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ROLE OF MACHINE LEARNING AND ORGANIZATIONAL STRUCTURE IN SCIENCE

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ABSTRACT

The progress of science increasingly relies on machine learning (ML) and machines work alongside humans in various domains of science. This study investigates the team structure of ML-related projects and analyzes the contribution of ML to scientific knowledge production under different team structure, drawing on bibliometric analyses of 25,000 scientific publications in various disciplines. Our regression analyses suggest that (1) interdisciplinary collaboration between domain scientists and computer scientists as well as the engagement of interdisciplinary individuals who have expertise in both domain and computer sciences are common in ML-related projects; (2) the engagement of interdisciplinary individuals seem more important in achieving high impact and novel discoveries, especially when a project employs computational and domain approaches interdependently; and (3) the contribution of ML and its implication to team structure depend on the depth of ML.

KEYWORDS

Team science; Machine Learning; Boundary Spanner; Collaboration; Artificial Intelligence; Interdisciplinary science

INTRODUCTION

Scientific knowledge shapes the foundation of the modern society, contributing to economic, social, and technological progress (Nelson, 2004; Stephan, 1996). The progress of science relies on various technical bases such as experimental techniques (Stephan, 2012: Ch.5). Among others, computational techniques play a crucial role in various parts of scientific research (Ding et al., 2010; Langley, 2000), and their role has been becoming more fundamental especially with the advancement of artificial intelligence, or more specifically machine learning (ML) (Cockburn et al., 2019).

Increasing examples have been reported in various domains, in which machines work alongside humans to push forward the progress of science (de Cock Buning 2017). For example, in life sciences, protein-protein interactions are predicted to understand disease mechanisms (Zeng et al., 2017); in chemistry, optimal chemical reaction paths are predicted (Service, 2017); and in material sciences, physical properties of new materials are predicted (Tshitoyan et al., 2019). These examples are characterized by ML, in which well-trained algorithms engage in complex tasks and directly contribute to making discoveries but not only merely automating the work process.

As contemporary science is usually based on a team activity (Wuchty et al., 2007), the integration of machine as a creative agent can influence the optimal design of work and organizations (King et al., 2009; Seeber et al., 2020; Yachie et al., 2017). While the interaction between human and machine has been studied at a micro (cognitive) level (Langley, 2000) or a at a macro level (Cockburn et al., 2019), the literature has been rather silent as to the role of machine in organization design (Orlikowski and Scott, 2008). Though a few studies described the patterns of collaboration (e.g., international vs. domestic collaboration) in ML-related projects (Hu et al., 2020; Xin et al., 2021), no previous study to the best of our knowledge has investigated the impact of ML on the organizational design of scientist teams. This study thus aims to investigate the team structure of ML-related projects and analyze the contribution of ML to the scientific knowledge production under different team structure.

To this end, we draw on bibliometric analyses. Our primary interest is how computational science techniques are integrated into the fields of conventional domains of science ("*domain science*" hereafter). Namely, our analysis includes six domains – agriculture, biology, chemistry, material sciences, medicine, and physics. To highlight the role of machine, we exploit a comparative approach, contrasting (1) ML-related projects (combination of computational and domain sciences) and (2) ML-unrelated projects (pure domain sciences). We collected approximately 2,500 ML-related and 22,000 ML-unrelated scholarly publications. With bibliometric and text analyses, we operationalized key variables of our interest. We investigated the quality (citation *impact* and *novelty*) of publication output produced by research teams with different team characteristics. Our results suggest (1) that interdisciplinary collaboration between domain scientists and computer scientists as well as the engagement of interdisciplinary individuals who have expertise in both domain and computer sciences are common in ML-related projects, (2) that the engagement of interdisciplinary individuals seem more important in achieving high impact and novel discoveries, especially when a project employs computational and domain approaches interdependently, and (3) that the contribution of ML and its implication to team structure depend on the depth of ML, in particular deep learning being associated with greater impact but with lower novelty.

This paper is structured as follows. The next section reviews literature on the use of ML and on the organizational design of science. The following section outlines the method and data. Then, the results from bibliometric analyses are presented. The final section discusses the results and concludes.

LITERATURE REVIEW

Role of Machine in Science

Though the use of ML in science has substantially grown in the 2010s (Cockburn et al., 2019), computational techniques have long been playing critical roles in science (Gibson and Ermus, 2019). In empirically driven domains of science such as physics and biology, statistical approaches have been actively used (Traweek, 1988), and enhanced computational power contributed to the progress of these fields (Gustafsson, 2018: p.233-238). Further, data have been accumulated for collective use in various fields (e.g., genome data in life sciences, material data in materials science), and access to large-scale data facilitated data-driven approaches in these fields (Libbrecht and Noble, 2015). These technical bases coupled with algorithmic breakthrough in the 2010 have transformed ML into a practical tool (Deng et al., 2013; Yu et al., 2010). ML has been applied to tackle broad areas of problems from industry to academia, including autonomous driving, robotics, communications, manufacturing, and medical diagnosis (Alsamhi et al., 2019; Kunze et al., 2018; Schwarting et al., 2018; Sharp et al., 2018).

The technical core of ML is a model based on neural network, decision trees, and so forth (Winston, 1992). A model is trained by data and then applied to additional data to make predictions. In academic research, domain scientists exploit this prediction capability to predict scientific laws of their interest, such as optimal chemical reaction paths, physical properties of materials, and protein-protein interactions (Service, 2017; Tshitoyan et al., 2019; Zeng et al., 2017).

Empirical research usually involves iterated cycles of hypothesis formulation, data collection, and data analysis (Latour and Woolgar, 1979; Shibayama et al., 2015). Domain scientists can incorporate ML into different parts or stages of this process. For example, ML can be used in later stages – data are generated through non-computational approaches (e.g., experiment) and fed into ML. In this case, the output of ML may become findings reported in publications. Alternatively, ML can be used in earlier stages – a hypothesis is formulated based on machine prediction and is tested by non-computational approaches. In this case, the role of ML is more exploratory and its output may be less explicitly presented in publications. Finally, ML may be used for data collection, to automate the process of collecting, cleaning, and coding the data. In such cases, the use of ML improves the efficiency of scientific research but its role may be less apparent in publications.

Only few studies have investigated the impact of ML on scientific knowledge production (Bianchini et al., 2020), but we argue that ML can bring various values depending on how it is incorporated into a research process. At the most primitive level, ML may make scientific research more efficient and productive, for example when ML is used for automation. ML is also expected to improve the quality of information extracted from the data. By selecting a right model and carefully tuning it, scientists may be able to extract more accurate or precise information than simpler statistical approaches can do. Finally, most fundamentally, ML may help domain scientists reach a discovery beyond their cognitive capacity. As a result of rapid progress of science, fully mastering domain knowledge has become a challenge for human scientists (Bloom et al., 2020). Increasing specialization of science also has made it challenging to integrate knowledge in multiple domains, even though such is an important route for scientific discoveries (Uzzi et al., 2013). With the computer processing power, ML may help overcome these challenges attributed to the limit of human cognition.

