The Use of AI in Science, Technology, Engineering, and Maths

Key themes identified in a breadth-focused literature review

Prepared for The Royal Society

Glen Berman, Jennifer Chubb, and Kate Williams

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Document aims

The Royal Society's *Disruptive Technology for Research* project aims to understand the landscape of data-driven and Artificial Intelligence-based technologies (AI) across different fields of scientific research. The project will further articulate the impact and risks data-driven technologies can have, outline cases of success, and improve understanding of factors that have slowed adoption of AI technologies across the sciences. The project uses applications of AI technologies across different fields as case studies to offer recommendations on how the UK government can best support the development, adoption, and uses of such technologies.

This document provides a brief summary of the literature of Artificial Intelligence (AI) related inventions and their application across different fields of scientific research. This research aims to enable end users to have an overview of the current state of application for artificial intelligence related inventions in scientific research - adding context to the challenges, opportunities and Royal Society's recommendations. Please refer to the full report for further information.

A note on 'AI' terminology

In this document we use 'AI' as a broad term, covering all efforts aiming to replicate and extend human capabilities for intelligence and reasoning in machines. Since the founding of the AI field at the 1956 Dartmouth Summer Research Project on Artificial Intelligence, many different techniques have been invented and studied in pursuit of this goal. Many of these techniques have developed into their own subfields within Computer Science, such as expert systems and symbolic reasoning. Machine Learning (ML) is one such technique, as is the dominant ML paradigm, Deep Learning (DL). Since the rise of Big Data and the advent of cost-effective parallel computing, ML and DL techniques have achieved remarkable successes in a wide variety of research and industry domains—so much so, that in modern parlance 'AI' is often treated as synonymous with ML. Reflecting this, this summary literature review—and the *Disruptive Technology for Research* project more generally—focus on the use of ML and DL techniques in the sciences.

Introduction: AI in STEM

AI is ubiquitous in society - it is part of our everyday lives. Crucially, AI, in particular ML, is being used across all fields and sectors from the creative arts through to cybersecurity and health diagnostics. In recent years, there has been a growing concern over the ethical implications of ML. This context is particularly important when exploring the use of AI in Science, Technology, Engineering, and Medicine (STEM) where much of the literature attempts to tackle both of these aspects though outside of the scope of this review.

Applications of AI can be found across all STEM fields, with concentration in digital health, medicine and dentistry, environment, materials science, engineering, computational and mathematical sciences, robotics, quantum information technologies, health informatics, computer aided design, nurse and health care professional education and training, sustainability, dynamical and control systems engineering, safety critical systems, genetics, agriculture, energy, conservation and efficiency, data analytics, mechanical engineering, smart innovation, physics and astronomy, and computer and information science. Crucially, the application of AI in STEM looks to consider its application from a range of perspectives from policy to practice.

Within STEM, AI is widely adopted in fields that have (1) substantial data infrastructure and (2) a history of using computer models. For adoption of AI techniques these two requirements are mutually reinforcing: data infrastructure means there is surfeit of data for training models, and a history of using modelling means there are scientists who feel comfortable translating and adopting AI techniques to their field.

Approach to the literature

To produce this summary of the key themes identified in the literature, the following subject categorisations were used:[1]

- **Physical sciences:** Chemical Engineering, Chemistry, Computer Science, Earth and Planetary Sciences, Energy, Engineering, Environmental Science, Material Science, Mathematics, Physics and Astronomy.
- **Health sciences:** Medicine, Nursing, Veterinary, Dentistry, Health Professions.
- **Life sciences:** Agricultural and Biological Sciences, Biochemistry, Genetics and Molecular Biology, Immunology and Microbiology, Neuroscience, Pharmacology, Toxicology and Pharmaceutics.

Literature searches were conducted by inputting AI related keywords (e.g. artificial intelligence, machine learning, deep learning) in combination with subject areas listed above. The focus was on recent systematic or comprehensive reviews in order to gain oversight into the key trends within each field.

[1] This is based on Elsevier's All Science Journal Classification Codes (ASJC). Full methodological details will be provided in the final report.

Summary of key themes identified in the literature

This section outlines the domains of use of AI across the subfields of STEM. Each area describes the ways in which AI is deployed, the benefits and key challenges highlighted in the literature.

Physical sciences

AI and the physical sciences are deeply entwined. Indeed, the physical sciences have a long history of deploying AI techniques to advance their research objectives. For example, expert systems, an AI technique which was actively researched throughout the 1970s and 1980s and aimed to replicate the decision-making processes of a domain expert, were adopted in chemical engineering and chemistry. Today, many subdomains in the physical sciences make substantial use of AI techniques to model natural and anthropogenic phenomena—from natural disasters to synthetic materials—and to help extract information from rapidly accumulating data streams, such as the data generated by experiments at the Large Hadron Collider. Meanwhile, subdomains in the physical sciences are also helping advance AI techniques, both by creating new challenges for AI techniques to address and by providing domain expertise to enable development of new classes of ML models. Of particular relevance to both the AI field and the physical sciences is the development of hybrid physics-based ML models—models that learn both from data and from domain-specific principles—as these models have demonstrated significant potential in addressing core AI challenges of model interpretability, robustness, and reliability.

