Pharmaceutical products formulation and it's optimization artificial intelligence much needed tool.

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ABSTRACT

Many businesses, including pharmaceuticals, are adopting AI . Such as in drug research and development, drug repurposing, pharmaceutical productivity, and clinical trials. The role of AI in the pharmaceutical industry is also examined, as are the present challenges and solutions. Artificial intelligence (AI) is reshaping businesses and how they handle innovation. Due to rapid technological development, AI may require management to rethink their whole innovation approach. In light of this, we examine future implications for innovation management. Based on Carnegie School and firm behavioural theories, we analyse the implications of AI technology and machine learning-based AI systems for innovation management. There are various elements to consider while transitioning from a traditional innovation organisation to a digital one. Finally, we'll look forward to what else we can learn.

INTRODUCTION

The pharmaceutical industry's future in AI. Neural networks have emerged as a viable option in recent years. Without any input from the user, neural networks are mathematical constructions that can "learn" correlations within data. Neural networks are able to build and evaluate a wide range of models to choose one that best fits the experimental data they are presented with, making no assumptions about the functional form of connections. Due to the complexity of pharmaceutical formulation and production, artificial neural networks (also known as ANNs) are increasingly being utilised to simulate behavior.[1] Using neural network models, "what if" scenarios may be easily explored. However, when combined with other technology, their powers are greatly boosted. Genetic algorithms and neural network models have shown to be extremely strong when the formulator must develop a formulation to fulfil strict, often competing, requirements. Fuzzy logic may be used to readily and clearly establish the goals for the optimization process. For example, hard tablets that dissolve fast can be created using fuzzy logic. [2] Recently, new approaches like neuro fuzzy logic have been developed that combine neural networks' ability to "learn" from data with fuzzy logic's capacity for expressing complicated notions in a simple manner. "Mining" data for information and presenting it in the form of actionable rules that may be used to guide future work is possible using these strategies.

PHARMACEUTICAL PRODUCT OPTIMIZATION

R&D cycles for small-molecule pharmaceuticals encounter various hurdles, including high costs to market, limited clinical trials success and extended cycle lengths. Despite record spending, the pharmaceutical industry's drug R&D productivity (here referring only to small molecule pharmaceuticals, unless otherwise specified) is declining. There are a variety of factors contributing to this trend, including the present saturation of the market, the difficulty of obtaining regulatory permission for new chemical substances, and the readiness to pay in both established and developing countries.[2,3] When it comes to drug discovery, there is an inherent difficulty in converting the process from fundamental science to clinical trials, which we shall address below. There is more relevant information available to researchers now than ever before, yet many scientists are unable to appropriately analyse and incorporate this information into their own workflows or study aims. When it comes to the analysis of multisource and multidimensional data, we can "outsource" our reasoning to a machine intelligence and avoid these issues altogether. For small-molecule drug development, machine learning and domain-specific "weak" artificial intelligence (AI) provide new avenues. Advances in both the core algorithms and applications of machine learning technologies that can be regarded examples of weak AI have been spectacular. There is no "strong" (generic) AI to yet, hence we shall use the word "AI" as a synonym for particular machine learning approaches. The focus of this study, therefore, will be on those components of this promising subfield that have already proved their utility and application, and on those technologies that look most promise for the next phase of AI in drug development.[3]