Organization of Science and Role of Machine

For fulfilling these values of ML in domain science, the expertise in computational science and that in domain science need to be integrated. ML algorithms may be able to improve themselves automatically through the use of data (Mitchell, 1997), and this autonomous nature makes machine a creative agent. Yet, machine requires a substantial care by human scientists, who develop, run, and assess a model as well as interpret output generated by the model (Deng et al., 2013; Langley, 2000). This process requires both the knowledge of domain science and that of computer science. In fact, a bibliometric analysis found that the vast majority of ML-based research involves collaboration (Hu et al., 2020), implying the integration of two sets of expertise is a key to success.

The application of ML for domain science can be considered a case of interdisciplinary research (NAS, 2004; Sonnenwald, 2007). Previous studies discussed various challenges associated with interdisciplinary research (Porac et al., 2004; Rafols et al., 2012). The studies consistently suggested organizational challenges for example in coordination of tasks and in communication between diverse scientists, as well as in trust building which is critical to share insights and research findings among members. In applying computational techniques into other domains, the same organizational challenges have been suggested (Larson and Dechurch, 2020; Rudko et al., 2021; Warner and Wäger, 2019).

Scientist teams set up various organizational arrangement to overcome such challenges. One potential solution concerns the proximity of collocation. Previous studies evaluated the impact of proximity of team members on team performance in various contexts, by and large suggesting that proximity facilitates communication and thus performance (Hall et al., 2018). In the context of science, collaboration may occur in proximity (e.g., intra-organizational collaboration) or remotely (e.g., inter-organizational collaboration) (Hu et al., 2020; Iglic et al., 2017). As an extreme case of proximity in science, collaboration can occur within a lab. A lab is an organizational unit more permanent than a project team, and it offers the organizational basis for scientific activities in traditional university systems (Carayol and Matt, 2004; Latour and Woolgar, 1979; Shibayama et al., 2015). Recent years have seen interdisciplinary labs being formed so that multiple disciplines can interact effectively (Bachnak and Steidley, 2002; Van Hecke et al., 2002). Apparently, effective and dense communication is expected among lab members who share the workspace on a daily basis. For example, members can monitor one another, which may allow a member to detect a problem that another member struggles with and quickly find a solution to it (Shibayama et al., 2015; Teasley et al., 2002).

As another route to tackle interdisciplinary research challenges, individual scientists may acquire expertise of multiple domains. If an individual scientist has skills both in computer science and in domain science, the aforementioned organizational challenges can be resolved within him/herself. In fact, some areas of domain science recognized the promising power of computational techniques and actively incorporated computational science, such as bioinformatics in the biology domain (Ditty et al., 2010). These domains tend to offer a curriculum to train for computational techniques, which systematically develops interdisciplinary scientists at the intersection of domain and computer sciences. This is becoming common, as computational techniques are increasingly available from external sources such as publicly shared codes and commands implemented in software, and thus, the skill requirement on computer science may be lowered.

Such interdisciplinary individuals can also play a boundary spanner role, who mediates members of different expertise (Bruns, 2013; Fleming and Waguespack, 2007). They translate the languages of domain scientists and computer scientists and facilitate their integration. Thus, the organizational challenges in interdisciplinary research are alleviated, which helps achieve expected interdisciplinary output (Leahey et al., 2017).

Among these organizational arrangements, the optimal form may depend on how computer science expertise is applied to domain science, or on the interdependency of the two areas of tasks (Benishek and Lazzara, 2019). On the one hand, task interdependency can be high if the output of domain science tasks is used as the input of computer science tasks, or vice versa. The two areas of tasks may be even repeated in an iterative way. In such a scenario with high task interdependency, organizational arrangement for interdisciplinary integration is expected to be more important. On the other hand, task interdependency can be low if the two areas of tasks are modularized. For example, computer scientists may apply their ML models to publicly available data from domain sciences. Domain scientists may use ML only for data preparation (cleaning, etc.) or may use established ML algorithms. In these cases, the interface between the two areas of tasks is minimized, and thus, the above discussed organizational arrangement becomes less relevant.

In summary, we hypothesize that scientist teams with such features that help integrate computer expertise and domain expertise, including collaboration in proximity and interdisciplinary individuals, tend to produce high-quality output, and that the features are more important when the computer-related tasks and domain tasks are interdependent.

METHODS AND DATA

Data

To test our hypotheses, we draw on bibliometric data collected from Web of Science (WoS).[1] Our primary interest is in the integration of computational science (ML) and domain science. To highlight the contribution of ML, we draw on a comparative approach, contrasting (1) ML-related projects (combination of computation and domain sciences) and (2) ML-unrelated projects (purely domain science). The unit of analysis is a project team, which is operationalized by a group of authors of a publication.

We employ the following sampling strategy. First, we chose six domains – agriculture, biology, chemistry, material sciences, medicine, and physics. The selection of these domains is based on WoS Subject Categories (SC). We chose 20 SCs in total within these domains (see Appendix 1).

Second, in these domains (SCs), we aimed to choose journals that are as mono-disciplinary as possible for two reasons. First, this is to lower the risk of sampling ML-related projects that are unrelated to domain science. We assume that mono-disciplinary journals set a clear scope of publication, with such a risk being mitigated. Second, to clarify the impact due to the integration of computer science and domain science, we minimized noise stemming from interdisciplinarity within a domain. To these ends, we chose up to five journals in each SC that are associated with a single SC (not associated with any other SC).

Third, in these journals we selected two sets of papers, ML-related and ML-unrelated. We first searched for ML-related papers with "machine learning", "deep learning", and "artificial intelligence" as search keywords, which resulted in 2,500 papers.[2] The majority of these papers were published in the last four years (Figure 1).

Next, we collected ML-unrelated papers that include none of the ML-related keywords. For clearer comparison, for each ML-related paper, we randomly selected up to 10 ML-unrelated

[1] To help interpret the result from the bibliometric analyses, we also interviewed two scientists employing both machine learning and conventional scientific approaches.
[2] We focus on papers whose document type is "Article", "Letter", or "Proceedings Paper" and whose language is English.

papers published in the same journal and in the same year. We found 22,300 ML-unrelated papers. In total, we sampled 25,000 papers with 10% of ML-related papers.

Measures

ML-related project. Part of the following analyses compare ML-related papers and ML-unrelated papers. For this comparison, we prepared a dummy variable, coded 1 if a paper is ML-related (i.e., including "machine learning", "deep learning", "artificial intelligence") and 0 otherwise (*ML-related*).

Scientific quality. As the dependent variables of our analyses, we prepared two measures of scientific quality. First, we use the citation count as of 2021 to assess the impact of the findings reported in the paper. To mitigate the skewness, we took a natural logarithm of citation count (*Impact*).

