

# Role of Artificial Intelligence in Scientific Research: Classification Framework and Empirical Insights

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## Abstract

Artificial intelligence (AI) represents the culmination of multidisciplinary scientific knowledge and, through its diverse technological capabilities, has significantly contributed to research across various fields. This study explores the bidirectional relationship between AI and scientific research, with a focus on the frequency and context in which AI is mentioned in research articles. A classification framework is developed to categorize the different ways AI is mentioned in articles. Empirical analysis is conducted in the fields of oncology, nanoscience and nanotechnology, as well as meteorology and atmospheric sciences. The findings indicate that while the mention of AI in research articles has become widespread, the distribution of different ways of mentions is relatively concentrated. We not only identify the conceptual differences in the focus of AI mentions, but also uncover the disparities in the intensity and ways of AI mentions across research articles from various countries. This study contributes to a deeper understanding of the complex interplay between AI and scientific research, advocating for the synergetic development of AI and scientific progress by leveraging the strengths of different nations.

## Introduction

The 2024 Nobel Prizes have marked a significant milestone in the convergence of artificial intelligence (AI) and scientific research. This year, the Nobel Prize in Physics was awarded to two pioneers in the field of AI, John Hopfield and Geoffrey Hinton, who utilized concepts and methods from physics to invent the Hopfield

network and Boltzmann machine, respectively, laying the foundation for machine learning and artificial neural networks. Simultaneously, the Nobel Prize in Chemistry was granted to David Baker, Demis Hassabis and John Jumper for their revolutionary advancements in protein structure prediction, achieved through the innovative integration of AI with computational chemistry. These awards not only emphasize the multidisciplinary collaboration driving AI innovation but also highlight AI's pivotal role in enabling scientific breakthroughs. Together, they exemplify the bidirectional synergy between AI and science, advancing both to remarkable new frontiers.

This development raises an important question: What role does AI play in science? For a long time, researchers have recognized how AI integrates interdisciplinary scientific knowledge, emphasizing the contributions of various scientific fields to the development of AI (Arencibia-Jorge et al., 2022). In recent years, increasing attention has been given to the enabling role of AI in scientific progress, with its growing use and benefits across diverse scientific domains (Gao et al., 2024). Researchers have recognized the emergence of the 5<sup>th</sup> Paradigm of Science – AI-driven science (Ioannidis, 2024), and discussed various ways in which AI supports scientific research in different research fields (He, 2024; Wang et al., 2023). Still remaining, however, are systematic and quantitative empirical investigations into the bidirectional relationship between AI and science, particularly regarding how AI both shapes and is shaped by scientific advancements (Miao et al., 2022; Xu et al., 2024). Further exploration is needed of the various manifestations of this reciprocal relationship across research domains and among research entities. Such analyses may provide practical insights for enhancing the interaction between AI and science in real-world research, thereby promoting their parallel development.

To advance knowledge in this direction, this study addresses two central questions: (1) How can we understand and distinguish the various roles of AI in science? (2) Do these roles vary across temporal periods, scientific fields and actors? To answer these questions, we will focus on textual mentions of AI in research articles, thereby taking one of the primary outputs of scientific research as an entry point. Such mentions may provide evidence of the roles of AI as currently recognized within the academic communities. By developing a classification framework and conducting an empirical analysis, we aim to map the landscape of AI influences across scientific fields and derive meaningful insights from the findings.

## **Classification framework**

Acknowledging the bidirectional relationship between AI and science, we classify research articles that mention AI into two primary categories: *Science for AI* (Type A) and *AI for Science* (Type B). The first category emphasizes the cross-disciplinary exchange and integration of scientific knowledge (Frank, 1988) and highlights the role of various scientific fields in supporting AI development, primarily reflecting the role of AI as the research subject. The second category draws on the theory of parallel intelligence (Miao et al., 2024) and suggests that AI can augment human capabilities in conducting scientific research in specific ways, mainly reflecting the

role of AI as the research tool. In addition to the two primary categories, we posit that there are other circumstances in which articles mention AI in a relatively inconsequential manner. Consequently, we establish a third category – *Other* (Type C), to encapsulate the more ambiguous relationships between AI and science. Below, we will elaborate on the subdivisions of the three categories and their meanings, as detailed in Table 1.

As for Type A, we distinguish different subtypes of *Science for AI* by examining the core issues encountered by AI throughout its various stages of development. As a general-purpose technology (Bresnahan et al., 1995), AI has developed a wide range of technological capabilities and permeated diverse industries and fields. Scientists are not only focused on the development and improvement of AI technology (e.g. establishing a deep learning model), but also on promoting its application in real-world scenarios (e.g. evaluating the effectiveness of using AI in disease diagnosis). Furthermore, there is an increasing necessity to recognize and address the unintended consequences that may arise from its deployment (e.g. investigating the issue of algorithmic bias). Following this understanding, we have identified three subtypes – *Science for the Development of AI* (Type A1), *Science for the Application of AI* (Type A2) and *Science for the Governance of AI* (Type A3).