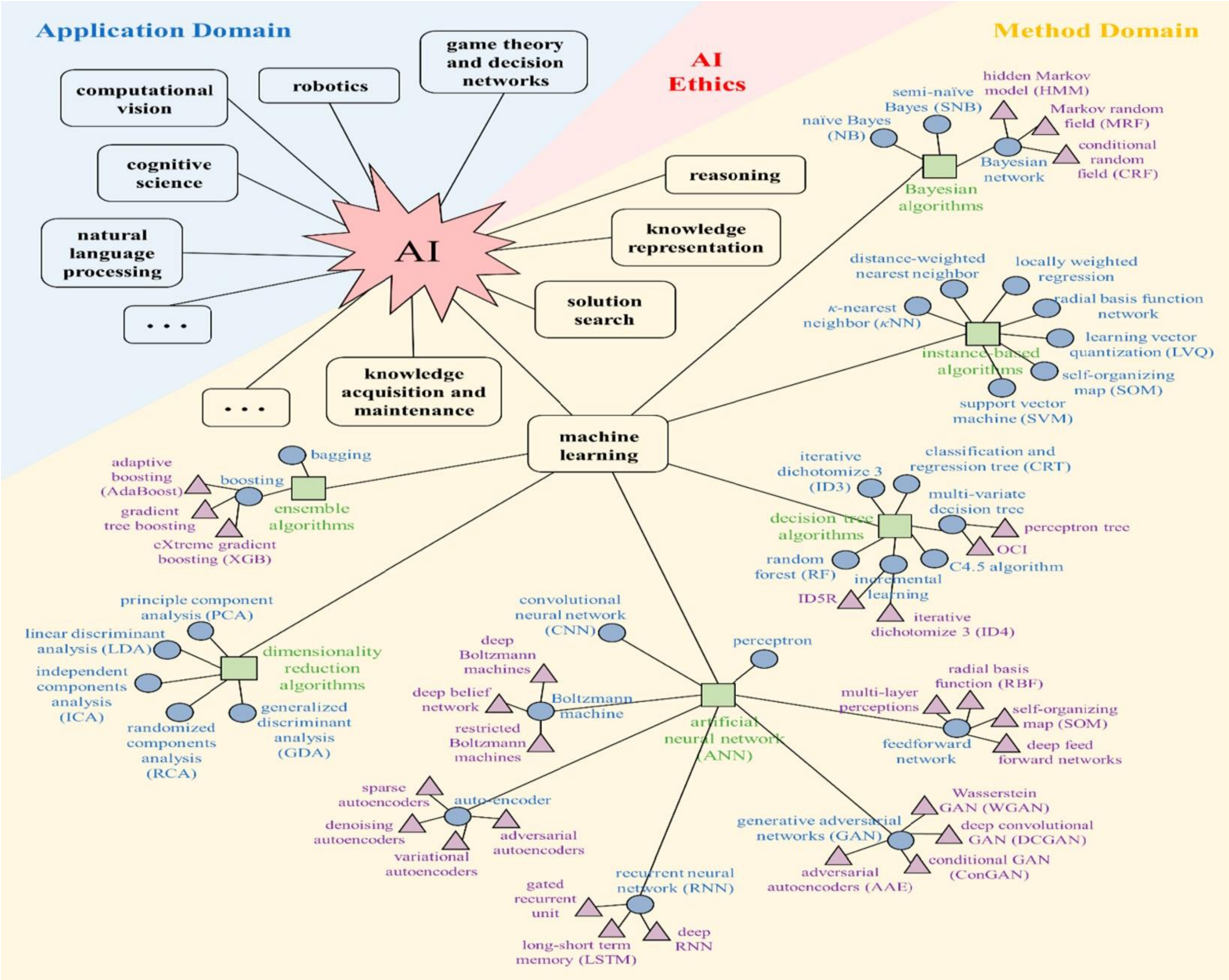

Fig: 1 Categories of Artifical Inteligence

When it comes to drug development, the use of artificial intelligence (AI) isn't new, but the use of AI in generalised structure-activity correlations is. QSAR has been around since Hammett's pioneering formula connecting reaction rates and equilibrium constants for benzene derivatives and Hansch, who is commonly considered the "father of QSAR" as practised in the pharmaceutical industry, began using computer-assisted identification and quantification of physicochemical properties of bioactive molecules. [4] When it comes to the evaluation and prediction of the biological effects of a drug, medicinal chemists have been using various AI methodologies ever since. In particular, the "pattern recognition" technique, which is based on the notion that molecules with similar structural patterns are likely to have comparable physicochemical characteristics and in vitro biochemical effects, is a strategy worth mentioning. A number of early neural network ideas and implementations (such as the Perceptron and its enhanced versions) have the potential to solve these issues.[4,5] The pharmaceutical business began using neural networks in the 1990s because of their ability to recognize patterns. In a paper from 1992, neural networks were constructed to anticipate the mechanisms of action in a cancer medication screening programme as a typical example from this time period. Neuronal networks and evolutionary algorithms were used for the first time in a completely automated molecular design process reported in 1994 The first examples of constructive machine learning are these integrated learning and decision-making models, which are capable of solving problems, learning from experience, and adapting to new conditions.[5]

