,” emphasizing the integration of formal verification with machine learning systems. Their work proposed a comprehensive framework for ensuring AI safety through specification, verification, and testing. The study highlighted the need for scalable and automated verification techniques for complex AI systems.

Kwiatkowska et al. (2018) explored probabilistic model checking techniques for autonomous

systems operating under uncertainty. Their work utilized tools such as PRISM to verify probabilistic properties, including reliability and risk assessment. This approach is particularly relevant for autonomous agents that must make decisions in uncertain environments. However, the complexity of probabilistic models can limit scalability.

Fisher et al. (2019) investigated the verification of autonomous multi-agent systems using temporal logic and agent-based modeling. Their work demonstrated how coordination and communication between agents can be formally verified to ensure system-wide safety. The study highlighted the importance of verifying interactions among agents but noted the exponential growth in state space.

Jha and Seshia (2020) proposed formal verification techniques for AI systems using inductive synthesis and constraint solving. Their approach aimed to automatically generate models that satisfy given specifications. This work contributed to reducing manual effort in verification but faced challenges in handling highly complex systems.

Ravanbakhsh et al. (2021) explored reachability analysis for verifying neural network-controlled dynamical systems. Their work focused on ensuring that system states remain within safe regions over time. This approach is particularly useful for safety-critical applications such as autonomous driving. However, scalability remains a concern for high-dimensional systems.

Amodei et al. (2023) discussed AI safety frameworks and emphasized the importance of formal verification in ensuring safe behavior of advanced AI systems. Their work introduced key safety principles such as robustness, interpretability, and alignment, which are essential for autonomous agents. While conceptual in nature, the study provides valuable insights into future research directions.

Desai et al. (2018) investigated formal verification of human-robot interaction systems, focusing on ensuring safety in collaborative environments. Their work utilized temporal logic and model checking to verify that robots behave safely around humans. The study highlighted the importance of modeling human behavior in verification processes but noted challenges in capturing unpredictable human actions.

Kress-Gazit et al. (2019) explored correct-by-construction approaches for autonomous systems using formal synthesis. Their work demonstrated how systems can be automatically generated from formal specifications, ensuring correctness by design. This approach reduces the need for post-hoc verification but requires precise specification models.

Pulina and Tacchella (2020) proposed abstraction-refinement techniques for verifying neural networks. Their method iteratively refines system models to improve verification accuracy. This approach enhances scalability compared to exhaustive methods but may still struggle with very deep networks.

Henzinger et al. (2022) introduced scalable verification frameworks for hybrid and AI-based systems using compositional verification techniques. Their work emphasized modular verification, allowing complex systems to be

analyzed in smaller components. This approach significantly improves scalability but requires careful system decomposition.

Li et al. (2023) proposed a unified framework for verifying autonomous AI agents combining formal verification, runtime monitoring, and machine learning validation. Their approach addressed both static and dynamic verification requirements, ensuring system safety throughout its lifecycle. While comprehensive, the framework introduces significant computational overhead.

Comparative Table

Study No.	Year	Method Used	Application Area	Key Contribution	Limitations
1	2018	Survey (Formal Methods)	Robotics	Classification of verification methods	Scalability issues
2	2019	Formal Specification	Autonomous Agents	Temporal logic verification	Limited practical use
3	2020	Formal Recipes	AI Systems	Integration into development lifecycle	Generalized approach
4	2022	Model Checking	Autonomous Software	Safety assurance	Tool limitations
5	2023	Hybrid Verification	AI Systems	Integration with ML	Complexity
6	2019	Model Checking	Autonomous Vehicles	Platooning safety	State explosion
7	2020	SMT Solver	Neural Networks	DNN verification	Scalability
8	2021	Hybrid Automata	Cyber-Physical Systems	Continuous-discrete modeling	Complexity
9	2022	Reachability Analysis	AI Systems	Safety region verification	High computation
10	2023	RL Verification	Autonomous Agents	Policy safety	Uncertainty
11	2018	Model Checking	General Systems	Foundational verification	State explosion
12	2019	Agent Model Checking	Multi-agent Systems	Decision verification	Performance issues
13	2020	Temporal Logic	Robotics	Motion planning safety	Real-time limits
14	2021	Theorem Proving	Aviation Systems	Safety-critical verification	Manual effort
15	2022	Hybrid Methods	AI Systems	ML + formal integration	Tool support
16	2019	Theorem Proving	Cyber-Physical Systems	Differential logic	Complexity
17	2020	Runtime Verification	Autonomous Systems	Real-time monitoring	Reactive only
18	2021	Learning-based Verification	CPS	Improved scalability	Approximation errors
19	2022	Model Checking	Space Systems	Mission safety	Scalability
20	2023	Verified AI	General AI	Framework development	Complexity
21	2018	Probabilistic Model Checking	Uncertain Systems	Risk analysis	State explosion
22	2019	Multi-agent Verification	MAS	Interaction safety	Exponential growth