As for Type B, we distinguish different subtypes of *AI for Science* by examining the various tasks that AI performs in scientific research. As AI is increasingly utilized in scientific research, several attempts have been made to characterize the ways in which AI enhances scientific pursuits. For example, the Royal Society (2024) has outlined three primary functions of AI in scientific research – a computational microscope, a resource for human inspiration, and an agent of understanding. The European Commission (2023) has summarized the most common applications of AI in the research process, including prediction problems, transformations of input data, optimal parameterization, literature review, literature-based discovery, and automation of tedious, routine laboratory tasks. A report released by Google DeepMind (2024) has pinpointed five opportunities to accelerate science with AI, namely knowledge, data, experiments, models and solutions. Wang et al. (2023) have reviewed the role of AI in scientific research from four aspects – AI-aided data collection and curation, learning meaningful representations of scientific data, AI-based generation of scientific hypotheses, and AI-driven experimentation and simulation. Messeri et al. (2024) have proposed four uses of AI in the research process – the use of AI as Oracle for the study design, as Surrogate for the data collection, as Quant for the data analysis, and as Arbiter for the peer review. By combining insights from such proposals for categorizations with our observations from empirical data (see Section 3), we have identified four subtypes – *AI for Data Collection* (Type B1), *AI for Data Representation* (Type B2), *AI for Generation* (Type B3), and *AI for Simulation* (Type B4).

As for Type C, we do not further subdivide the category. Research articles under this type may mention AI in specific contexts, but AI is not an indispensable component in the conduct of the research, thereby neither being the subject of study as in Type A nor serving as the research tool as in Type B. Nevertheless, this type of research

remains of notable importance. AI may be mentioned to provide a contextual backdrop, reflecting its status as a current hot topic, or it could be indirectly supported by the research, indicating a special and potential relationship between the research and AI. The characteristics of studies under this type will be further explored in the empirical analysis to reveal more nuanced insights.

**Table 1. Classification framework of AI mentions in research articles.**

<i>Categories</i>		<i>Description</i>
A. Science for AI	A1. Science for the Development of AI	This type of study provides theoretical or methodological support for the technological development, improvement, and application of AI.
	A2. Science for the Application of AI	This type of study provides an overview, comment or evaluation of the progress, dilemmas, challenges, and potentials in applying AI to solving the problems within certain fields.
	A3. Science for the Governance of AI	This type of study provides a discussion on ethical, legal and policy problems arising from AI technologies and possible solutions to these problems.
B. AI for Science	B1. AI for Data Collection	The application of AI technologies for gathering data for further processing and in-depth analysis, to solve the problems in certain research fields.
	B2. AI for Data Representation	The application of AI technologies for structuring, modeling, and feature extraction from data, to solve the problems in certain research fields.
	B3. AI for Generation	The application of AI technologies for emulating human reasoning and cognition to generate creative content by calculating and mining large datasets, to solve the problems in certain research fields.
	B4. AI for Simulation	The application of AI technologies for simulating experimental or real-world scenarios to conduct predictive analysis of potential situations and outcomes, to solve the problems in certain research fields.
C. Other		Studies where AI is mentioned without having an indispensable role in the research.

## Empirical data

### *Sample selection*

This study uses research articles mentioning AI in representative fields within years from 2014 to 2023 as samples<sup>1</sup>. The data source is Web of Science (WoS) Core Collection. We selected three fields representing different areas of research by using three WoS categories – *Oncology* (ON), *Nanoscience and Nanotechnology* (NN), and *Meteorology and Atmospheric Sciences* (MA) – for exploratory analysis.

In selecting the case fields, we have considered three aspects. Firstly, given the varying sizes of fields within the WoS categories, we need to focus on fields that are relatively targeted and of moderate granularity. The fields of ON, NN and MA meet our need, with the detailed descriptions of the samples provided in the following subsection. Secondly, these three fields cover natural sciences, engineering sciences, and life sciences, encompassing both basic and applied value, and are capable of reflecting the research characteristics of different disciplinary domains. Thirdly, a more important consideration is that these fields feature typical examples of the intersection between AI and scientific research, such as the AI-assisted cancer screening in the ON field (McKinney et al., 2020), the AI-driven material discovery in the NN field (Szymanski et al., 2023), and the AI-supported weather forecasting in the MA field (Bi et al., 2023). In November 2024, Google announced nine ways in which AI is advancing science. Several of them involve the three representative fields mentioned above, including protein structure prediction, accelerating materials science, saving lives with accurate flood forecasting, predicting weather faster and with more accuracy, etc. Promoting the application of AI in health, environment, climate, and other fields, has become a focal point for academia, industry and policymaking circles (CB Insights, 2024; OECD, 2023). Based on our bidirectional classification framework, we will further explore and reveal the complex interactive relationships between AI and scientific research in these three fields.