Second, we measure the novelty of a paper. This is because we are interested in to what extent ML contributes to creating new knowledge beyond human cognition. We drew on the recombinant novelty concept (Fleming, 2001; Uzzi et al., 2013) and followed the operationalization by Matsumoto et al. (2021). The method considers a paper to be novel when it cites a pair of references that have rarely been cited together before. For easier interpretation we transformed the measure into a rank measure so that its values uniformly distribute between 0 and 1, with 0 being the least novel and 1 being the most novel (*Novelty*).[3]

Team size. We prepared several variables concerning the structure of scientist teams. As the base characteristic of a team, we first measured the team size. We counted the number of authors of each paper (*#Author*), the number of organizations (university, firms, etc.) included in the author address (*#Org*), and the number of countries included in the author address (*#Country*).

Form of collaboration. Second, since we are interested in the integration of computational expertise and conventional expertise, we investigated the forms of collaboration. To this end, we scrutinized the names of authors' affiliated organizations to distinguish if an organization has a computational background or not. Then, we consider an organization to be computational if the name includes "computation", "information", or "system", and we consider an

[3] We were unable to compute this variable for part of our sampled papers due to lack of access to citation network information. The regression analyses on novelty thus draws on a subset (67%) of our sample.

organization to be in a traditional domain if the name includes none of them.[4] Using this distinction of organizations, we prepared three variables. We first measured if a team involved both computational and domain organizations (instead of involving only domain organizations). A dummy variable is coded 1 if at least one affiliated organization is computational and 0 otherwise (*Comp-Domain Collab*). To further investigate the proximity in collaborating parties, we examined whether a team involved computational and domain organizations inside the same parent organization (i.e., a computational department and a domain department in the same university). In such teams, a dummy variable is coded 1 and otherwise 0 (*Intra-Org Collab*). Similarly, if a team involved computational and domain organizations in two different organizations, another dummy variable is coded 1 and otherwise 0 (*Inter-Org Collab*). Note that one team can involve both intra-organizational collaboration and inter-organizational collaboration.

Interdisciplinary individuals. Third, we measured whether an individual team member has both computational and domain expertise in two ways. One measure is based on organizational affiliation. If an individual member of a team (an author of a paper) is affiliated to both computational and domain organizations, we consider that the member has both computational and conventional expertise and plays a boundary spanner role at the individual level. A dummy variable is coded 1 if a team has at least one author affiliated to both types of organizations and 0 otherwise (*Multi-Affiliation*). The other measure is based on previous experience of individual members. For feasibility, we focused on the corresponding author of each paper and tracked WoS Subject Categories (SCs) associated to their previous publications. We grouped SCs into computer-related and domain-related SCs,[5] and coded a dummy variable 1 if previous paper is associated with both a computer-related SC and a domain-related SC, and 0 otherwise (*Multi-Expertise*).[6]

Interdependency of computer and domain science. ML may be used in different ways in domain sciences. We sampled ML-related papers[7] and categorized them into two groups by reading the method section of the papers. The first group of papers integrates both

[4] In this analysis we disregard the types (universities, firms, etc.) of organizations, but such distinction is of interest for future research. For example, industries and universities may use ML differently.
[5] Computer-science-related SCs are all SCs including "Computer Science", "Mathematical & Computational Biology", and "Information Science & Library Science"
[6] Preparing this variable requires at least one previous publication. The corresponding authors of 18% of our sampled papers had no previous publications and are excluded from regression analyses.
[7] We used only a subset of ML-related papers for this variable because this categorization requires access to the full text of the papers.

computational approaches and domain approaches (e.g., experiment, observation), whereas the second group uses mainly computational approaches, typically based on secondary data.[8] We assume that this is a critical distinction in that the former group (*Computer-Domain Integrated*) should require a greater extent of integration between computer and domain expertise compared with the latter group (*Computation-Focused*).

Depth of ML. ML can mean various technologies. In fact, common technical keywords in our selected papers include, for example, "neural network", "classification", "regression", "support vector machine", and "random forest." Some of these have been used traditionally (e.g., regression analyses). To highlight the impact of machines, we attempted to differentiate the complexity or the depth of models on which ML is carried out. Hence, we aim to contrast "deep" learning (DL) and "non-deep" learning (non-DL). This is because the distinction should affect the computer-science expertise required in a team, and because deeper learning might provide new values for science beyond what traditional statistical techniques can do. Making this technical distinction based on text information is challenging because papers do not always describe the ML model in detail. For feasibility, we consider that a project involved DL if a paper includes "deep learning" or "neural network" in the abstract or in the keywords (*DL-related*).[9]

Other variables. In the regression analyses, we include publication year dummies as well as journal dummies. Part of the following analyses are broken down by countries and fields. As for countries, we distinguish seven major countries: the USA, Canada, the UK, Germany, France, Japan, and China. As to fields, we used the aforementioned six fields: agriculture, biology, chemistry, material sciences, medicine, and physics (Figure 2). Table 1 presents the descriptive statistics and correlation matrix of all the variables.

RESULTS

Description of Team Structure

We first analyze whether ML-related projects exhibit different organizational features than ML-unrelated projects.

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[8] We also identified a few review papers that involve neither computational nor domain approaches and excluded them from this categorization.
[9] The use of "neural network" can be misleading as "neural network" may be shallow.

Team size. Figure 3 first shows the team size of ML-related and ML-unrelated projects. We regressed the size variables on *ML-related* and other control variables. The top bars indicate that ML-related projects involve slightly fewer authors than ML-unrelated projects (5.3 vs. 5.5, p<.001). This may be because ML-related projects require less physical work, and thus, fewer members. The second bars, however, indicate that ML-related project involve more organizations (3.1 vs. 3.0, p <.05) probably because the ML-related projects tend to require a broader set of expertise (i.e., computational and domain). Finally, the bottom bars show no significant difference in the number of involved countries.

Collaboration form. Then, we analyze the collaboration forms between computational and conventional organizations (Figure 4). As expected, domain-computer collaboration is more common in ML-related projects than in ML-unrelated projects (39% vs. 15%, p<.001). Domain-computer collaboration is broken down into intra-organizational and inter-organizational collaborations, both of which are more common in ML-related projects (20% vs. 7%, p<.001 and 33% vs. 14%, p<.001).

Interdisciplinary individuals. Finally, Figure 5 compares ML-related and unrelated projects in terms of individual team members having both computational and domain expertise. The figure indicates that ML-related projects are more likely to involve one or more individuals who are affiliated to domain and computer departments (21% vs. 9%, p<.001). Similarly, ML-related projects are more likely to engage individuals who had previous experience in computer and domain sciences (38% vs. 13%, p<.001). These results indicates that ML-related projects do incorporate combination of computational and domain expertise.