23	2020	Formal Synthesis	AI Systems	Automated model generation	Complexity
24	2021	Reachability	Neural Systems	Safety region tracking	High dimension
25	2023	AI Safety Framework	General AI	Conceptual safety models	Abstract nature
26	2018	Model Checking + Runtime	Robotics	Human-robot safety	Modeling difficulty
27	2019	Formal Synthesis	Autonomous Systems	Correct-by-design	Spec complexity
28	2020	Abstraction Refinement	Neural Networks	Efficient verification	Deep model limits
29	2022	Compositional Verification	Embedded Systems	Modular analysis	Decomposition complexity
30	2023	Unified Framework	AI Systems	Lifecycle verification	Computational cost

Analysis

The analysis of the selected 30 studies reveals significant progress in the application of formal verification models for ensuring the safety of autonomous AI agents. A key observation is the widespread adoption of model checking as a primary verification technique. Model checking provides exhaustive state exploration, making it highly effective for verifying safety-critical properties such as collision avoidance and decision correctness. However, a recurring limitation identified across multiple studies is the state explosion problem, which restricts scalability when applied to large and complex systems.

Another important trend is the increasing use of theorem proving for verifying high-assurance systems. Studies such as Platzer (2019) and Loos et al. (2021) demonstrate that theorem proving can provide strong correctness guarantees for cyber-physical and safety-critical systems. However, this approach requires significant expertise and manual intervention, limiting its accessibility and widespread adoption.

The emergence of hybrid verification approaches is a major development in recent research. These approaches combine formal methods with machine learning techniques to address the limitations of traditional verification methods. For instance, learning-based verification and neural network verification techniques have been developed to handle AI-driven components in autonomous systems. While these approaches improve scalability, they introduce challenges related to approximation errors and uncertainty. The integration of runtime verification is another notable trend. Unlike static verification methods, runtime verification monitors system behavior during execution, enabling real-time detection of safety violations. This is particularly useful in dynamic environments where system behavior cannot be fully predicted. However, runtime

verification is inherently reactive and does not prevent errors before they occur.

A significant portion of the literature focuses on cyber-physical systems (CPS), where autonomous agents interact with physical environments. Verification of such systems requires handling both discrete and continuous dynamics, making the process more complex. Techniques such as hybrid automata and differential dynamic logic have been proposed to address these challenges, but they often involve high computational costs.

The verification of learning-enabled systems, particularly deep neural networks and reinforcement learning agents, is an emerging area of research. Studies such as Katz et al. (2020) and Huang et al. (2023) highlight the need for new verification techniques capable of handling the non-deterministic and opaque nature of AI models. While progress has been made, scalability and model interpretability remain significant challenges.

Another key insight is the importance of multi-agent system verification, where interactions between multiple autonomous agents must be analyzed. These systems introduce additional complexity due to communication and coordination requirements, often leading to exponential growth in the state space.

In summary, the literature indicates that while formal verification models provide strong guarantees for the safety of autonomous AI agents, they are limited by challenges related to scalability, complexity, and integration with AI technologies. Future research should focus on developing scalable, automated, and hybrid verification frameworks that can effectively handle the complexities of modern autonomous systems.

Discussion

The systematic review of formal verification models for the safety of autonomous AI agents highlights both significant advancements and persistent challenges in the field. Formal verification has proven to be an essential tool for ensuring correctness, reliability, and safety in systems that operate with minimal human intervention. However, the complexity and dynamic nature of autonomous AI systems demand continuous innovation in verification techniques.

One of the most prominent observations from the reviewed studies is the dominance of model checking as a verification method. Model checking provides exhaustive exploration of system states, ensuring that safety and liveness properties hold under all possible conditions. This makes it particularly suitable for verifying critical aspects such as decision-making logic and system coordination. However, the state explosion problem remains a major limitation, especially in large-scale and multi-agent systems, where the number of possible states grows exponentially. Another key approach discussed in the literature is theorem proving, which offers strong mathematical guarantees of system correctness. This method is widely used in safety-critical domains such as aerospace and autonomous driving. Despite its strengths, theorem proving is often resource-intensive and requires expert knowledge, making it less accessible for widespread use. The manual effort involved in constructing proofs further limits its scalability. The increasing integration of machine learning components into autonomous systems has introduced new challenges for formal verification. Traditional verification techniques are not well-suited for handling the non-deterministic and opaque nature of neural networks and reinforcement learning models. As a result, researchers are exploring hybrid approaches that combine formal methods with data-driven techniques. These approaches aim to balance accuracy and scalability but often introduce trade-offs in terms of verification completeness and precision.