It should be noted that by focusing our study on research articles that mention AI, we may overlook some specific connections between AI and science. For instance, prior to the popularization of the term of AI, numerous research fields have laid foundational theoretical and methodological groundwork for the development of AI, such as probability and information theory in mathematics, genetic phenomena and neural networks in biology, etc. These efforts, in a broader sense, constitute a form of *Science for AI*, yet they fall outside the scope of this study. In addition, AI may assist researchers in tasks such as literature review, hypothesis formulation and academic writing. However, these contributions of AI are often not explicitly discussed in papers and, therefore, are not included in our analysis. Recognizing the

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<sup>1</sup> On the one hand, we aim to obtain the latest data that reflects contemporary trends. Given that our research was conducted in 2024, the most recent year covered is 2023. On the other hand, we strive to encompass key milestones in the development of AI over recent years, such as the emergence of BERT in 2018, hence we have selected a time window spanning a decade.

boundaries of our research sample is essential for a proper understanding of the subsequent analyses and results of this research.

*Search strategy*

We use two approaches to retrieve articles mentioning AI. One is to select articles that explicitly mention the term “artificial intelligence” or its abbreviations in certain contexts (considering that the abbreviation “AI” can refer to different concepts across various disciplines) in the title, keywords, or abstract. These three information fields are the ones that WoS can provide directly reflecting the content of the articles. The other approach is to include terms referring to representative sub-technologies of artificial intelligence as search keywords. Considering the broad definition of AI, traditional machine learning techniques such as Naive Bayes are not the focus of this study. According to a survey targeting scientists across various academic disciplines worldwide, ChatGPT and its LLM cousins are the tools that researchers mentioned most often when asked to type in the most impressive or useful example of AI tools in science (van Noorden et al., 2023). To a certain extent, ChatGPT and LLM represent a landmark moment in the development of AI, with the potential to disrupt existing paradigms and, optimistically, exert a positive influence on humanity (Vert, 2023). Therefore, terms related to ChatGPT and large language models (LLM) are selected for inclusion in the search terms.

Based on the above two approaches, we have developed a set of search terms by referencing existing search queries (Arencibia-Jorge et al., 2022; Mariani et al., 2024), performing manual filtering and supplementary additions, as well as consulting experts in the relevant fields, as shown in Table 2. We conducted searches in the *Title* (TI), *Author Keywords* (AK) and *Abstract* (AB) fields of the WoS database. After excluding six papers with false positives by manual checking, a total of 1,251, 1,189 and 364 articles mentioning AI were retrieved in the fields of *Oncology*, *Nanoscience and Nanotechnology*, and *Meteorology and Atmospheric Sciences*, respectively. These articles were subsequently utilized as the analytical samples for this study. The data retrieval date is January 3<sup>rd</sup>, 2025.

**Table 2. Search terms of research articles mentioning AI.**

<i>Search strategies</i>	<i>Search terms</i>
Full name	“artificial intelligen*”
Abbreviations in certain contexts	“strong AI” OR “full AI” OR “human-level AI” OR “AI for science” OR “AI4S” OR “AI4Science” OR “generative AI” OR “AI-generated content*” OR “AIGC” OR “AI-based research”
Keywords for representative AI technologies	“large language model*” OR “generative language model*” OR “generative pretrained transformer*” OR “generative pretrained language model*” OR “ChatGPT*” OR “GPT-1*” OR “GPT-2*” OR “GPT-3*” OR “GPT-4*” OR “GPT-5*” OR “GenAI” OR “OpenAI GPT” OR “Midjourney*”

*Data annotation*

Based on the classification framework shown in Table 1, this study categorizes 2,794 research articles with abstracts through manual annotation, carried out by two authors with significant experience in data annotation. After thoroughly understanding the connotations and characteristics of different types of articles among three selected fields, the annotators read the abstracts independently and labeled each article with the type of mentioning AI. During the annotation process, the annotators prioritized sentences that mention AI or its sub-technologies. The type of article is determined by analyzing the key terms within these sentences and the surrounding context. If a single sentence mentioning AI or its sub-technologies does not provide enough information to classify the article, the classification is further refined based on the overall content of the abstract.

For the results of manual annotation, the Kappa consistency test was conducted using the SPSS software. The annotation results of two annotators in the three research fields are statistically consistent, as shown in Table 3, indicating that the annotation results are usable for further analysis. In cases where discrepancies in the annotation results arose, the two annotators discussed the articles together until a consensus was reached.

**Table 3. Kappa statistics of manual annotation results.**

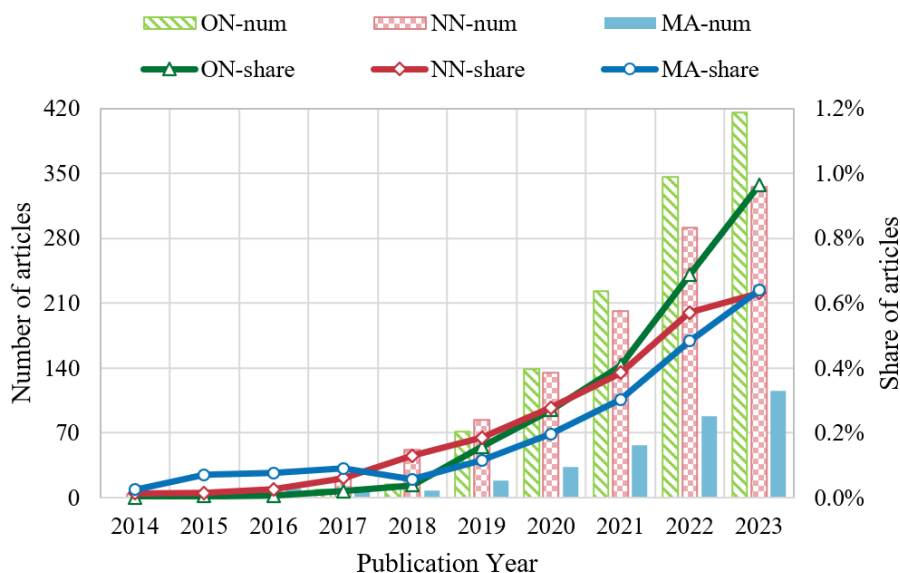
<i>Research field</i>	<i>Kappa value</i>
Oncology	0.982***
Nanoscience and Nanotechnology	0.997***
Meteorology and Atmospheric Sciences	0.908***

