

# Data, measurement and empirical methods in the science of science

Received: 30 June 2022

Accepted: 17 February 2023

Published online: 1 June 2023

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The advent of large-scale datasets that trace the workings of science has encouraged researchers from many different disciplinary backgrounds to turn scientific methods into science itself, cultivating a rapidly expanding ‘science of science’. This Review considers this growing, multidisciplinary literature through the lens of data, measurement and empirical methods. We discuss the purposes, strengths and limitations of major empirical approaches, seeking to increase understanding of the field’s diverse methodologies and expand researchers’ toolkits. Overall, new empirical developments provide enormous capacity to test traditional beliefs and conceptual frameworks about science, discover factors associated with scientific productivity, predict scientific outcomes and design policies that facilitate scientific progress.

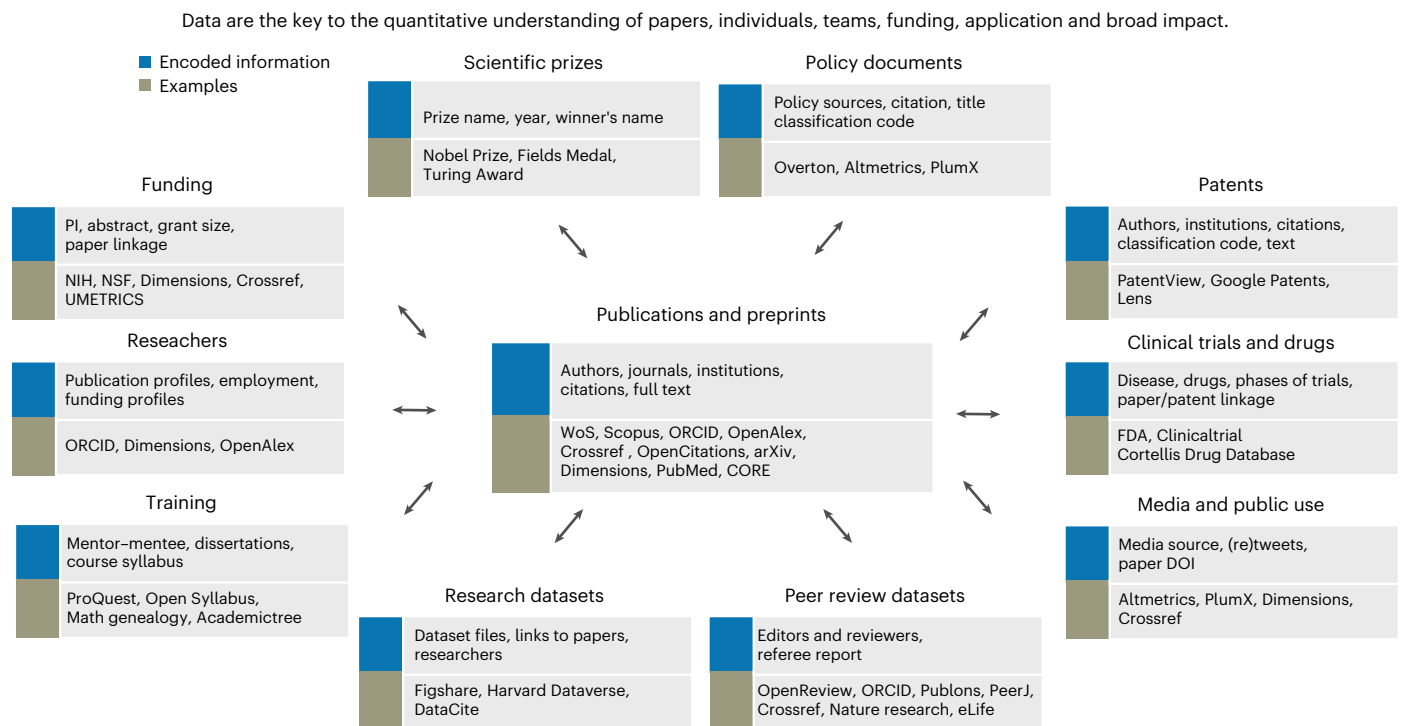
Scientific advances are a key input to rising standards of living, health and the capacity of society to confront grand challenges, from climate change to the COVID-19 pandemic<sup>1–3</sup>. A deeper understanding of how science works and where innovation occurs can help us to more effectively design science policy and science institutions, better inform scientists’ own research choices, and create and capture enormous value for science and humanity. Building on these key premises, recent years have witnessed substantial development in the ‘science of science’<sup>4–9</sup>, which uses large-scale datasets and diverse computational toolkits to unearth fundamental patterns behind scientific production and use.

