A Comprehensive Review of Generative AI Applications in Drug Safety:
Predicting Interactions and Adverse Effects

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ABSTRACT

The forecast of drug-drug interactions (DDIs) and adverse drug reactions (ADRs) is something that has a direct relationship with the safety of the patient. Boom in polypharmacy is an additional justification for the above statement. The objective of the traditional models, such as clinical trials and post-market surveillance, is to identify the DDIs and ADRs. However, these models are limited mainly in the diversity, granularity, and timeliness of the data that they rely on. Generative AI has come on the plate as a possible option as it is capable of creating new drug combinations and thus predicting the likely perils by applying machine learning methodologies. This survey on the continued developments related to the use of generative AI in both DDI and ADR will cover GANs, VAEs, and specifically, transformers. The authors discuss the ethical and legal implications of using these models in clinical practice in addition to outlining data sources and methodological difficulties. Future directions to enhance generative AI in pharmacovigilance are also highlighted.

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1. INTRODUCTION

With the number of patients medicated with more than one drug, polypharmacy has grown in frequency, polypharmacy is the concurrent usage of multiple drugs, particularly in the case of elderly people and those with chronic diseases. Polypharmacy, a contributive factor of drug-drug interactions (DDIs) as well as adverse drug reactions (ADRs), in turn, may result in serious clinical outcomes (Alizadehsani et al., 2024). The traditional methods of DDIs- and ADRs-detection and prediction are based on data obtained from clinical trials, observational studies, and pharmacovigilance databases. Existing techniques are restricted by the uniquely preprogramed, the yet to be discovered observational data, and the lack of rapid learning from ADRs expressed post-marketing. Besides the fact that the number of approved drugs is constantly expanding, it is obvious that forecasting possible interactions will be difficult to do so (Bowskill et al., 2024).

Artificial intelligence (AI) is accelerating the process of change in a wide range of sectors among which healthcare and pharmacology are the leaders (Atance et al., 2022). One of the AI applications which is capable of creating new data through the learning of existing data has the potential to revolutionize drug safety procedures within the field. This work aims to find out how generative AI is training machines to anticipate drug interactions and adverse effects, with the goal of advancing patient safety, reducing drug development time, and minimizing healthcare costs (Brown et al., 2023). The pharmacy industry, on the other hand, considers drug safety as a key measure in the development of a new drug which is further compounded by the adverse drug reactions (ADRs) that still remain are recurrent fears among researchers. However, they are the consequences of the increased healthcare demands and the worst case, deaths have also been reported as the possible disastrous aftermaths (Buterez et al., 2024). Correct and accurate forecast of ADRs can help to avoid or stop harm and minimize drug withdrawals on the market afterward. Nevertheless, due to the highly complicated nature of biological systems, human variability, and vast diversity of drug combinations, this process of implementation gets difficult(Buterez et al., 2024). The conventional approaches in ADRs prediction – clinical trials, external studies after the marketing stage – take considerable time and money. Lately, AI-based techniques are being reported to be very successful as additional tools in the treatment. In particular, generative AI proposes new techniques for reproducing the human body processes and can be used for large-scale predictions of drug safety issues, which in turn, will enhance proactive risk assessment and pharmacovigilance.

Generative AI is the healthcare application of several different mechanisms and models, including GANs, VAEs, and transformer-based models, to synthetically create data or mimic real-world patterns visualized in Fig1. The broad applications in health care are artificial intelligence-based imaging, the generation of synthetic data for personalized medicine, and natural language processing in medical documents. These algorithms can study complicated data, make a realistic simulation & give predictions to support decision-makers. Generative AI can analyze a wide variety of biomedical data such as clinical trials, electronic health records, and scientific literature to find drug safety signals including drug toxicity and drug-drug reaction patterns (Carlini et al., 2023). Its models are not only capable of traditional predictive tasks but also advance in the modelling of hypothetical cases, simulate the effects of new drugs, and explore the entire chemical space beyond the laboratory. Drug-drug interactions (DDIs) are the ones that can lead to either the improved effectiveness of the medication or the occurrence of adverse effects or failures of therapy. As they are those patients undergoing a multitude of therapies the major aspect of risk factor in the treatment of diseases (DiMasi, 2020). As the total number of possible drug combinations and the possible interaction pathways is a very dynamic and complicated entity, it has