Note: \*\*\* indicates that the result is statistically significant.

**Results**

*Overview of articles mentioning AI*

Figure 1 illustrates the number of articles mentioning AI and their proportion within the total number of articles in the fields of *Oncology* (ON), *Nanoscience and Nanotechnology* (NN), and *Meteorology and Atmospheric Sciences* (MA) from 2014 to 2023. It can be observed that, over time, the frequency of AI mentions in research articles has steadily increased, especially since 2018, reflecting the growing integration of AI in scientific research. Specifically, the proportion of articles mentioning AI in the ON field has shown a more significant increasing trend.

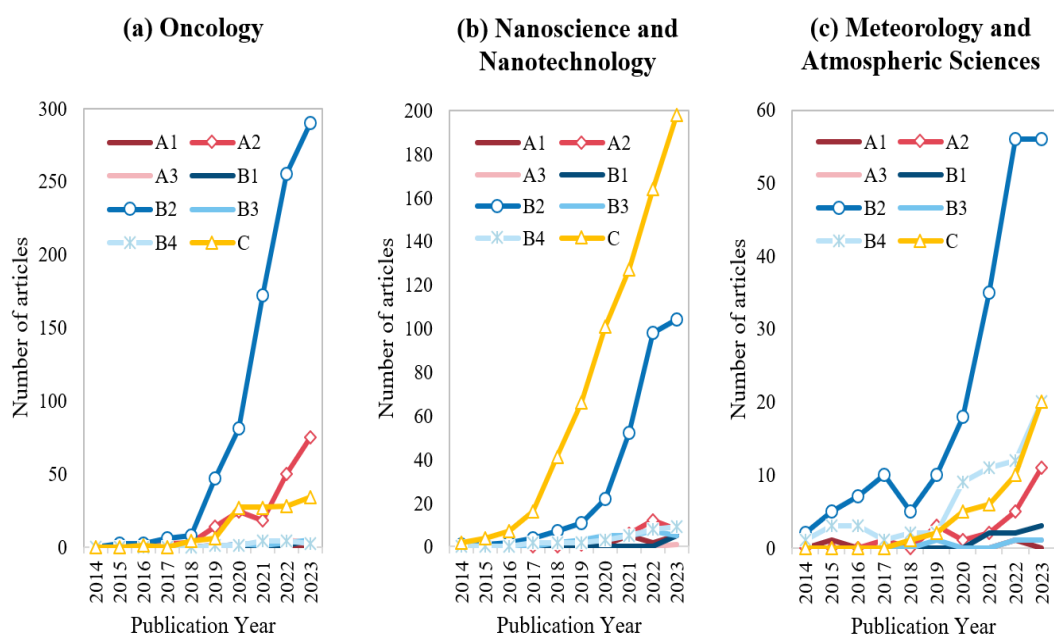


**Figure 1. Number of articles mentioning AI and their proportion within the total articles in the corresponding fields.**

Note: The full names and abbreviations of three fields are as follows – Oncology (ON), Nanoscience and Nanotechnology (NN), Meteorology and Atmospheric Sciences (MA).

When examining the different types of AI mentions, both commonalities and differences emerge across the three research fields, as shown in Figure 2. Our first observation is that the data representation is the primary way through which AI contributes to scientific research, with Type B2 articles accounting for 70%, 26% and 59% of the overall samples in the fields of ON, NN and MA respectively. At the same time, we observe that the ways AI is mentioned vary in emphasis across the three fields. Specifically, the ON field exhibits a relatively higher proportion of Type A2 research (15%), the NN field generates a substantial amount of Type C research (64%), and the MA field produces relatively more Type B4 research (18%).





