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PRESCRIPTION

Latest news and updates from the Faculty of Pharmacy

REVOLUTIONISING PHARMACY THROUGH MACHINE LEARNING: THE PROGRESS AND PERILS

By: Assoc. Prof. Dr. Yuslina Zakaria

Machine learning (ML) is transforming pharmacy, enhancing accuracy in drug discovery, personalised medicine, and patient care. ML, a branch of artificial intelligence (AI), uses algorithms such as neural networks, decision trees, and support vector machines to learn from large datasets and make predictions. In pharmaceutical research, ML accelerates the identification of potential drug candidates, improves design optimisation, and increases research efficiency. Additionally, ML in predictive analytics for pharmacy practice shows promising results, highlighting the need for further research and adoption to improve patient care (1).

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ML significantly impacts pharmacy, offering benefits over conventional statistical techniques. It accelerates drug-target affinity predictions, expediting the selection of suitable drug molecules and streamlining the discovery process. Deep learning, a subset of ML, reduces costs and speeds up research by efficiently analysing complex datasets, predicting bioactivity, and aiding in virtual screening, proving more effective than traditional experiments (2). Additionally, ML can predict drug-drug interactions early, optimising treatment regimens and improving patient outcomes.

A notable example is the discovery of Halicin, an antibiotic identified by an ML model trained on over 100 million molecules (3). The process involved training the model on existing chemical and biological data, enabling it to predict effective compounds against specific targets. Halicin's discovery through deep learning and in vitro validation highlights ML's transformative impact on pharmaceutical science, underscoring its role in predicting and validating new drug candidates (4).

Implementing ML in pharmacy, however, faces several challenges. Key issues include data security and privacy, given the sensitive nature of healthcare information. Regulatory and ethical concerns, such as patient consent and data usage, also present significant obstacles. Another significant hurdle is the scarcity of comprehensive, high-quality data essential for accurate ML model training (5). Reliable and diverse datasets are crucial for developing robust ML algorithms for effective analysis and prediction in pharmacy settings. Ensuring data quality, integrity, and relevance throughout ML development is essential for generating meaningful insights (6). The "black box" nature of some ML models hinders interpretability and transparency, causing mistrust among healthcare professionals and patients. While deep learning models can make highly accurate predictions, understanding how they arrive at these predictions is often challenging.

Strategies to mitigate the challenges of implementing ML in pharmacy include strict access controls and robust encryption to enhance data privacy and security. Protecting patient confidentiality, data encryption, and compliance with regulations like HIPAA is vital for handling sensitive healthcare information. Enhancing access to diverse, high-quality datasets through data-sharing collaborations addresses the data quantity problem effectively. To tackle "black box" issues, it is essential to enhance the interpretability and reliability of ML models through collaborative efforts (7). Effective communication within interdisciplinary teams is vital for developing and implementing AI solutions. Clear roles and communication channels,

with cultivating authentic teamwork, significantly enhance collaboration. By promoting data-sharing, ensuring data privacy, and maintaining transparency in ML models, researchers can fully leverage ML's potential to advance drug discovery and healthcare outcomes.

ML in pharmacy addresses numerous challenges and offers significant advantages over traditional methods. Integrating ML with emerging technologies like blockchain and the Internet of Things (IoT) enhances patient care and operational efficiency. IoT devices can collect real-time health data for personalised medical advice, while blockchain ensures secure, transparent medical records. These innovations promise improved patient outcomes and comprehensive healthcare solutions. Utilising ML, IoT, and blockchain can transform pharmacy practice, drive innovation, and tackle industry challenges effectively.

References

1. Adeghe EP. A Review of the Use of Machine Learning in Predictive Analytics for Patient Health Outcomes in Pharmacy Practice. Open Access Res J Life Sci. 2024;
2. Liu Y, Lim H, Xie L. Exploration of Chemical Space With Partial Labeled Noisy Student Self-Training for Improving Deep Learning Performance: Application to Drug Metabolism. 2020;
3. Almallah Z, El-Lababidi R, Shamout FE, Doyle DJ. Artificial Intelligence: The New Alexander Fleming. Healthc Inform Res. 2021;
4. Fernandes PO. Machine Learning-Based Virtual Screening of Antibacterial Agents Against Methicillin-Susceptible and Resistant Staphylococcus Aureus. J Chem Inf Model. 2024;
5. Bacelar MO. Monitoring Bias and Fairness in Machine Learning Models: A Review. 2021.
6. Alosert H, Savery J, Rheaume J, Cheeks M, Turner R, Spencer C, et al. Data Integrity Within the Biopharmaceutical Sector in the Era of Industry 4.0. Biotechnology Journal. 2022.
7. Husnain A. Revolutionizing Pharmaceutical Research: Harnessing Machine Learning for a Paradigm Shift in Drug Discovery. Int J Multidiscip Sci Arts. 2023;

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Assoc. Prof. Dr. Yuslina Zakaria earned her PhD in Bioinformatics from University of New South Wales (UNSW) Australia in 2015. She began her career as an academician since 2006 at Faculty of Pharmacy, UiTM. Her research expertise includes bioinformatics and network pharmacology, big data analytics, text mining, machine learning, and financial technology (FinTech).

Questions

Let's dive deeper into the article and evaluate your comprehension. We have three questions for you here.

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