Cross-national comparison. To investigate potential differences between countries, we present a breakdown by countries (Figure 6). Figure 6A indicates that the majority of ML-related papers are published by the USA (34%) and China (23%). Japan accounts for 4.4% of the all ML-related papers. Comparing with ML-unrelated papers, it is clear that the USA is leading ML-related research (the standardized ratio of ML-related to unrelated papers = 1.18). On the other hand, ML-related research accounts for a relatively smaller portion of entire research activities in Japan (ratio = 0.80) and France (ratio = 0.79). In terms of team size (Figure 6B), data suggest that the team size in Japan is relatively smaller than European counterparts but is comparable to the USA. In terms of interdisciplinary expertise (Figure 6D), Japanese scientists have lower levels of interdisciplinarity (i.e., more likely to specialize in either computer science or domain science).

Quality of Output from ML-related Projects

ML-related vs. ML-unrelated projects. Next, we analyze the quality of scientific output produced by ML-related and unrelated projects. We predicted citation impact and novelty by *ML-related* with controlling for the team size and other variables (Table 2A). Model 1 shows a significantly positive coefficient of *ML-related* (b = .481, p <.001), suggesting that ML-related papers tend to receive more citations than ML-unrelated papers. On the other hand, Model 2 finds no significant coefficient of *ML-related* (b = -.007, p >.1), suggesting that ML-related papers do not necessarily present novel discoveries. We further repeated the same set of analyses with a matching approach, in which ML-related papers are compared with ML-unrelated papers published in the same journal in the same year, finding a consistent result (Table 2B).

Team structure. We then examine how different collaboration forms affect the quality of publications from ML-related projects (Table 3A). First, Models 1-4 use citation impact as the dependent variable. Model 1 suggests that computer-domain collaboration is associated with higher citation impact (b = .112, p <.01). Breaking down such collaboration into intra-organizational and inter-organizational ones, Model 2 finds both coefficients weakly significant (b = .086, p<.1 and b = .069, p<.1). The result suggests no significant difference between the two forms of collaboration, and thus, proximity in collaboration does not seem to play a role in this context.

Model 3 further breaks down computer-domain collaboration into ones involving individuals affiliated to both computer and domain departments (*Multi-Affiliation*) and ones not involving such individuals (*Comp-Domain Collab without Multi-Affiliation*), finding that only the former group is associated with higher citation impact (b = .160, p <.001) but not the latter (b = .055, p>.1). This suggests that interdisciplinary individuals are important to achieve high citation impact. Similarly, Model 4 breaks down computer-domain collaboration into ones involving individuals having previous experience in computer and domain sciences (*Multi-Expertise*) and ones not involving such individuals (*Comp-Domain Collab without Multi-Expertise*). The result shows significantly positive coefficients for both variables (b = .119, p <.001 and b = .139, p <.001), suggesting that high citation impact requires either computer-domain collaboration or interdisciplinary individuals.

Models 5-8 repeat the same set of analyses with novelty as the dependent variable. The result presents no significant pattern, except that Model 4 shows that interdisciplinary individuals having both computer and domain science expertise are weakly associated with higher novelty ($b = .129$, $p <.1$).

These results seem to imply relatively greater importance of interdisciplinary individuals rather than interdisciplinary collaboration. Thus, we further test whether the role of interdisciplinary individuals is specific to ML-related projects. To this end, we compare the impact of *Multi-Affiliation* and *Multi-Expertise* between ML-related and ML-unrelated projects (Table 3B). In all four models, we find that the coefficients are larger for ML-related projects than for ML-unrelated projects. In particular, Model 1 shows that individuals having both computer and domain affiliations (*Multi-Affiliation*) are significantly associated with higher citation impact ($b = .120$, $p <.001$); and Model 4 shows that individuals having both computer and domain expertise (*Multi-Expertise*) are significantly associated with higher novelty ($b = .026$, $p<.05$).

Interdependency of computer and domain science. Next, we test whether the role of interdisciplinary individuals differs due to different uses of ML. Table 4 draws on the subsamples of ML-related projects – *computation-focused* projects (Models 1, 2, 5, and 6) and *computer-domain integrated* projects (Models 3, 4, 7, and 8) – and shows that both *Multi-Affiliation* and *Multi-Expertise* have significantly positive coefficients only in the latter group. This suggests that interdisciplinary individuals are particularly important when projects employ both computational and domain approaches interdependently.

We also ran the same models as in Table 3A with the computation-focused and computer-domain-integrated subsamples (Table S4) and confirmed that interdisciplinary individuals rather than interdisciplinary collaboration are important in the latter subsample.

Depth of ML. Finally, we break down ML technologies. In particular, Table 5A regresses the publication quality on *DL-related* in addition to *ML-related*. Model 1 shows that DL-related papers are even more cited compared to DL-unrelated papers ($b = .201$, $p <.001$). However, Model 2 indicates that DL-related papers are less novel compared to DL-unrelated papers ($b = -.054$, $p <.001$). Thus, it appears that DL does not necessarily allow scientists to gain novel insights beyond human cognition. DL rather seems to be applied to an agenda that humans have relatively good understanding (and thus lower novelty). Our interviewee suggested that DL tends to provide better model performance (e.g., accuracy, precision), facilitating further uses of DL models, which is consistent with the positive coefficient of DL-related on citation count (Model 1).

Table 5B further investigates the contribution of interdisciplinary individuals in DL-related and DL-unrelated projects by distinguishing computation-focused projects and computer-domain integrated projects. The result shows almost no effect of interdisciplinary individuals in computation-focused projects (Models 1, 2, 5, and 6), as in Table 4. In contrast, in computer-domain integrated projects, interdisciplinary individuals seem to play different roles between DL-related and DL-unrelated projects. In terms of citation impact, Models 3 and 4 show that interdisciplinary individuals are more important in DL-unrelated projects (but ML-related) than in DL-related projects. On the other hand, in terms of novelty, Models 5 and 6 show that interdisciplinary individuals are more important in DL-related projects than in DL-unrelated ones. A plausible interpretation is that greater novelty is rooted in inspiration from DL facilitated by the integration of computer and domain expertise, whereas greater citation results from higher model performance due to DL, which may not necessarily require the fundamental integration of computer and domain expertise.

DISCUSSION AND CONCLUSION

The progress of science increasingly relies on computational expertise and particularly on ML (Cockburn et al., 2019), and machines work alongside humans in various domains (de Cock Buning 2017). As the integration of machine as a creative agent in science can influence the optimal design of work and organizations (King et al., 2009; Seeber et al., 2020; Yachie et al., 2017), this study investigated the team structure of ML-related projects and analyzed the contribution of ML to scientific knowledge production under different team structure. Drawing on bibliometric analyses of 25,000 scientific publications in six domains, we found (1) that interdisciplinary collaboration and the engagement of interdisciplinary individuals are common in ML-related projects, (2) that the engagement of interdisciplinary individuals is associated with higher impact and novelty especially when a project employs computational and domain approaches substantially, and (3) that the contribution of ML and its implication to team structure depend on the depth of ML.