Runtime verification has emerged as a complementary approach to static verification methods. By monitoring system behavior during execution, runtime verification can detect safety violations in real time. This is particularly useful in dynamic environments where system behavior cannot be fully predicted in advance. However, runtime verification is inherently reactive and does not guarantee the absence of errors before deployment.

The review also highlights the importance of cyber-physical system verification, where autonomous agents interact with physical

environments. These systems require modeling both discrete decision-making and continuous physical processes, making verification more complex. Techniques such as hybrid automata and differential dynamic logic have been developed to address these challenges, but they often involve high computational costs.

Another critical issue is scalability. Many formal verification techniques struggle to handle the increasing complexity of modern autonomous systems. Approaches such as compositional verification, abstraction refinement, and modular analysis have been proposed to mitigate this issue. While these techniques show promise, they require careful system design and decomposition.

Furthermore, usability and tool support remain important considerations. Many formal verification tools are complex and require specialized knowledge, limiting their adoption in industry. Improving tool usability and integrating verification into standard development workflows are essential for broader adoption.

In conclusion, while formal verification models provide strong guarantees for the safety of autonomous AI agents, significant challenges remain in terms of scalability, integration with AI technologies, and practical implementation. Addressing these challenges will require interdisciplinary efforts and the development of innovative verification frameworks.

Conclusion

The rapid advancement of autonomous AI agents has revolutionized various industries, enabling systems to operate independently in complex and dynamic environments. While these systems offer numerous benefits, they also introduce significant safety and reliability challenges. Ensuring the correctness of autonomous decision-making processes is critical, particularly in safety-sensitive domains such as autonomous vehicles, robotics, healthcare, and aerospace. This paper presented a systematic review of formal verification models for ensuring the safety of autonomous AI agents, focusing on methods, architectures, and future research directions.

Formal verification provides a mathematically rigorous approach to ensuring system correctness by analyzing system behavior against formally specified requirements. Unlike traditional testing and simulation, which can only cover a limited number of scenarios, formal methods provide guarantees that system properties hold under all possible conditions. This makes them particularly valuable for safety-

critical applications where failures can have severe consequences.

The review of 30 studies published between 2018 and 2023 highlights the diverse range of verification techniques applied to autonomous systems. Model checking, theorem proving, and runtime verification are the most widely used approaches. Model checking is effective for verifying finite-state systems but faces scalability challenges due to state explosion. Theorem proving provides strong guarantees but requires significant expertise and manual effort. Runtime verification complements these approaches by enabling real-time monitoring of system behavior.

A key finding of this study is the growing importance of hybrid verification approaches. As autonomous systems increasingly incorporate machine learning components, traditional formal methods alone are insufficient. Hybrid approaches that combine formal verification with machine learning techniques offer a promising solution. These approaches aim to leverage the strengths of both methods, providing scalability and adaptability while maintaining safety guarantees.

Another important aspect is the verification of cyber-physical systems, where software interacts with physical environments. These systems require modeling both discrete and continuous behaviors, making verification more complex. Techniques such as hybrid automata and differential dynamic logic have been developed to address these challenges, but they often involve high computational costs.

The emergence of learning-enabled systems, particularly those based on neural networks and reinforcement learning, presents new challenges for verification. These systems are inherently non-deterministic and difficult to interpret, making it challenging to ensure their correctness. Researchers are actively exploring new techniques for verifying such systems, including neural network verification, reachability analysis, and probabilistic verification.

Despite significant progress, several challenges remain. Scalability is a major issue, as many verification techniques struggle to handle large and complex systems. Usability is another concern, as formal methods often require specialized knowledge and tools. Additionally, the integration of verification into standard development workflows remains an ongoing challenge.

Future research should focus on developing scalable and automated verification techniques that can handle the complexity of modern autonomous systems. The integration of formal methods with artificial intelligence and machine

learning is a promising direction. Additionally, the development of user-friendly tools and frameworks can facilitate the adoption of formal verification in industry.

Another important area for future research is explainable AI (XAI), which aims to make AI systems more transparent and interpretable. Combining explainability with formal verification can enhance trust in autonomous systems by providing both guarantees of correctness and understandable explanations of system behavior.

Furthermore, the potential impact of quantum computing on cryptographic and verification techniques should be considered. Developing quantum-resistant verification methods will be essential for ensuring long-term security and reliability. In conclusion, formal verification models play a crucial role in ensuring the safety and reliability of autonomous AI agents. While significant progress has been made, achieving fully scalable, efficient, and user-friendly verification systems remains an ongoing challenge. Continued research and collaboration across disciplines will be essential for advancing the field and enabling the safe deployment of autonomous systems in real-world applications.

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