The idea of turning scientific methods into science itself is long-standing. Since the mid-20th century, researchers from different disciplines have asked central questions about the nature of scientific progress and the practice, organization and impact of scientific research. Building on these rich historical roots, the field of the science of science draws upon many disciplines, ranging from information science to the social, physical and biological sciences to computer science, engineering and design. The science of science closely relates to several strands and communities of research, including metascience, scientometrics, the economics of science, research on research, science and technology studies, the sociology of science, metaknowledge and quantitative science studies<sup>5</sup>. There are noticeable differences between some of these communities, mostly around their historical origins

and the initial disciplinary composition of researchers forming these communities. For example, metascience has its origins in the clinical sciences and psychology, and focuses on rigour, transparency, reproducibility and other open science-related practices and topics. The scientometrics community, born in library and information sciences, places a particular emphasis on developing robust and responsible measures and indicators for science. Science and technology studies engage the history of science and technology, the philosophy of science, and the interplay between science, technology and society. The science of science, which has its origins in physics, computer science and sociology, takes a data-driven approach and emphasizes questions on how science works. Each of these communities has made fundamental contributions to understanding science. While they differ in their origins, these differences pale in comparison to the overarching, common interest in understanding the practice of science and its societal impact.

Three major developments have encouraged rapid advances in the science of science. The first is in data<sup>9</sup>: modern databases include millions of research articles, grant proposals, patents and more. This windfall of data traces scientific activity in remarkable detail and at scale. The second development is in measurement: scholars have used data to develop many new measures of scientific activities and examine theories that have long been viewed as important but

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**Fig. 1 | Science of science data and linkages.** This figure presents commonly used data types in science of science research, information contained in each data type and examples of data sources. Datasets in the science of

science research have not only grown in scale but have also expanded beyond publications to integrate upstream funding investments and downstream applications that extend beyond science itself.

difficult to quantify. The third development is in empirical methods: thanks to parallel advances in data science, network science, artificial intelligence and econometrics, researchers can study relationships, make predictions and assess science policy in powerful new ways. Together, new data, measurements and methods have revealed fundamental new insights about the inner workings of science and scientific progress itself.

With multiple approaches, however, comes a key challenge. As researchers adhere to norms respected within their disciplines, their methods vary, with results often published in venues with non-overlapping readership, fragmenting research along disciplinary boundaries. This fragmentation challenges researchers' ability to appreciate and understand the value of work outside of their own discipline, much less to build directly on it for further investigations.

Recognizing these challenges and the rapidly developing nature of the field, this paper reviews the empirical approaches that are prevalent in this literature. We aim to provide readers with an up-to-date understanding of the available datasets, measurement constructs and empirical methodologies, as well as the value and limitations of each. Owing to space constraints, this Review does not cover the full technical details of each method, referring readers to related guides to learn more. Instead, we will emphasize why a researcher might favour one method over another, depending on the research question.

Beyond a positive understanding of science, a key goal of the science of science is to inform science policy. While this Review mainly focuses on empirical approaches, with its core audience being researchers in the field, the studies reviewed are also germane to key policy questions. For example, what is the appropriate scale of scientific investment, in what directions and through what institutions<sup>10,11</sup>? Are public investments in science aligned with public interests<sup>12</sup>? What conditions produce novel or high-impact science<sup>13–20</sup>? How do the reward systems of science influence the rate and direction of progress<sup>13,21–24</sup>, and what governs scientific reproducibility<sup>25–27</sup>? How do contributions

evolve over a scientific career<sup>28–32</sup>, and how may diversity among scientists advance scientific progress<sup>33–35</sup>, among other questions relevant to science policy<sup>36,37</sup>.

Overall, this review aims to facilitate entry to science of science research, expand researcher toolkits and illustrate how diverse research approaches contribute to our collective understanding of science. Section 2 reviews datasets and data linkages. Section 3 reviews major measurement constructs in the science of science. Section 4 considers a range of empirical methods, focusing on one study to illustrate each method and briefly summarizing related examples and applications. Section 5 concludes with an outlook for the science of science.

## Data

Historically, data on scientific activities were difficult to collect and were available in limited quantities. Gathering data could involve manually tallying statistics from publications<sup>38,39</sup>, interviewing scientists<sup>16,40</sup>, or assembling historical anecdotes and biographies<sup>13,41</sup>. Analyses were typically limited to a specific domain or group of scientists. Today, massive datasets on scientific production and use are at researchers' fingertips<sup>42–44</sup>. Armed with big data and advanced algorithms, researchers can now probe questions previously not amenable to quantification and with enormous increases in scope and scale, as detailed below.