**Figure 2. Number of articles with different AI-mention types in three research fields.**

### *Thematic features of AI mentions*

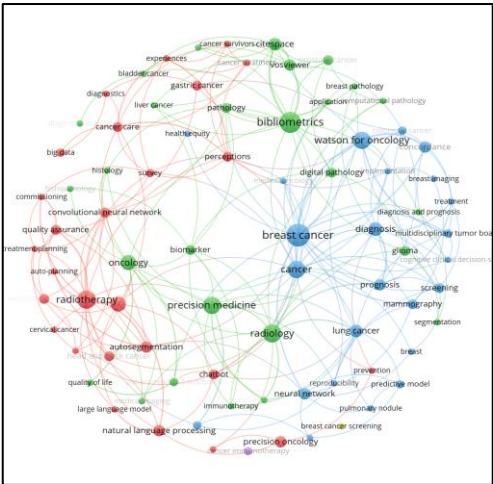
As AI is increasingly mentioned across a wide range of research articles, often by diverse ways, it is essential to investigate the specific problems these studies seek to address with the mention of AI. This section will analyze articles with representative types from three distinct fields, constructing keyword co-occurrence networks to identify and elucidate the core thematic features of these studies, as shown in Figure 3.

In the field of *Oncology* (ON), the primary focus is on Types A2 and B2. Type B2 constitutes the most prevalent category of articles within the field, whereas Type A2, though less dominant, exhibits a comparatively higher volume of publications relative to the other two fields. Type A2 (Science for the Application of AI) includes topics such as the bibliometric analysis on the research progress of AI usage in specific scenarios (green cluster), evaluating the effectiveness of AI applications (blue cluster), and investigating the attitudes of different stakeholders towards the use of AI (red cluster). These discussions aim to promote the more effective utilization of AI in real-world scenarios by examining the current status and impacts of AI usage. The prevalence of studies under this type reflects a cautious academic stance toward the application of AI in areas involving human health and life. Type B2 (AI for Data Representation) includes topics such as disease identification and classification (red cluster), organ segmentation (blue cluster), and tumor metastasis prediction (green cluster), primarily focused on medical image analysis and processing. The concentration on this type highlights that the ways of applying AI in oncology research are still relatively narrow in scope.

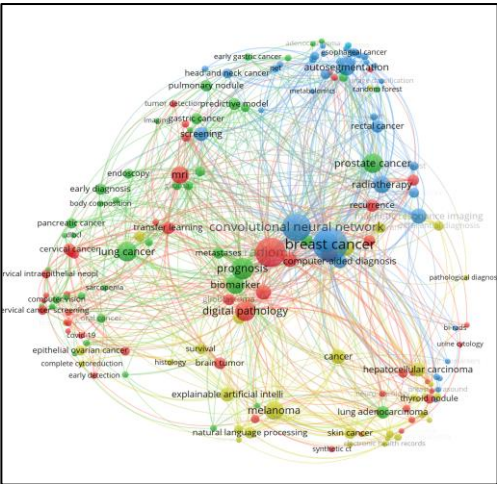
In the field of *Nanoscience and Nanotechnology* (NN), the primary focus is on Types B2 and C. These two types are the most prevalent categories of articles in this field, with the number of articles with the Type C being particularly prominent. Type B2 (AI for Data Representation) includes topics such as motion, odor and status detection (blue cluster), material structure analysis (green cluster) and related areas, though the topics in this category tend to be fragmented. In contrast, Type C (AI without a clear role in the research) encompasses topics such as artificial synapses (yellow cluster), memristors (blue cluster) and flexible materials (red cluster), with these technologies playing a significant role in advancing AI. For example, research on flexible materials can enhance the application of AI in sensor devices. Keyword analysis of a substantial body of Type C research reveals that the NN field is underpinned by robust foundational support, positioning it as a fundamental area within basic research for the development of AI. The inclusion of AI in studies within this field highlights the bidirectional relationship between AI and interdisciplinary knowledge, demonstrating how AI not only integrates insights from various disciplines but also drives the advancement of multiple fields.