This study contributes to the literature by illustrating the role of machines in a scientist team. Previous literature on the use of machines has been either at a macro level (Cockburn et al., 2019) or at a micro (cognitive) level (Langley, 2000), with the meso-level discussion in scientist teams remaining to be understudied (Orlikowski and Scott, 2008). Although a few recent studies described the patterns of collaboration (e.g., international vs. domestic collaboration) in ML-related projects (Hu et al., 2020; Xin et al., 2021), our understanding has been scarce as to how ML affects the quality of scientific knowledge production under different organizational designs. Drawing on the literature of scientific collaboration and interdisciplinarity (Fleming and Waguespack, 2007; Latour and Woolgar, 1979; Rafols et al., 2012; Shibayama et al., 2015), we argue that team features that help integrate computer expertise and domain expertise are associated with higher output quality, and that these features are more important when the computer-related tasks and domain tasks are interdependent. Our empirical analyses support this hypothesis.

A potential challenge in integrating computer and domain sciences is lack of incentive. While our analysis shows that interdisciplinarity contributes to higher impacts and novelty, it is not obvious whether scientists with computational expertise and those with domain expertise are willing to work together. In fact, our interview suggested that scientists working on ML tended to appreciate publications in computer science rather than publications in other fields. It is also suggested that domain scientists do not always appreciate research approaches based upon ML because it is difficult to explain how prediction is made by a model that could be considered a black box. It is thus critical to understand what motivates ML scientists to collaborate with domain scientists and what obstacles exist in their collaboration.

It is particularly interesting to find that ML can contribute to the *novelty* of scientific discoveries with the engagement of interdisciplinary individuals. Our empirical work further suggests that interdisciplinary individuals are critical in delivering novel discoveries based on deeper ML (DL). ML can bring various values, such as efficiency of data analysis or greater precision of model prediction. However, supplementing humans' cognitive capacity and delivering novel discoveries is a fundamental benefit of machines under the burden of knowledge (Bloom et al., 2020). Our result highlights a critical role played by interdisciplinary individuals in achieving novelty. Thanks to the continued advancement of computational science, more sophisticated and potentially more complex and deeper ML approaches are likely to become available for domain scientists. Our result implies that engaging interdisciplinary individuals is crucial in exploiting the full capacity of computational techniques. Indeed, our interviewee referred to a critical "liaison" role played by a scientist who studied computer science and genetics in a project utilizing ML for detecting cancers. Such interdisciplinary scientists may begin their careers either as domain scientists or as computer scientists. For example, domain sciences have invested in computational techniques (e.g., bioinformatics) to systematically train interdisciplinary scientists (Ditty et al., 2010). Our cross-national comparison shows that interdisciplinary individuals are more common in some countries than others, suggesting that the latter countries need to further invest in training interdisciplinary scientists who can integrate computer and domain sciences (e.g., support for educational programs).

Our results need to be interpreted with a few limitations. First, our bibliometric approach cannot fully capture how machines are used and how teams are formed. Future research should look into more detailed or precise information. Second, we have to be cautious about potential changes in the role of machines over time. The vast majority of our sampled papers were published in the last four years (2017-2021) because ML is a rather recent phenomenon. The role of machines and how it affects the team design might change in the future with the advancement of computational techniques. Third, our results are based on cross-sectional analyses, and thus, the causal mechanism behind our findings cannot be completely clear.

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FIGURES AND TABLES

Figure 1 **Publication year of ML-related papers**

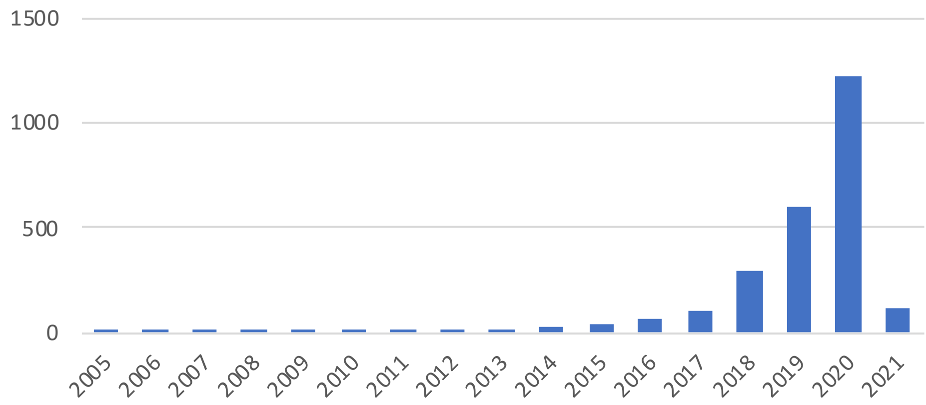


Figure 2 **Distribution across disciplines**

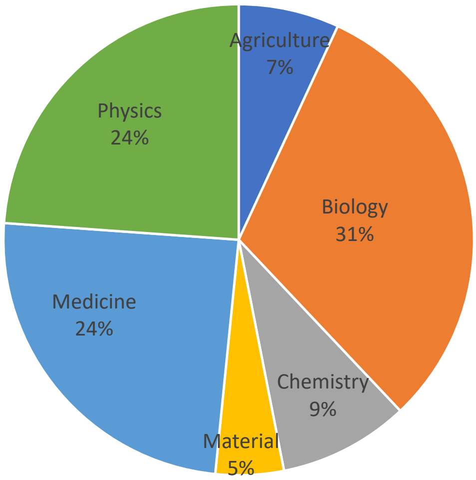
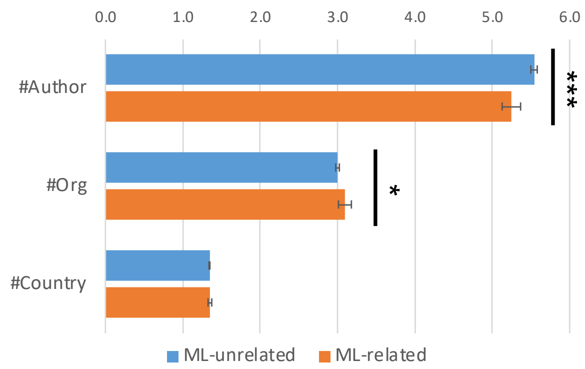
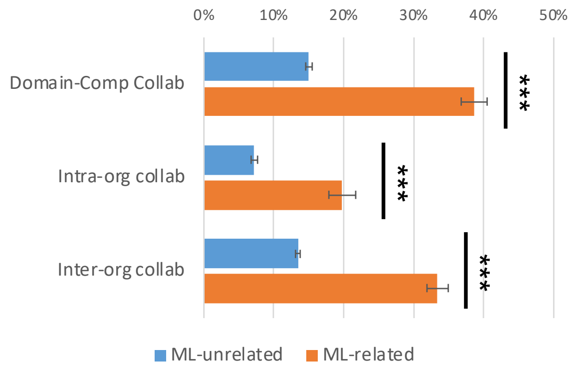