METHODS FOR PRODUCT OPTIMIZATION

In order to enhance production speed while minimising faults, process optimization optimises the variables in the process. To achieve completely automated process optimization, there are a number of steps to take. From a commercial perspective, each stage has its own set of advantages and drawbacks. A machine that requires no human intervention may be the ultimate aim, but we'll cover each stage in the process below.[6] It is important to point out that machine learning is not a substitute for simulations when it comes to process optimization. Calculations based on physical or chemical attributes are a good starting point for the first optimization of parameters. As a result, machine learning may be more useful in situations where physical simulations are compared to real-world operational circumstances and mistakes are present. It's important to utilise both at the same time. As a result, this is a good time to get started on process improvement. Guardrails must be put in place before we can begin optimising the parameters of the process. If the model advises raising the line speed of a machine, it first needs to ensure that the suggested line speed does not result in faulty components or unscheduled stoppages owing to low quality. In the quality metric following, we'll explore this quality prediction application in further detail. A quality prediction model should initially be created using previous failures and supporting data, such as setpoints and environmental sensor readings. This is the simplest way to put it. We may now start manually improving some processes thanks to our quality prediction model. It is possible for an operator to set up their machine in a way that they feel would boost productivity while still fulfilling the quality standards. Despite the fact that the current production line appears to be the same as it was a few years ago, a subtle revolution is taking place: the manufacturing industry is moving online. Big and small firms alike are already using sensors to capture data throughout the manufacturing process because of the significant decline in sensor prices in recent years. The sheer volume of data generated by each assembly line is too much for humans to process, thus artificial intelligence is needed to make sense of it all. Unstructured and structured datasets can be recognised by machine learning algorithms since they are too complicated for humans to analyse. Value generated by smart factories might reach up to $3.7 trillion per year by 2025, according to a McKinsey report. AI-enabled smart factories allow manufacturing to run at a phenomenal pace while cutting costs and improving customer satisfaction. Anticipating failures, managing inventories, predicting delivery times, and working with artificial intelligence are just some of the benefits of using the newest digital technology in the workplace .[1,3,6]

A. It's possible to utilise computer vision to keep an eye on the manufacturing process and spot mistakes like small fractures in manufacturing equipment or irregular machine movement.

B. The use of artificial intelligence in generative design has had a significant impact on the way manufacturing businesses build goods. Detailed design information is fed to the AI algorithms in an iterative design process. Some of these design characteristics may include the product's production technique, material, time limits or a budget.[6]

C. Reactive maintenance has been used by the industrial sector for many years to fix machine components that have broken down. Predictive maintenance is now possible because to the rise of artificial intelligence in the manufacturing industry. [6]

CONNECTIVITY OF SOFTWARE AND PRODUCT OPTIMIZATION

Hardware advancements have been the primary driver of AI optimization and acceleration to date. AI start-up and research groups, however, have lately produced new solutions that act at the software level in the machine learning technology stack, reducing training length, inference time, energy consumption, and memory utilization of AI and ML models.[7]

The AI industry is being disrupted by these technologies, therefore understanding how to benchmark, implement, and use them is essential for corporate success.

1. Reduce AI hardware ownership costs by improving the performance of ML models on CPUs.
2. Optimizing AI accelerators that are already in use (GPUs, FPGAs, DSPs etc.)
3. Supporting the complete implementation of additional data science and machine learning initiatives
4. Increasing the competitiveness of edge devices and IoT goods

It will be demonstrated how to use the newest software optimization tools in AI/ML workflows at the Software for AI Optimization Summit This means that AI and ML models may be trained and inferred more quickly, cost-effectively, and with high levels of performance and accuracy by innovators and early adopters of data science and machine learning. [8]