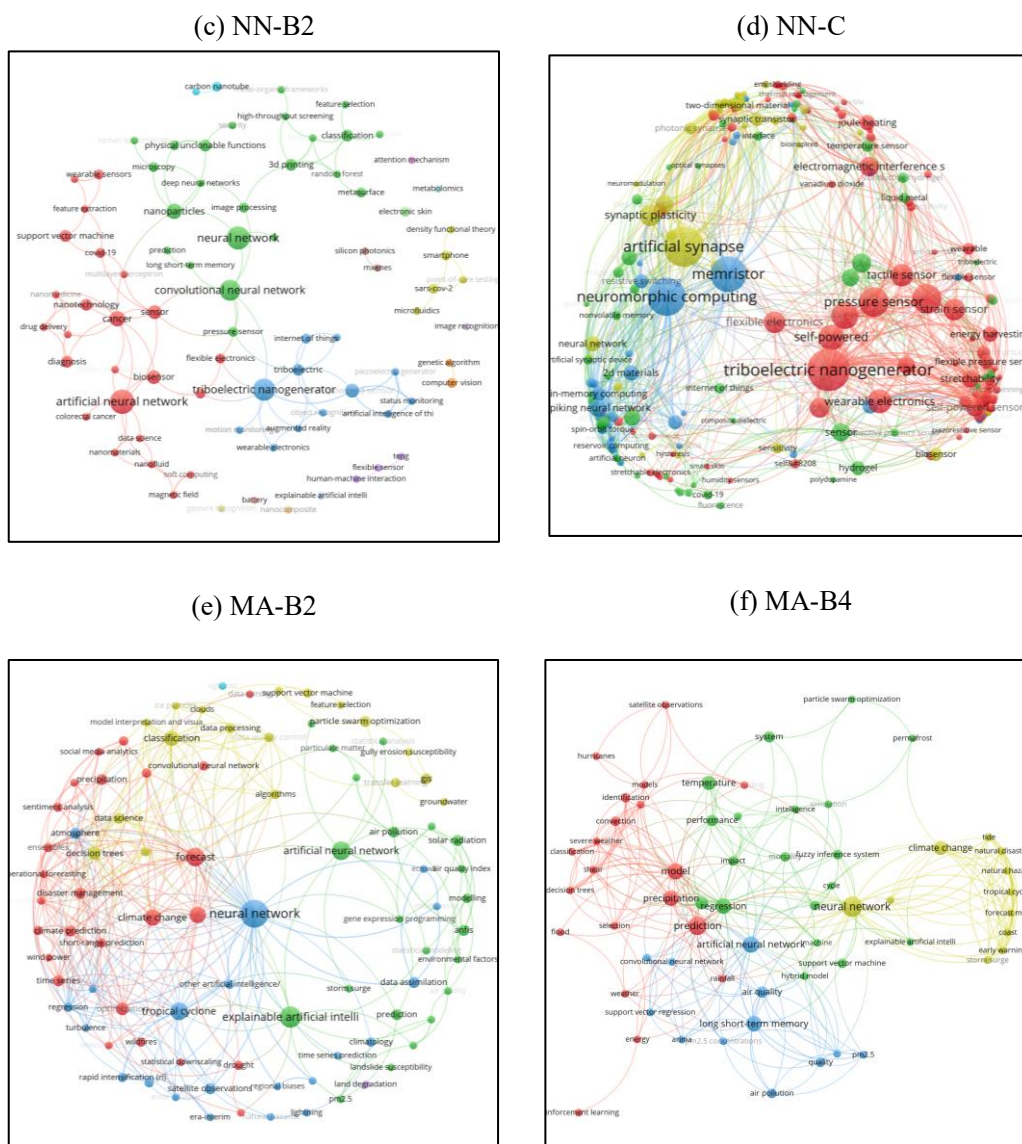
In the field of *Meteorology and Atmospheric Sciences* (MA), the primary focus is on Types B2 and B4. While Type B2 (AI for Data Representation) represents the most prevalent category of articles within the field, Type B4 (AI for Simulation) exhibits a comparatively higher volume of publications relative to the other two fields. The topics arising from these two types of research are relatively consistent, both addressing issues such as weather forecasting (blue cluster in subgraph (e) and green cluster in subgraph (f)), disaster management (red clusters in subgraphs (e) and (f)), and air quality monitoring (green cluster in subgraph (e) and blue cluster in subgraph (f)). However, given the specialized nature of these topics, AI can contribute to addressing specific challenges through a range of methodologies, including data representation and simulation techniques. This underscores the diverse and multifaceted enabling capabilities of AI in advancing research within the MA field.

(a) ON-A2



(b) ON-B2



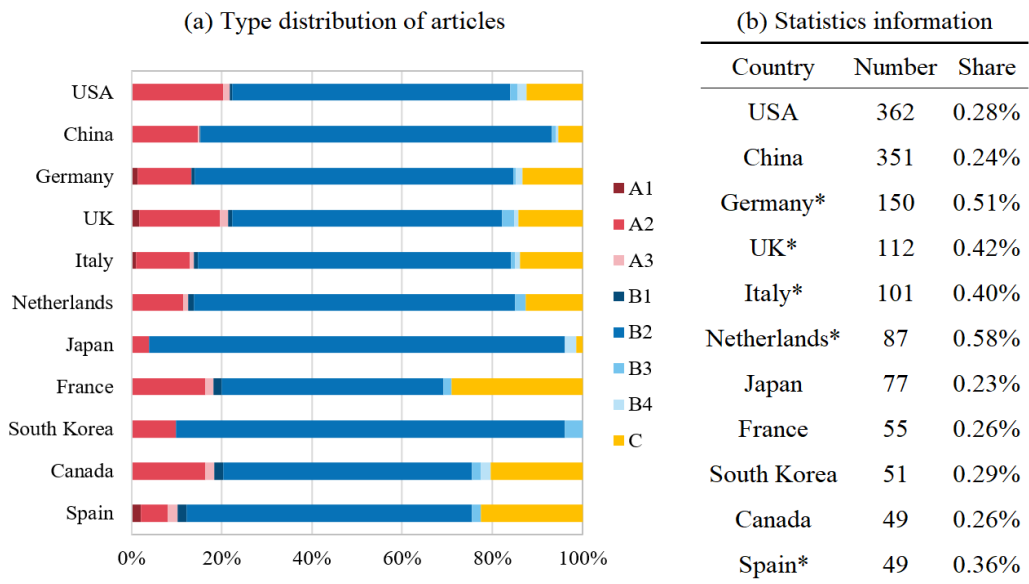


**Figure 3. Keyword co-occurrence networks of articles with different types in three research fields.**

Note: (1) The network is constructed using the VOSViewer software. (2) The nodes represent keywords; the size of each node indicates the frequency of keyword occurrence; nodes with different colors belong to different topic clusters; the thickness of the edges between nodes reflects the frequency of keyword co-occurrence. (3) Due to the limited number of articles with Type B4 in the MA field, Subgraph (f) uses both author keywords and WoS supplementary keywords, while the other subgraphs rely solely on author keywords. (4) The terms “artificial intelligence”, “machine learning” and “deep learning”, which are frequently occurring and highly generalizable technical keywords, are excluded to prevent overshadowing other thematic terms in the network.