Figure 3 Team Size



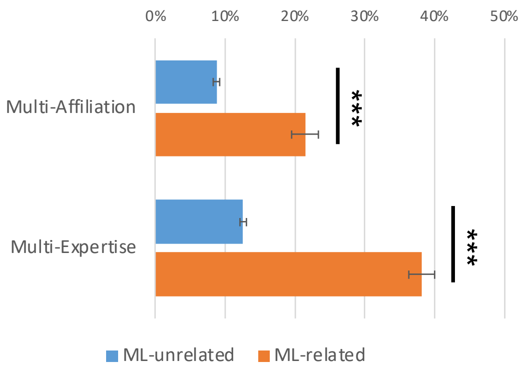
Notes: Team size is estimated by ordinary least squares (OLS) regressions controlling for publication years and journals (see Table S1). The error bars indicate one standard error. Two-tailed test: $^{*}p<0.05$, $^{***}p<0.001$.

Figure 4 Collaboration Form



Notes: Collaboration forms are estimated by logit regressions controlling for publication years and journals (see Table S2). The error bars indicate one standard error. Two-tailed test: $^{***}p<0.001$.

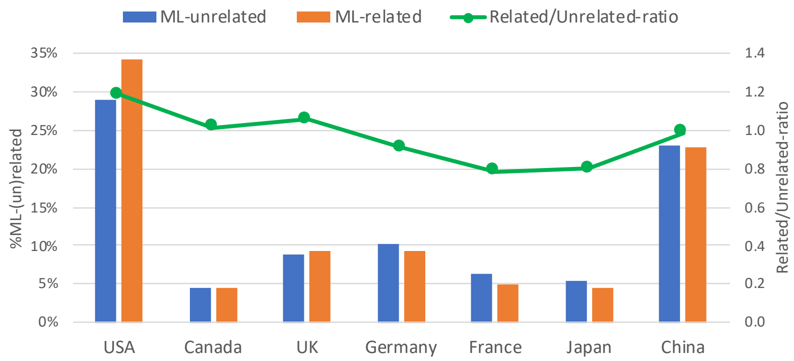
Figure 5 Interdisciplinary Expertise



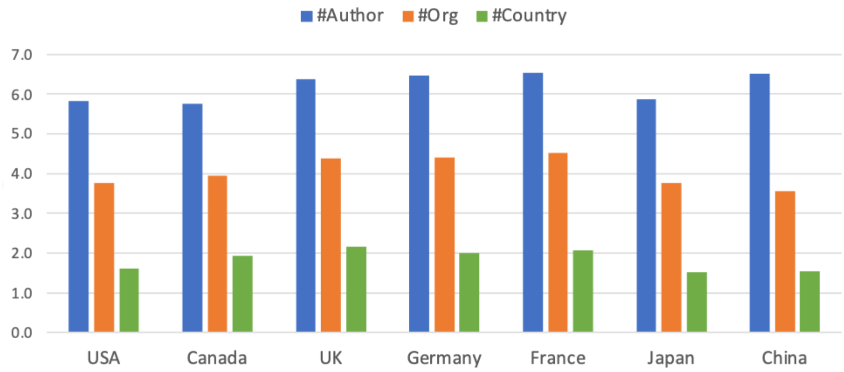
Notes: Collaboration forms are estimated by logit regressions controlling for publication years and journals (see Table S3). The error bars indicate one standard error. Two-tailed test: ***p<0.001.

Figure 6 Cross-National Comparison

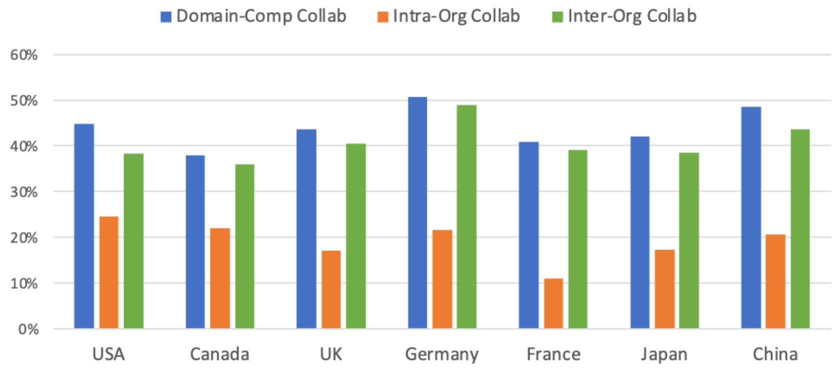
(A) Proportion of country



(B) Team size



(C) Collaboration form



(D) Interdisciplinary Expertise

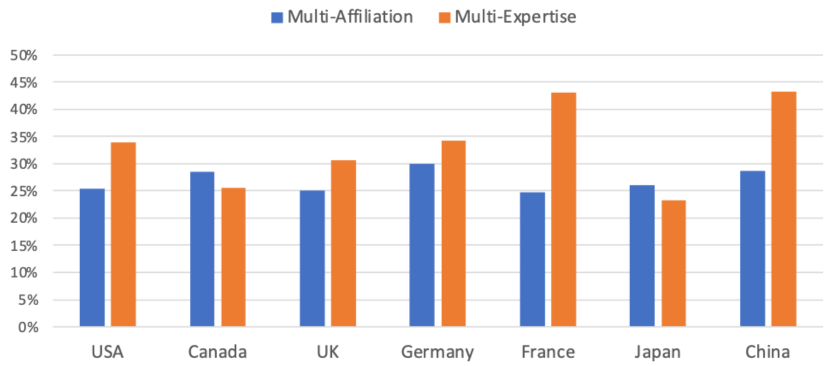


Table 1 **Descriptive Statistics and Correlation Matrix**

	Variables	Mean	S.D.	Min	Max	1	2	3	4	5	6	7	8	9	10	11
1	Impact	1.010	1.180	.000	8.220											
2	Novelty	.500	.290	.000	1.000	-.053										
3	Ln(#Author)	1.710	.680	.000	5.200	.078	.071									
4	Ln(#Org)	1.100	.730	.000	5.180	.071	.049	.668								
5	Ln(#Country)	.300	.460	.000	3.300	.095	.008	.327	.515							
6	Comp-Domain Collab	.170	.380	.000	1.000	.070	.011	.105	.256	.152						
7	Intra-Org Collab	.080	.280	.000	1.000	.064	.023	.103	.212	.045	.660					
8	Inter-Org Collab	.150	.360	.000	1.000	.064	.010	.124	.274	.193	.932	.515				
9	Multi-Affiliation	.100	.300	.000	1.000	.071	.019	.075	.226	.131	.727	.582	.684			
10	Multi-Expertise	.150	.360	.000	1.000	.017	-.018	-.131	-.044	.015	.227	.142	.210	.161		
11	ML-related	.100	.300	.000	1.000	.095	.005	-.030	.009	-.010	.192	.134	.171	.130	.230	
12	DL-related	.040	.200	.000	1.000	.046	-.020	-.030	-.020	-.014	.130	.082	.117	.086	.156	.601

Notes: N = 24,641 (except for N = 16,440 for Novelty).

