Chapter 15

Accelerating Precision Medicine Through Advanced Computational Techniques:

Hyper Soft Computing in Drug Discovery

B. M. Parashiva Murthy
https://orcid.org/0000-0001-8808-8366
Department of Computer Science and Engineering, SJCE, JSS Science and Technology University, India

Saba Fatima
School of Electrical and Communication Sciences, JSPM University, Pune, India

Harishchander Anandaram
https://orcid.org/0000-0003-2993-5304
Department of Artificial Intelligence, Amrita Vishwa Vidyapeetham, Coimbatore, India

B. J. Job Karuna Sagar
Department of Computer Science and Engineering, Joginpally B.R. Engineering College, Hyderabad, India

Deepshree Buchade
https://orcid.org/0009-0008-4621-0034
Department of Artificial Intelligence and Machine Learning, Dayananda Sagar College of Engineering, Bangalore, India

ABSTRACT

Hyper soft computing techniques are revolutionizing drug discovery by enhancing speed, accuracy, and efficiency in identifying potential candidates in the pharmaceutical industry. This chapter discusses how hyper soft computing, representing the merge of fuzzy logic, neural networks, evolutionary algorithms, and probabilistic reasoning, is addressing complex, uncertain, and imprecise data inherent in drug discovery. Optimization of computational models for the tasks, such as molecular docking, SAR analysis, and virtual screening, would therefore greatly reduce time and cost from that of conventional

DOI: 10.4018/979-8-3693-7112-1.ch015

drug development. Chapter 2 Discusses the ability of machine learning algorithms in predicting drug efficacy and toxicity, which eventually lead to precision medicine. The integration of quantum-inspired algorithms with bioinformatics is being discussed for potential future pharmaceutical research using hyper soft computing. This chapter explores the current applications and future opportunities of advanced computing methodologies in accelerating drug development.

INTRODUCTION

Finding new drugs is a challenging, time-consuming process involving limitless resources. Traditionally, drug discovery had relied heavily on experimental approaches requiring much trial and error, high costs, and long timelines. In recent years, however, advancements in computational approaches have opened up new possibilities for improving the speed and efficacy of drug discovery programs. Among them, the hyper soft computing paradigm has emerged, which is very likely to revolutionize the process by overcoming those inherent complexities, uncertainties, and imprecisions present in biological systems (A. Tripathi et al., 2023).

Hyper soft computing is an interdisciplinary field encompassing multiple soft computing techniques-fuzzy logic, neural networks, evolutionary algorithms, and probabilistic reasoning-to solve complex, nonlinear problems that traditional computing approaches fail to cope with. With this approach of hybridization, hyper soft computing presents a versatile framework for handling vague or imprecise information, a challenge very common in the case of biological data. The methodology has emerged quite promising in various fields including optimization problems, decision-making, and pattern recognition-all tasks that belong to top priorities of drug discovery (Nag et al., 2022).

Among the significant challenges of drug discovery is the extent to which one needs to search through immense chemical spaces for compounds that may show the desirable pharmacological properties: high efficacy, for example, with low toxicity. Such an estimation is considerably critical in being as early as possible within drug discovery so as not to raise the possibility of failure at later stages of drug development. This is where hyper soft computing comes in, meaning powerful algorithms that are capable of dealing with tremendous volumes of data; and besides it is capable of generating predictive models for identifying potential drug candidates (Nayarisseri et al., 2021). Techniques such as fuzzy logic and neural networks in hyped soft computing enable scientists to construct more accurate models of the complex relationship formed between molecular structures and their associated biological activities, even when based on incomplete or noisy data (N. Tripathi et al., 2021).

A more significant application of hyper soft computing comes in the form of fuzzy logic, which is exceptionally useful in drug discovery, especially since it handles all forms of uncertainty and approximate reasoning. Fuzzy logic brings a degree of truth to its systems, which contrasts the binary logic in traditional systems due to the biological nature of the interacting entities. For example, fuzzy logic can be adapted in modeling the affinity between the drug molecule and its target protein to include flexibility and dynamic nature in molecular interactions in molecular docking. This would allow more subtle understandings of binding interactions, in turn making better predictions for drug efficacy (Jiménez-Luna et al., 2021).

Neural networks, another core technique within the framework of hyper soft computing, are particularly useful for QSAR modeling and virtual screening. These networks are particularly well-suited to the pattern recognition operations required for the identification of subtle relationships between structural

22 more pages are available in the full version of this document, which may be purchased using the "Add to Cart" button on the publisher's webpage:
www.igi-global.com/chapter/accelerating-precision-medicine-through-advanced-computational-techniques/374516

Related Content

Harnessing Higher Generative Artificial Intelligence for Educational Pedagogy: Human-AI Collaboration in ChatGPT Experiences
Daniel Emakporuena, Victor Omoboye Oluwasegun, Ogheneruona Maria Esegbona-Isikeh, Williams Ogochukwu Ugbomeh, Morgan Nwaiku, Eboesomi Esther Bunmi, Oyedemi Oluyemisi Adenikeand Ugochukwu Okwudili Matthew (2026). *Integrating ChatGPT Into System Applications and Services (pp. 23-58).*
www.irma-international.org/chapter/harnessing-higher-generative-artificial-intelligence-for-educational-pedagogy/385312

Mining Competitors and Finding Winning Plans Using Feature Scoring and Ranking-Based CMiner++ Algorithm: Finding Top-K Competitors
Sujatha T., Wilfred Blessing N. R.and Suresh Palarimath (2023). *International Journal of Intelligent Information Technologies (pp. 1-11).*
www.irma-international.org/article/mining-competitors-and-finding-winning-plans-using-feature-scoring-and-ranking-based-cminer-algorithm/318670

Self Adaptive Particle Swarm Optimization for Efficient Virtual Machine Provisioning in Cloud
R. Jeyarani, N. Nagaveniand R. Vasanth Ram (2013). *Organizational Efficiency through Intelligent Information Technologies (pp. 88-107).*
www.irma-international.org/chapter/self-adaptive-particle-swarm-optimization/71962

Educational Program for AI Literacy
Mageshkumar Naarayanasamy Varadarajan (2024). *Improving Library Systems with AI: Applications, Approaches, and Bibliometric Insights (pp. 134-154).*
www.irma-international.org/chapter/educational-program-for-ai-literacy/347645

Leveraging AI Tools to Enhance Writing Skills and Assessment in Language Education
Christina Kitsonand Nabat Erdogan (2026). *Harnessing AI for Multigenerational English Language Learning (pp. 65-96).*
www.irma-international.org/chapter/leveraging-ai-tools-to-enhance-writing-skills-and-assessment-in-language-education/384092