*Actor characteristics of AI mentions*

Up to this point, we have observed that AI has been mentioned in research articles focused on various topics in different ways. The next question that arises is: who is conducting these studies? This section will examine the actor characteristics at the national level, with the aim of exploring the differences and similarities in the extent and specific ways that AI is mentioned in research articles across different countries. Figure 4 presents the distribution of the types of articles mentioning AI that were published in the field of *Oncology* (ON) by the eleven largest contributing countries<sup>2</sup>, along with the proportion of articles mentioning AI within the total of articles from each country in the corresponding field. Our first observation is that, compared to countries such as the United States, the United Kingdom and Canada, which place greater emphasis on conducting research for advancing AI, countries like China, Japan and South Korea focus more on the specific utilization of AI in scientific research, with a more concentrated distribution of AI mentions within the Type B2. Our second observation is that, although China and the United States have the highest number of articles mentioning AI, European countries such as Germany, the United Kingdom, Italy, the Netherlands and Spain have higher proportions of articles mentioning AI in their total oncology articles.



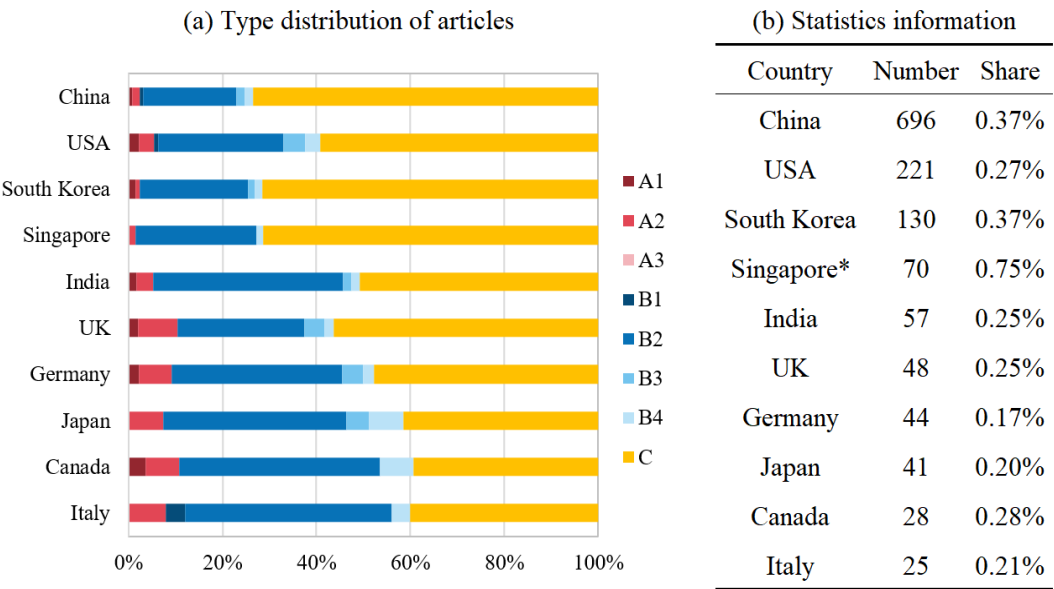
**Figure 4. Number, distribution of types and share in all articles in the ON field of the largest contributing countries.**

Note: \* indicates that the proportion of articles mentioning AI in the total publications of the country is relatively prominent among all countries.

<sup>2</sup> Canada and Spain are tied for tenth in the number of papers, so both have been included.

1518

Figure 5 presents the distribution of the types of articles mentioning AI published in the field of *Nanoscience and Nanotechnology* (NN) by the ten largest contributing countries, along with the proportion of articles mentioning AI within the total of articles from each country in the corresponding field. It is evident that Asian countries are particularly dominant in the number of articles mentioning AI within this field. In contrast to the ON field, countries with a high number of articles mentioning AI in the NN field tend to publish a greater proportion of Type C studies. These studies are more focused on advancing the field itself and only have an indirect connection to AI, suggesting that the high-ranking countries may exhibit stronger research capabilities within the NN field, rather than necessarily demonstrating superior expertise in leveraging AI for scientific research. However, it is worth noting that Singapore distinguishes itself with the highest proportion of articles mentioning AI in relation to its total articles in the NN field. This may be attributed to Singapore’s advanced information technology infrastructure and its prioritization of artificial intelligence (Zahra et al., 2021), which has facilitated considerable activity both in using AI for NN research and in conducting NN research to advance AI.