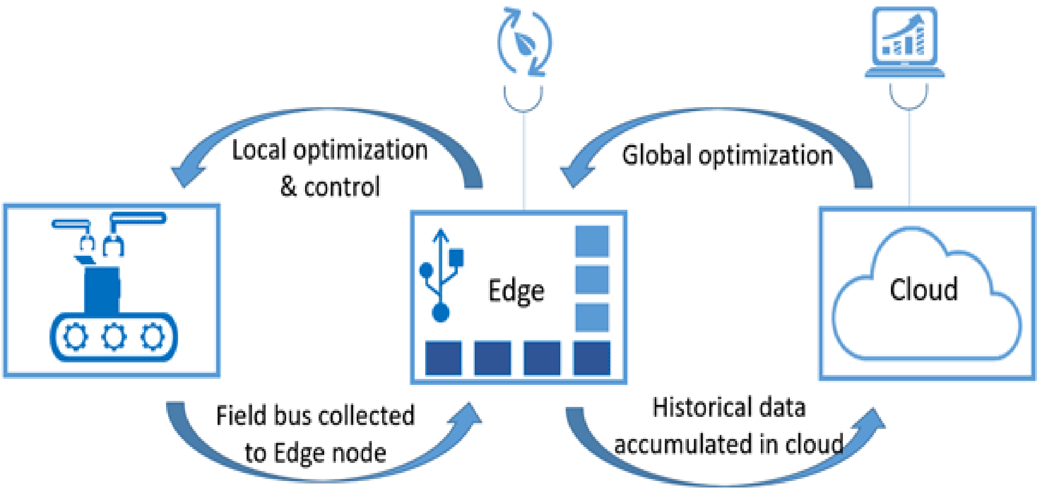

Fig: 2 AI model Close to loop and product optimization

SOFTWARE RELATED WITH PRODUCT OPTIMIZATION FOR AI DEVICE

Many businesses face the challenge of product optimization. We define optimization as any action, process, or approach that aims to make anything as excellent, functional, or effective as possible, such a design, system, or choice. Optimization is a term used to describe the process of making decisions that minimise costs, maximise quality, and minimise energy use. There is a strong emphasis on digitization and analytics in the sector right now. [8] Even in a single manufacturing site, thousands of sensors generate enormous volumes of data every day, fueling this laser-like concentration. Data from sensors and other systems was previously limited in its use because of a lack of expertise and the lack of appropriate technologies and data pipelines for gathering data for further analysis. Developing an app from the ground up is easy with the AI platform. This can be done with the built-in formula. It's easy to use because of the drag and drop approach. An increasing number of people are using chatbots, which are computer programmes that mimic the actions of a human. Speech and picture recognition can also benefit from deep learning software. [9] Using machine learning software, a computer is able to learn from the information it has access to. To put it another way, artificial intelligence is the science and technology that makes a system or programme or any machine execute the intellectual and inventive tasks of a human, autonomously solving problems and making decisions. [9,10] Artificial Intelligence Software Systems are designed to help people improve their productivity and performance over time by allowing them to find new information. Machine learning and deep learning are two examples of artificial intelligence systems that provide an analytical report to improve planning, reasoning, thinking, problem-solving, and learning. [11]

SOME TOOL USED IN AI: [11,12,13]

- Artificial Intelligence (AI) tool Ayasdi is used in financial, healthcare, and government sectors. •
- Open-source data analysis tool Scikit learn is used for classification, a grouping of objects, regression and dimensionality reduction, among other functions. Python is the programming language used in this instance.
- If you're an engineer, you can use Meya to design and build your system or product, test it, and deploy it.
- Viv is a Siri-powered personal assistant that assists developers in launching their products.
- For digital banking, the block chain serves as a wallet that may be used to transmit, store, and collect digital currency.

USE OF AI TOOLS FOR BETTER PRODUCT DEVELOPMENT

Artificial intelligence (AI) enables digital testing of product prototypes before spending time and money on actual product testing. Future goods frequently have diverse qualities. From startups to huge enterprises, AI and ML are helping to speed up product development. Job postings for DevOps and product development engineers utilizing AI and machine learning total 15,400.[14] According to Capgemini, the connected product industry will be between $519 billion to $685 billion this year. With the fast advancement of AI-based apps, goods, and services, the IoT platform sector will also consolidate. [2] Most likely to survive the next shakeout are IoT platform vendors that focus on solving business challenges in vertical markets. Now is the time for IoT platforms and ecosystems to plan for the emergence of AI and ML in product development. [15] [16] In the future, relying on technology alone won't suffice, as many IoT solutions do now. Here are five ways artificial intelligence (AI) assists today's new product creation: Most advanced AI and ML product developers earn over 30% of their revenue from digital goods or services, and they lead their peers in exploiting nine key technologies and methods. According to PwC, more than a quarter of Digital Champions (29%) earn over 30% of revenues from new goods and services within two years. As a result, Digital Champions are optimistic about personalization's benefits. [17][18][19]