Table 2 Prediction of Publication Quality: ML-related vs. ML-unrelated Projects

(A) Base Model

	Impact		Novelty	
	Model 1		Model 2	
ln(#Author)	.172***	(.010)	.019***	(.005)
ln(#Org)	.015	(.009)	.006	(.004)
ln(#Country)	.081***	(.011)	-.005	(.005)
ML-related	.481***	(.014)	-.007	(.006)
Year dummies	Yes		Yes	
Journal dummies	Yes		Yes	
F stat	504.299***		37.187***	
R2_adjusted	.660		.172	
N	24641		16433	

Notes: Unstandardized coefficients (standard errors in parentheses). Two-tailed test: ***p<0.001. Ordinary least squares (OLS).

(B) Matched Sample

	Impact		Novelty	
	Model 1		Model 2	
ln(#Author)	.162***	(.009)	.018***	(.005)
ln(#Org)	.013	(.009)	.009*	(.004)
ln(#Country)	.067***	(.011)	-.006	(.005)
ML-related	.496***	(.016)	-.001	(.008)
F stat	242.001***		155.908***	
R2_adjusted	.828		.797	
N	24405		15938	

Notes: Unstandardized coefficients (standard errors in parentheses). Two-tailed test: ***p<0.001. Ordinary least squares (OLS). ML-related papers are paired with ML-unrelated papers published in the same journal in the same year.

Table 3 Prediction of Publication Quality by Team Structure

(A) ML-related Projects Only

	Impact								Novelty							
	Model 1		Model 2		Model 3		Model 4		Model 5		Model 6		Model 7		Model 8	
ln(#Author)	.111**	(.037)	.111**	(.037)	.111**	(.037)	.106*	(.042)	-.015	(.013)	-.015	(.013)	-.013	(.013)	-.013	(.015)
ln(#Org)	.006	(.037)	.002	(.038)	.010	(.037)	.053	(.039)	.032*	(.013)	.030*	(.013)	.026*	(.013)	.014	(.013)
ln(#Country)	.144***	(.044)	.149***	(.044)	.134**	(.044)	.100*	(.048)	-.003	(.015)	-.000	(.015)	-.003	(.015)	.000	(.016)
Comp-Domain Collab	.112**	(.037)							-.000	(.013)						
Intra-org Collab			.086+	(.048)							.016	(.016)				
Inter-org Collab			.069+	(.041)							-.008	(.014)				
Multi-Affiliation					.160***	(.046)							.018	(.016)		
Comp-Domain Collab without Multi-Affiliation					.055	(.046)							-.018	(.016)		
Multi-Expertise							.119**	(.044)							.029+	(.015)
Comp-Domain Collab without Multi-Expertise							.139**	(.053)							-.012	(.018)
Year dummies	Yes		Yes		Yes		Yes		Yes		Yes		Yes		Yes	
Journal dummies	Yes		Yes		Yes		Yes		Yes		Yes		Yes		Yes	
F stat	42.830***		42.366***		42.394***		31.752***		5.987***		5.935***		5.713***		5.254***	
R2_adjusted	.611		.611		.606		.587		.180		.180		.172		.185	
N	2530		2530		2505		2034		2137		2137		2117		1724	

(B) ML-related vs. ML-unrelated Projects

	Impact				Novelty			
	Model 1		Model 2		Model 3		Model 4	
ln(#Author)	.171***	(.010)	.161***	(.011)	.020***	(.005)	.024***	(.005)
ln(#Org)	.009	(.009)	.013	(.010)	.005	(.004)	.002	(.005)
ln(#Country)	.081***	(.011)	.070***	(.012)	-.004	(.005)	-.000	(.006)
ML-related	.460***	(.016)	.464***	(.020)	-.010	(.007)	-.013	(.009)
Multi-Affiliation (ML-unrelated)	.006	(.017)			.003	(.008)		
Multi-Affiliation (ML-related)	.120***	(.033)			.016	(.014)		
Multi-Expertise (ML-unrelated)			-.006	(.016)			-.006	(.008)
Multi-Expertise (ML-related)			.005	(.031)			.026*	(.013)
Year dummies	Yes		Yes		Yes		Yes	
Journal dummies	Yes		Yes		Yes		Yes	
F stat	491.678***		416.598***		34.573***		30.836***	
R2_adjusted	.654		.665		.163		.175	
N	24392		20095		16250		13386	

Notes: Unstandardized coefficients (standard errors in parentheses). Two-tailed test: $^{\dagger}p<0.1$, $^{*}p<0.05$, $^{**}p<0.01$, $^{***}p<0.001$. Ordinary least squares (OLS). (B) To compare the impact of *Multi-Affiliation* and *Multi-Expertise* between ML-related and ML-unrelated projects, we interacted *Multi-Affiliation* (*-Expertise*) with *ML-related.* For example, *Multi-Affiliation (ML-unrelated)* is 1 if *Multi-Affiliation* = 1 and *ML-related* = 0.

Table 4 **Use of Machine: Computation-focused vs. Computer-Domain Integrated Projects (ML-related projects only)**

	Impact								Novelty							
	Computation-focused				Computer-Domain Integrated				Computation-focused				Computer-Domain Integrated			
	Model 1		Model 2		Model 3		Model 4		Model 5		Model 6		Model 7		Model 8	
ln(#Author)	.004	(.082)	.014	(.098)	.105	(.071)	.110	(.080)	-.017	(.030)	-.018	(.037)	-.011	(.023)	-.003	(.026)
ln(#Org)	-.010	(.084)	.046	(.091)	-.020	(.068)	.038	(.073)	.001	(.031)	-.015	(.033)	-.034	(.022)	-.026	(.024)
ln(#Country)	.152	(.095)	.157	(.107)	.172*	(.078)	.114	(.084)	.017	(.033)	.037	(.037)	.049+	(.025)	.049+	(.027)
Multi-Affiliation	.080	(.098)			.182*	(.074)			.037	(.036)			.055*	(.024)		
Multi-Expertise			.006	(.089)			.166*	(.074)			-.014	(.032)			.064**	(.024)
Year dummies	Yes		Yes		Yes		Yes		Yes		Yes		Yes		Yes	
Journal dummies	Yes		Yes		Yes		Yes		Yes		Yes		Yes		Yes	
F stat	19.466***		11.424***		21.710***		18.771***		2.909***		2.798***		3.401***		3.204***	
R2_adjusted	.611		.533		.665		.662		.161		.189		.202		.213	
N	613		476		751		646		487		380		664		572	

Notes: Unstandardized coefficients (standard errors in parentheses). Two-tailed test: †p<0.1, *p<0.05, **p<0.01, ***p<0.001. Ordinary least squares (OLS).