Within the physical sciences, the fields of computer science and mathematics are particularly closely associated with the AI field. ML, in particular, is often considered a subfield of computer science. Current research focuses across computer science include the development of new ML modelling approaches, including advanced DL and generative ML, and the application of these approaches to highly generalisable tasks, such as natural language processing, image processing and computer vision, game playing, and model explanation and interpretation. Additionally, within applied subfields of computer science, particularly cybersecurity, video game development, and software engineering, a major focus has been the integration of ML techniques into workflows and data processing. Current research focuses across mathematics, meanwhile, include addressing some of the fundamental research challenges in AI: identifying optimal model training processes, model interpretability and robustness, and quantifying the extent of model generalisability. These challenges reflect, in particular, the ongoing search for a mathematical foundation for DL, to complement the growing empirical evidence of DL's effectiveness.

The physical sciences have been particularly receptive to the current wave of ML and DL research. In part, this is because the development of ML models to ingest and identify patterns in very large datasets, and the maturation of open-source software to build ML models, has coincided with explosive growth in data generated by various physical science fields. In high energy particle physics, for example, the Large Hadron Collider is producing a vast volume of data, and the search for new particles requires the ability to detect minute signals within this data. Similarly, in astronomy data generated by the Event Horizon Telescope is of such a scale that information extraction is only possible with the support of custom-built ML models. Comparable advances in data generation can be found in the fields of environmental science, energy, earth and planetary sciences, chemistry, and chemical engineering. In all these fields significant growth in the array of sensors used to monitor and observe physical phenomena has resulted in comparably significant growth in the volume of data generated, creating clear use cases for the deployment of ML techniques.

An additional factor in the enthusiastic adoption of ML and DL research in the physical sciences is the extant centrality of computer-based modelling to many fields. Pre-dating the current wave of ML, modelling was already used in many physical sciences to complement and extend physical experiments, and to manage industrial processes. In chemical engineering, models are critical to understanding chemical reactions, and are used to monitor chemical manufacturing processes. Similarly, a core focus of research in the Earth and planetary sciences has been the development of models of the climate, water systems, and mineral deposits. ML and DL techniques are extending the capacity of the physical sciences to model complex phenomena, particularly in instances where many variables interact. In chemical engineering and material science, ML and DL techniques have thus been applied to the problems of forward and inverse modelling of molecular structures, enabling more efficient and accurate prediction of the properties of a given molecular structure and the prediction of new molecular structures that are likely to produce specific desirable properties. In engineering, energy, chemistry, and environmental sciences, ML and DL techniques have been applied to problems of fault detection in industrial processing (e.g. chemical synthesising) and health monitoring of industrial and natural systems (e.g. structural health of infrastructure, health of waterways).

Three challenges to further use of AI techniques in the physical sciences stand out. First, while many physical sciences have strong data infrastructures in place, there are data gaps relating to publicly-accessible datasets for model training, benchmark datasets for model evaluation, and benchmarks for the collection and curation of new datasets. Second, although researchers have shown interest in adopting ML and DL techniques, field-specific training in the appropriate use of these techniques is still under development. Finally, as ML and DL techniques are deployed in the physical sciences, limitations inherent in these techniques are also surfaced. Limitations of particular concern to the physical sciences are: scientific interpretation of model outputs; determination of model generalisability; and, most importantly, the potential for ML models to produce outputs that do not accord with known principles of natural phenomena. This final limitation has spurred the development of hybrid physics-informed ML models, which attempt to hard code into the neural network relevant laws of physics, to ensure model compliance. In the Earth and planetary sciences, energy, engineering, and physics and astronomy, physics-informed models are a significant area of ongoing research and collaboration with computer scientists.

Health sciences

AI is rapidly spreading across healthcare. The literature suggests that healthcare professionals prefer to use AI as a tool which must be used in complement with human judgement and exposes concerns about AI explainability and transparency with frequent references to AI as a 'black-box' technology. This is reinforced by frequent references to the implications of algorithmic historical bias and discriminatory data. Indeed, much of the literature on healthcare and AI use reveals ethics and AI to be deeply intertwined requiring patient and public involvement in the research process. Further, the literature reveals concerns over a lack of communication and understanding between clinicians and health professionals, and AI scientists.

Across the field of health sciences, the main subdomains where AI is used includes: mental health and psychiatry, pharmaceutical industries, physiology, neuroscience and neurology, infectious diseases, biotechnology, genetics, oncology, stem cell research, radiography, perinatal and gynaecology. To do this, fields rely on big data, machine learning, deep learning, and natural language processing as examples of AI-based technologies.