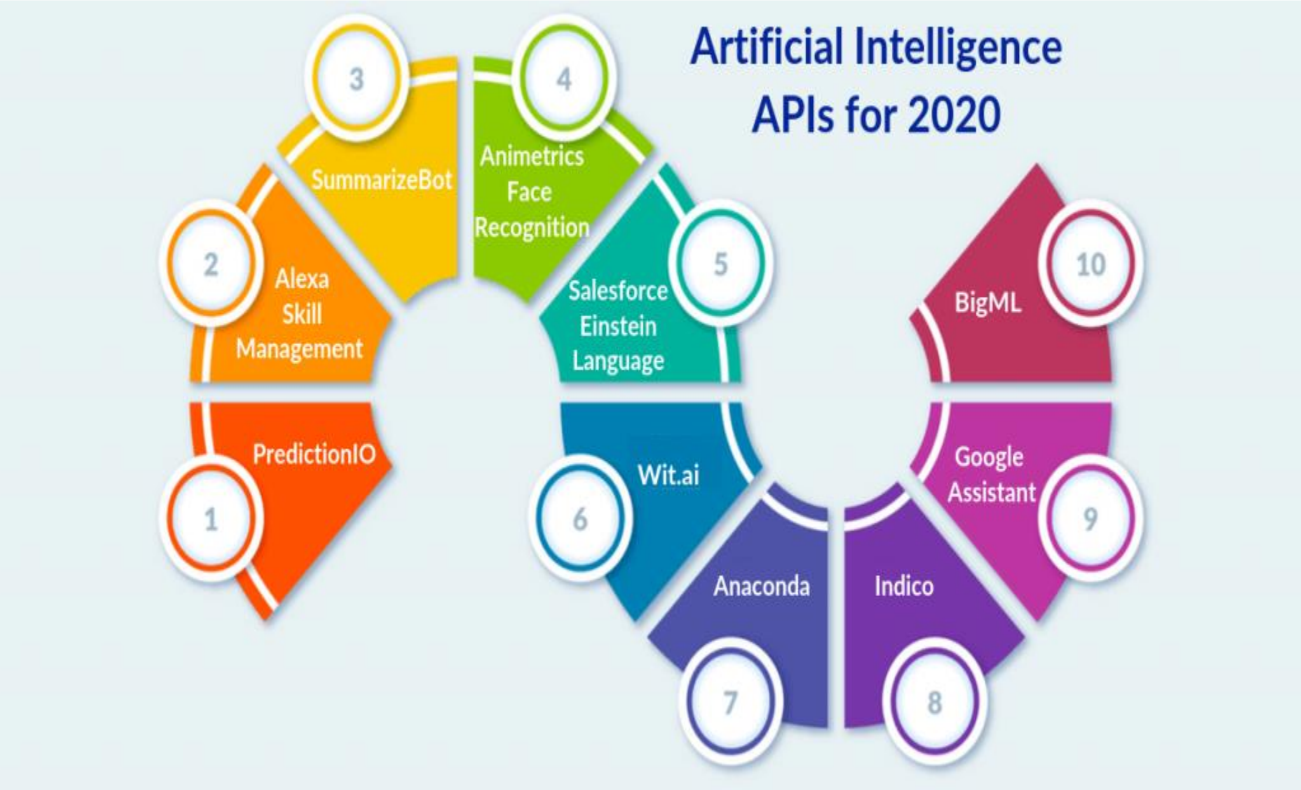

Fig: 3 AI MODEL OF APIs CONSIDERATION

FUTURE PROSPECTIVE OF AI IN PHARMACEUTICAL

Pharmaceutical firms are turning to AI to reduce the financial burden and risk of VS. With a forecast of $5 billion by 2024, the AI market is predicted to grow from US$200 million in 2015 to US$700 million in 2018. [1,2,21] AI is expected to expand 40% between 2017 and 2024, revolutionising the pharmaceutical and medical industries. Several pharmaceutical corporations have invested in AI and worked with AI businesses to build important healthcare technologies. [20,22] A cooperation between Deep Mind Technologies, a Google company, and the Royal Free London NHS Foundation Trust for acute kidney damage is one example. Figure 4 shows major pharmaceutical and AI businesses. The success of AI depends on the availability of large amounts of data since these data are required to train the system. [23] Data from several database sources can be expensive, and data must be dependable and of high quality to provide accurate result prediction. Others holding back AI adoption in the pharmaceutical industry are a lack of skilled personnel to operate AI-based platforms, limited budgets for small organisations, fear of AI replacing humans and resulting in job losses, scepticism about the data generated by AI and the black box phenomenon (how the AI platform reaches conclusions). However, this is all 'narrow AI'; where AI has to be educated using a vast volume of data and so is ideal for a certain job. Human interaction is required to successfully install, develop, and operate the AI platform. Currently, AI is taking over repetitious occupations, leaving human intellect free to generate more complex insights and creativity. [24] Nonetheless, numerous pharmaceutical businesses have implemented AI, and it is projected that AI-based solutions would generate US$2.199 billion in revenue by 2022, with an industry investment of over US$7.20 billion over 300+ acquisitions between 2013 and 2018. Pharmaceutical companies need to know how AI technology may help solve problems and what feasible goals can be accomplished once it is applied. Skilled data scientists and software engineers that understand the company's commercial goals and R&D goals may be developed to fully exploit the AI platform. [25]