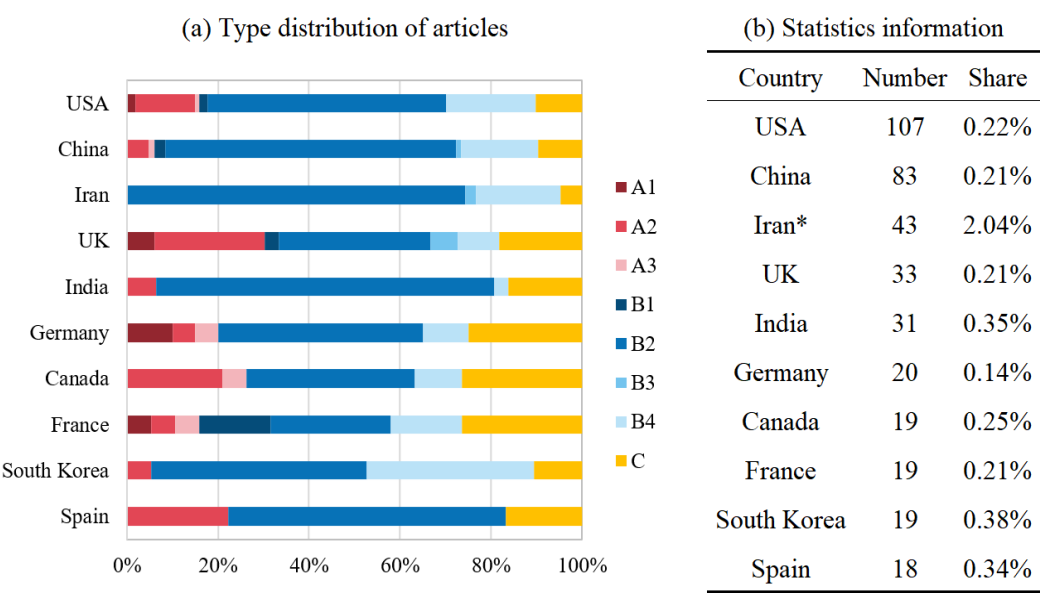
**Figure 5. Number, distribution of types and share in all articles in the NN field of the largest contributing countries.**

Note: \* indicates that the proportion of articles mentioning AI in the total publications of the country is relatively prominent among all countries.

Figure 6 presents the distribution of types of articles mentioning AI published in the field of *Meteorology and Atmospheric Sciences* (MA) by the ten largest contributing countries, along with the proportion of articles mentioning AI within the total of articles from each country in the corresponding field. An intriguing finding is that



Iran has published 43 articles mentioning AI, accounting for 12% of all articles mentioning AI in this field. Moreover, the proportion of articles mentioning AI among Iran’s total publications in this field is notably high (2%), significantly surpassing that of other countries. Furthermore, we conducted a search of Iran’s publications across all disciplines and found that articles mentioning AI make up only 3% of its total output. These findings indicates that the integration of AI in Iran’s MA research is exceptionally pronounced. Upon further examination of the thematic features of these studies, we found that they cover topics such as drought, flood and landslide prediction. However, the underlying factors contributing to Iran’s exceptional performance in MA articles mentioning AI warrant further investigation. In addition, the contrast between the greater emphasis on “Science for AI” in Western countries and the focus on “AI for Science” in Asian countries is also evident in MA research.



**Figure 6. Number, distribution of types and share in all articles in the MA field of the largest contributing countries.**

Note: \* indicates that the proportion of articles mentioning AI in the total publications of the country is relatively prominent among all countries.

### Conclusions and discussion

This study examines the bidirectional relationship between AI and science, using the frequency and context of AI mentions in research articles as a source of information. It constructs a classification framework for the various ways in which AI is mentioned in research articles, with the aim of providing a quantitative approach to elucidating the role of AI in scientific research. This framework contributes to a clearer understanding of the interactive relationship between AI and science, revealing that AI emerges from the cross-disciplinary integration of knowledge and,

in turn, empowers and enhances research across different academic fields in diverse ways.

We conducted empirical research in three representative fields of research. The findings indicate that the mentions of AI in research articles becomes increasingly prevalent but also varies across countries with different levels of research capacity, geographic locations, and national contexts. These differences not only reflect the unique characteristics of each country but may also offer insights into potential collaborations between nations in the scientific discovery in the age of AI.

A limitation in our study is that it is confined to analyzing mentions to AI within research articles, which may not fully encompass the diverse ways in which AI contributes to scientific research and vice versa. However, the inclusion of AI mentions in research articles reflects the forms of AI engagement in scientific research that are widely recognized and accepted within the academic community, thereby providing significant indications of the relationship between AI and science. Another limitation arises from the search terms used to identify articles mentioning AI, which were based primarily on general representations and did not explore specific AI sub-technologies commonly employed in particular research fields. A more thorough investigation into the characteristics of individual fields would enable us to conduct a more comprehensive search for AI-related research within those specific domains. Moving forward, we aim to improve the classification framework by observing a broader range of samples from additional fields, and develop approaches to achieve automatic annotation. It will facilitate the exploration of more nuanced patterns over extended time periods, across diverse domains, and within larger datasets.

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