As a result of the COVID-19 pandemic, perhaps unsurprisingly, there has been an explosion of research about AI and digital health in the area of infectious disease and clinical management. Beyond this, a high level analysis of the ways in which AI is used in health shows that most commonly the areas of application are explored through the lens of disease detection, disease prediction, modelling, diagnosis, treatment, discovery, repair, data visualisation, surgery, training, robotics, precision, treatment, risk stratification, clinical management and decision making and health care 'futures' such as considerations of major grand challenges including risk prevention of infectious disease, ageing population and obesity.

AI offers huge potential for improving healthcare in supporting clinical decision making and new techniques for diagnostics and detection as well as clinical evaluation. However, its deployment is often opaque, and adoption can be 'inhibited by the use of 'black box' AI systems where it is not understood why AI is an effective technique or how far it protects the rights of patients to confidentiality, consent and autonomy. Indeed, the rapid integration of AI in health has occurred with little communication between those developing it, computer scientists and doctors where, for instance, historical and algorithmic bias may widen healthcare inequalities.

Life sciences

AI and the life sciences have benefited from strongly intertwined progress. The literature shows two key areas. First, in the life sciences around agriculture and the food industry, advancements in the Internet of Things (IoT) have provided a range of sophisticated sensors and physical devices that in turn have provided a wealth of data that can be analysed using supervised and unsupervised AI models. The insights derived from these models are used in creating automated 'smart machines' or in informing human interventions. Second, in the life sciences oriented towards improving health outcomes and knowledge on biological and molecular systems, advancements in computing capability and algorithms have allowed the integration of big data, artificial intelligence, and multi-scale modelling techniques to improve all stages of the process from research to clinical practice.

Across the field of the life sciences, the main subdomains include a focus on; food security, climate change, agriculture, farming, e-waste, water, energy, oceans, fish farming, analysis of power usage, soil management, water management, biochemistry, molecular biology including genetics, genomics, drug interactions and discoveries, immunology and neuroscience as well as modelling in pharmacology and toxicology. The sector particularly relies on the IoT, big data, neural networks, modelling and image recognition.

A high-level analysis of the ways in which AI is used in the life sciences shows the areas of application relate to autonomous farming, crop management, water management, soil management, livestock management, laboratory processes and care pathways, imaging and laboratory services, diagnosis and disease monitoring, patient eligibility, genomic analysis, diagnosis, prediction and treatment for psychiatric, neural and developmental disorders as well as drug development.

Overall, the life sciences are faced with two key challenges, which differ depending on the goals and processes of the subfield. Within the life sciences focused on agriculture and food, data is plentiful thanks to the relatively low cost of sensors and devices, however the use of advanced technologies are localised to highly developed countries, particularly large factory farms in North America and Europe, while making a livelihood remains extremely difficult for most farmers around the world. On the other hand, a challenge for the life sciences oriented towards improving health outcomes is a lack of data, which is exacerbated by strict controls over databases held by big pharma companies, plus the high resource and time costs of experiments and optimization processes. Furthermore, as with healthcare above, the literature highlights the implications of bias and discriminatory data and emphasises the role of ethics and interpretable AI in progressing the field.

Conclusion

This review demonstrates that applications of AI in Science and Technology can be found across all STEM fields. AI presents many potential opportunities to transform the way research is done, and to extend the capabilities of industries associated with the life sciences, health sciences, and physical sciences. The enthusiastic adoption of AI, however, should be tempered with a view to managing risks and unintended consequences associated with AI. Of particular concern are data systems and practices that discriminate against particular social groups. There are concentrations of AI use in digital health, medicine and dentistry, environment, materials science, engineering, computational and mathematical sciences, robotics, quantum information technologies, health informatics, computer aided design, nurse and health care professional education and training, sustainability, dynamical and control systems engineering, safety critical systems, genetics, agriculture, energy, conservation and efficiency, data analytics, mechanical engineering, smart innovation and computer and information science. Crucially, the application of AI in science and technology looks to consider its application from a range of perspectives, indicative of the AI ecosystem comprising actors across the research community, policy and practice.

The use of AI in certain domains, particularly to support resource allocation decisions (e.g. in health) and to monitor critical infrastructures and processes (e.g. in engineering), is especially high stakes. As such, much of the material we describe inevitably refers to ethical implications in their findings and conclusions, and engages with the broader literature on ethical implications and governance of ML.

Further, there is a clear theme relating to the collective need for multi and interdisciplinary working practices across the research landscape, and the development of shared data infrastructures. In AI, this extends further too, with research involvement from public and private sectors who comprise the AI ecosystem. While it is clear that AI can transform STEM, caution should be taken in applying a broad brush to its implementation. This is where AI futures and related work in the fields of the humanities and social sciences can support research and development, addressing issues of biases and inequalities emerging from the field of AI research.

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