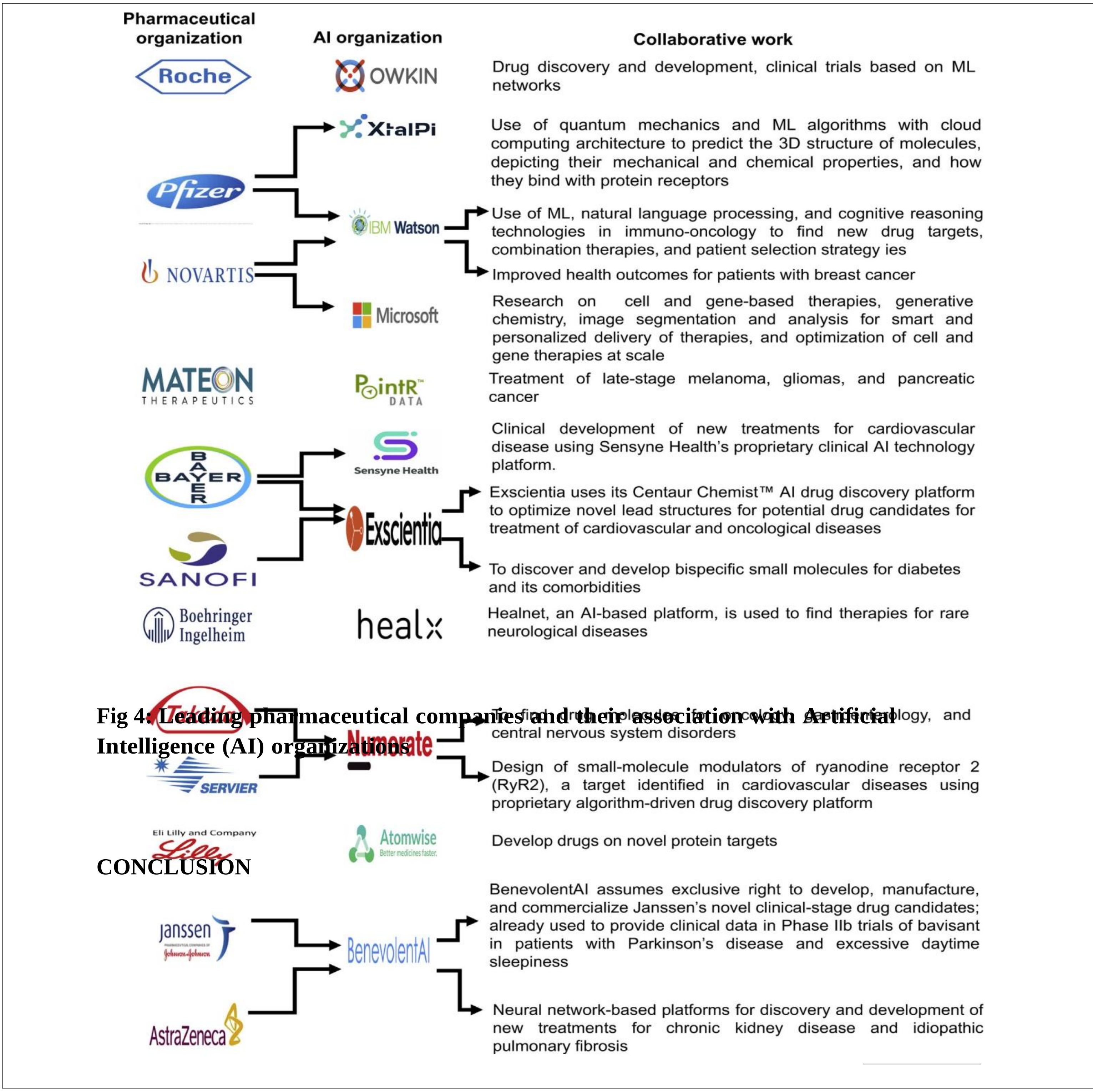

Fig 4: Leading pharmaceutical companies and their association with Artificial Intelligence (AI) organizations

CONCLUSION

In this study, we analyze how AI may help with innovation management. Conventional human-centered innovation management systems have flaws in their capacity to properly meet information demands and deal with complexity. Artificial intelligence is used in everyday life in areas such as communication, time management, education, cognition, health, traffic control, purchasing, marketing, shopping, and planning. Science uses AI to design experiments, train resources, evaluate results, and minimise complexity. We built a framework around the firm's behavioural theory's information processing restrictions. We used that to establish the AI information processing capability tiers required to build digital companies. Finally, we defined the obstacles innovation management has in deploying AI systems in connection to the technology, the personnel applying it, and the technology–human nexus. A positive function for artificial intelligence is evident when traditional innovation management resources are overburdened, unattainable due to digitalization, or when AI is clearly the preferred alternative. Our research shows that the evident promise of AI is in integrating AI into firms that are pursuing innovation. As a result of our research, the future organization of innovation will be illuminated by AI and machine learning algorithms. Our findings hint to places where AI systems may already help organizations innovate, specifically when information processing restrictions prevent new ideas from being developed. Anomaly detection AI systems can aid organizations that are battling with information processing limits while looking for new prospects. Finally, we discuss recent AI algorithm advances that show AI's ability to handle increasingly severe innovation management difficulties. Overcoming local search and developing new ideas are two examples. We are excited to watch how new AI advances expand the opportunities and places where AI can be employed in innovation management.

