

Artificial Intelligence in Predicting Clinical Trial Failure

Sashank Sharma^{1*}, Priyanka Mishra^{1*}, and Mohit Nigam²

¹Department of Pharmaceutical Sciences, School of Pharmaceutical & Biological Sciences, Harcourt Butler Technical University, Kanpur-208002, U.P., India

²Department of Biotechnology, School of Pharmaceutical & Biological Sciences, Harcourt Butler Technical University, Kanpur-208002, U.P., India

*Corresponding author

ABSTRACT

Clinical trials are essential for evaluating the safety and efficacy of novel drugs and new treatments. However, they face several major challenges such as patient recruitment delays affecting nearly 80% of studies, rising pharmaceutical research and development costs exceeding USD 200 billion, low success rates of less than 12%, and poor data quality impacting almost 50% of datasets. Artificial intelligence (AI) has emerged as a promising approach to address these issues by enabling early prediction of clinical trial failure and success. AI-based methods, including machine learning and large language models (LLMs) such as GPT-3.5, GPT-4, and HINT, have shown significant potential in analysing complex clinical data and predicting trial outcomes. Proper data cleaning, processing, and integration are essential for developing accurate AI-based prediction models. The integration of electronic health records with patient-specific genetic data is a growing area of interest with considerable future potential. De novo AI approaches that focus on predicting drug-target interactions further assist in novel drug discovery and optimization of clinical trial design. Applications of AI in clinical research can be grouped into three main areas: drug discovery and preclinical development, clinical development and precision medicine, and post-marketing safety monitoring. Machine learning algorithms such as random forest and XGBoost, along with deep learning models including multilayer and recurrent neural networks, are particularly effective in generating predictions from high-dimensional, multimodal datasets. Overall, AI offers a promising approach to improve clinical trial success and make drug development more efficient.

Keywords: *Clinical trial, Artificial Intelligence, Large language model, de novo drug design, XGBoost*