Table 5 **ML Technologies**

(A) Base model

	Impact		Novelty	
	Model 1		Model 2	
ln(#Author)	.171***	(.010)	.019***	(.005)
ln(#Org)	.016+	(.009)	.006	(.004)
ln(#Country)	.080***	(.011)	-.005	(.005)
ML-related	.404***	(.018)	.014+	(.008)
DL-related	.201***	(.028)	-.054***	(.012)
Year dummies	Yes		Yes	
Journal dummies	Yes		Yes	
F stat	500.598***		37.061***	
R2_adjusted	.661		.173	
N	24641		16433	

(B) Interdisciplinary Expertise (ML-related projects only)

	Impact								Novelty							
	Computation-focused				Computer-Domain Integrated				Computation-focused				Computer-Domain Integrated			
	Model 1		Model 2		Model 3		Model 4		Model 5		Model 6		Model 7		Model 8	
ln(#Author)	-.018	(.081)	-.003	(.097)	.106	(.071)	.104	(.080)	-.014	(.031)	-.013	(.037)	-.013	(.023)	.000	(.026)
ln(#Org)	-.004	(.083)	.037	(.090)	-.017	(.068)	.044	(.073)	.001	(.030)	-.014	(.033)	-.036	(.022)	-.029	(.023)
ln(#Country)	.164+	(.094)	.174+	(.105)	.173*	(.078)	.112	(.084)	.015	(.033)	.034	(.037)	.048+	(.025)	.047+	(.027)
DL-related	.235**	(.079)	.198+	(.109)	.082	(.084)	.106	(.098)	-.022	(.029)	-.026	(.040)	-.056*	(.027)	-.072*	(.032)
Multi-Affiliation (DL-unrelated)	-.018	(.137)			.193*	(.085)			.098+	(.052)			.042	(.027)		
Multi-Affiliation (DL-related)	.111	(.124)			.131	(.135)			.001	(.046)			.102*	(.044)		
Multi-Expertise (DL-unrelated)			-.137	(.125)			.212*	(.086)			.005	(.047)			.040	(.028)
Multi-Expertise (DL-related)			.100	(.113)			.047	(.133)			-.026	(.040)			.125**	(.043)
Year dummies	Yes		Yes		Yes		Yes		Yes		Yes		Yes		Yes	
Journal dummies	Yes		Yes		Yes		Yes		Yes		Yes		Yes		Yes	
F stat	19.378***		11.643***		21.104***		18.258***		2.896***		2.727***		3.377***		3.207***	
R2_adjusted	.619		.548		.665		.661		.166		.189		.205		.218	
N	613		476		751		646		487		380		664		572	

Notes: Unstandardized coefficients (standard errors in parentheses). Two-tailed test: †p<0.1, *p<0.05, **p<0.01, ***p<0.001. Ordinary least squares (OLS).

Appendix 1 Selection of Fields and Journals

Field	Subject category	Journal 1	Journal 2	Journal 3	Journal 4	Journal 5
Agriculture	Food Science & Technology	Foods	LWT Food Science and Technology	Food Research International	International Journal of Food Science and Technology	Food Control
	Plant Sciences	Frontiers in Plant Science	Plants Basel	New Phytologist	Plant Disease	Journal of Experimental Botany
Biology	Biochemistry & Molecular Biology	Biomolecules	Journal of Biological Chemistry	Nucleic Acids Research	FEBS Journal	Metabolites
	Neurosciences	Frontiers in Neuroscience	Brain Sciences	Journal of Neuroscience	Journal of Alzheimers Disease	Neuroscience
	Biotechnology & Applied Microbiology	Applied Microbiology and Biotechnology	Applied and Environmental Microbiology	Journal of Applied Microbiology	Biotechnology and Bioengineering	Nature Biotechnology
	Cell Biology	Cells	Cell Reports	Cell Death & Disease	Oxidative Medicine and Cellular Longevity	Journal of Cell Science
	Biology	ELife	Journal of Experimental Biology	Biology-Basel	Saudi Journal of Biological Sciences	Philosophical Transactions of the Royal Society B-Biological Sciences
	Immunology	Frontiers in Immunology	Journal of Immunology	Journal of Clinical Immunology	Cellular Molecular Immunology	Nature Immunology
Chemistry	Chemistry, Physical	Catalysts	ACS Catalysis	Colloids and Surfaces A Physicochemical and Engineering Aspects	Journal of Colloid and Interface Science	Journal of Physical Chemistry B
	Chemistry, Multidisciplinary	RSC Advances	Angewandte Chemie International Edition	ASC Omega	Chemical Communications	Journal of The American Chemical Society
	Chemistry, Organic	Organic Letters	Journal of Organic Chemistry	Organic Biomolecular Chemistry	European Journal of Organic Chemistry	Tetrahedron Letters
Material Sciences	Materials Science, Multidisciplinary	Materials	Journal of Materials Science	Materials Chemistry and Physics	Materials Today Communications	Materials Design
Medicine	Pharmacology & Pharmacy	Frontiers in Pharmacology	European Review for Medical and Pharmacological Sciences	Pharmaceutics	International Journal of Pharmaceutics	Clinical Pharmacology Therapeutics
	Surgery	British Journal of Surgery	Journal of The American College of Surgeons	Surgical Endoscopy and Other Interventional Techniques	Obesity Surgery	Plastic and Reconstructive Surgery
	Oncology	Journal of Clinical Oncology	Cancers	Annals of Oncology	Frontiers in Oncology	Cancer Research
	Clinical Neurology	Neurology	Movement Disorders	Journal of Neurology	Parkinsonism Related Disorders	Multiple Sclerosis and Related Disorders
	Medicine, General & Internal	Journal of Clinical Medicine	BMJ British Medical Journal	BMJ Open	Jama Journal of the American Medical Association	New England Journal of Medicine
Physics	Physics, Applied	Journal of Applied Physics	Applied Physics Letters	Journal of Physics D Applied Physics	Physical Review Applied	Applied Physics Express
	Physics, Condensed Matter	Journal of Physics Condensed Matter	Annual Review of Condensed Matter Physics	Solid State Physics	Advances in Physics	
	Physics, Multidisciplinary	Physical Review Letters	Entropy	Physica A Statistical Mechanics and Its Applications	European Physical Journal Plus	Physica Scripta

Note. In each SC, we selected up to five journals that are associated with only a single SC. We further selected only Tier-1 and Tier-2 journals in the WoS journal ranking. In one SC (Physics, Condensed Matter), we found only four journals that satisfy the conditions. Thus, we selected 99 journals in total.