REFERECES

1. *Paul, D., Sanap, G., Shenoy, S., Kalyane, D., Kalia, K., & Tekade, R. K. (2021). Artificial intelligence in drug discovery and development. Drug discovery today, 26(1),80–93. https://doi.org/10.1016/j.drudis.2020.10.010*
2. *Miles, J. C., & Walker, A. J. (2006, October). The potential application of artificial intelligence in transport. In IEE Proceedings-Intelligent Transport Systems (Vol. 153, No. 3, pp. 183-198). IET.*
3. *Yang, Y., & Siau, K. (2018). A qualitative research on marketing and sales in the artificial intelligence age. Midwest United States Association for Information Systems (MWAIS) 2018 proceedings.*
4. *Brooks, R. (2018). The artificial life route to artificial intelligence: building embodied, situated agents. Routledge.*
5. *Blasiak, A., Khong, J., & Kee, T. (2020). CURATE. AI: optimizing personalized medicine with artificial intelligence. SLAS TECHNOLOGY: Translating Life Sciences Innovation, 25(2), 95-105.*
6. *Hikaru G. Jolliffe and Dimitrios I. Gerogiorgis Journal: Industrial & Engineering Chemistry Research, 2017, Volume 56, Number 15, Page 4357 DOI: 10.1021/acs.iecr.6b02146*
7. *Castle, B. C., & Forbes, R. A. (2013). Impact of quality by design in process development on the analytical control strategy for a small-molecule drug substance. Journal of Pharmaceutical Innovation, 8(4), 247-264.*
8. *Barmpalexis, P., Kachrimanis, K., & Georgarakis, E. (2011). Solid dispersions in the development of a nimodipine floating tablet formulation and optimization by artificial neural networks and genetic programming. European Journal of Pharmaceutics and Biopharmaceutics, 77(1), 122-131.*
9. *JOUR,Papavasileiou, V.Koulouris, A.Siletti, Charles, Petrides, Demetri 2007/07/01 1086 – 1097 Optimize Manufacturing of Pharmaceutical Products with Process Simulation and Production Scheduling Tools10.1205/cherd06240 Chemical Engineering Research & Design - CHEM ENG RES DES*

10. *Achilleos, E.C., Calandranis, J.C., and Petrides, D.P., 2006,Quantifying the impact of uncertain parameters in the batch manu-facturing of active pharmaceutical ingredients,PharmaceuticalEngineering, 34–40.*

11. *Vaghani, S. S., Patel, S. G., Jivani, R. R., Jivani, N. P., Patel, M. M., & Borda, R. (2012). Design and optimization of a stomach-specific drug delivery system of repaglinide: application of simplex lattice design. Pharmaceutical development and technology, 17(1), 55-65.*
12. *Prajapati, S., Patel, L., & Patel, C. (2011). Floating matrix tablets of domperidone formulation and optimization using simplex lattice design. Iranian journal of pharmaceutical research: IJPR, 10(3), 447.*
13. *Chaudhury, A., Barrasso, D., Pandey, P., Wu, H., & Ramachandran, R. (2014). Population balance model development, validation, and prediction of CQAs of a high-shear wet granulation process: towards QbD in drug product pharmaceutical manufacturing. Journal of Pharmaceutical Innovation, 9(1), 53-64.*
14. *Jarrahi, M. H. (2018). Artificial intelligence and the future of work: Human-AI symbiosis in organizational decision making. Business Horizons, 61(4), 577-586.*
15. *Velmourougan, S., Dhavachelvan, P., Baskaran, R., & Ravikumar, B. (2014, September). Software development Life cycle model to build software applications with usability. In 2014 International Conference on Advances in Computing, Communications and Informatics (ICACCI) (pp. 271-276). IEEE.*
16. *Fenton, N., Hearty, P., Neil, M., & Radlinski, L. (2010). Software project and quality modelling using Bayesian networks. In Artificial intelligence applications for improved software engineering development: New prospects (pp. 1-25). IGI Global.*
17. *Wenyan Song, Tomohiko Sakao, A customization-oriented framework for design of sustainable product/service system Journal of Cleaner Production, Volume 140, Part 3, 2017, Pages 1672-1685 https://doi.org/10.1016/j.jclepro.2016.09.111.*
18. *Cinar, D., Gakis, K., & Pardalos, P. M. (2016). A 2-phase constructive algorithm for cumulative vehicle routing problems with limited duration. Expert Systems with applications, 56, 48-58.*
19. *Ahmad, S. G., Liew, C. S., Munir, E. U., Ang, T. F., & Khan, S. U. (2016). A hybrid genetic algorithm for optimization of scheduling workflow applications in heterogeneous computing systems. Journal of Parallel and Distributed Computing, 87, 80-90.*
20. *Chiang, T. C., & Hsu, W. H. (2014). A knowledge-based evolutionary algorithm for the multiobjective vehicle routing problem with time windows. Computers & Operations Research, 45, 25-37.*
21. *Dal, B., Tugwell, P., & Greatbanks, R. (2000). Overall equipment effectiveness as a measure of operational improvement–a practical analysis. International Journal of Operations & Production Management.*
22. *Ngo, Q. H., & Schmitt, R. H. (2016). A data-based approach for quality regulation. Procedia CIRP, 57, 498-503.*
23. *Wang, Z. H., Liu, Y. M., Gong, D. Y., & Zhang, D. H. (2018). A New Predictive Model for Strip Crown in Hot Rolling by Using the Hybrid AMPSO-SVR-Based Approach. steel research international, 89(7), 1800003.*

24. *Kelly, A. E., Sleeman, D. H., & Gilhooly, K. J. (1993). Artificial intelligence in education: using state space search and heuristics in mathematics instruction. International journal of man-machine studies, 38(4), 725-746.'*
25. *Aiken, R. M., & Epstein, R. G. (2000). Ethical guidelines for AI in education: Starting a conversation. International Journal of Artificial Intelligence in Education, 11, 163-176.*