Publication datasets cover papers from nearly all scientific disciplines, enabling analyses of both general and domain-specific patterns. Commonly used datasets include the Web of Science (WoS), PubMed, CrossRef, ORCID, OpenCitations, Dimensions and OpenAlex. Datasets incorporating papers' text (CORE)<sup>45–47</sup>, data entities (DataCite)<sup>48,49</sup> and peer review reports (Publons)<sup>33,50,51</sup> have also become available. These datasets further enable novel measurement, for example, representations of a paper's content<sup>52,53</sup>, novelty<sup>15,54</sup> and interdisciplinarity<sup>55</sup>.

Notably, databases today capture more diverse aspects of science beyond publications, offering a richer and more encompassing view of research contexts and of researchers themselves (Fig. 1). For example,

some datasets trace research funding to the specific publications these investments support<sup>56,57</sup>, allowing high-scale studies of the impact of funding on productivity and the return on public investment. Datasets incorporating job placements<sup>58,59</sup>, curriculum vitae<sup>21,59</sup> and scientific prizes<sup>23</sup> offer rich quantitative evidence on the social structure of science. Combining publication profiles with mentorship genealogies<sup>60,61</sup>, dissertations<sup>34</sup> and course syllabi<sup>62,63</sup> provides insights on mentoring and cultivating talent.

Finally, today's scope of data extends beyond science to broader aspects of society. Altmetrics<sup>64</sup> captures news media and social media mentions of scientific articles. Other databases incorporate marketplace uses of science, including through patents<sup>10</sup>, pharmaceutical clinical trials and drug approvals<sup>65,66</sup>. Policy documents<sup>67,68</sup> help us to understand the role of science in the halls of government<sup>69</sup> and policy making<sup>12,68</sup>.

While datasets of the modern scientific enterprise have grown exponentially, they are not without limitations. As is often the case for data-driven research, drawing conclusions from specific data sources requires scrutiny and care. Datasets are typically based on published work, which may favour easy-to-publish topics over important ones (the streetlight effect)<sup>70,71</sup>. The publication of negative results is also rare (the file drawer problem)<sup>72,73</sup>. Meanwhile, English language publications account for over 90% of articles in major data sources, with limited coverage of non-English journals<sup>74</sup>. Publication datasets may also reflect biases in data collection across research institutions or demographic groups. Despite the open science movement, many datasets require paid subscriptions, which can create inequality in data access. Creating more open datasets for the science of science, such as OpenAlex, may not only improve the robustness and replicability of empirical claims but also increase entry to the field.

As today's datasets become larger in scale and continue to integrate new dimensions, they offer opportunities to unveil the inner workings and external impacts of science in new ways. They can enable researchers to reach beyond previous limitations while conducting original studies of new and long-standing questions about the sciences.

## Measurement

Here we discuss prominent measurement approaches in the science of science, including their purposes and limitations.

### Citations

Modern publication databases typically include data on which articles and authors cite other papers and scientists. These citation linkages have been used to engage core conceptual ideas in scientific research. Here we consider two common measures based on citation information: citation counts and knowledge flows.

First, citation counts are commonly used indicators of impact. The term 'indicator' implies that it only approximates the concept of interest. A citation count is defined as how many times a document is cited by subsequent documents and can proxy for the importance of research papers<sup>75,76</sup> as well as patented inventions<sup>77–79</sup>. Rather than treating each citation equally, measures may further weight the importance of each citation, for example by using the citation network structure to produce centrality<sup>80</sup>, PageRank<sup>81,82</sup> or Eigenfactor indicators<sup>83,84</sup>.

Citation-based indicators have also faced criticism<sup>84,85</sup>. Citation indicators necessarily oversimplify the construct of impact, often ignoring heterogeneity in the meaning and use of a particular reference, the variations in citation practices across fields and institutional contexts, and the potential for reputation and power structures in science to influence citation behaviour<sup>86,87</sup>. Researchers have started to understand more nuanced citation behaviours ranging from negative citations<sup>86</sup> to citation context<sup>47,88,89</sup>. Understanding what a citation actually measures matters in interpreting and applying many research findings in the science of science. Evaluations relying on citation-based indicators rather than expert judgements raise questions regarding misuse<sup>90–92</sup>. Given the importance of developing indicators that can

reliably quantify and evaluate science, the scientometrics community has been working to provide guidance for responsible citation practices and assessment<sup>85</sup>.

Second, scientists use citations to trace knowledge flows. Each citation in a paper is a link to specific previous work from which we can proxy how new discoveries draw upon existing ideas<sup>76,93</sup> and how knowledge flows between fields of science<sup>94,95</sup>, research institutions<sup>96</sup>, regions and nations<sup>97–99</sup>, and individuals<sup>81</sup>. Combinations of citation linkages can also approximate novelty<sup>15</sup>, disruptiveness<sup>17,100</sup> and interdisciplinarity<sup>55,95,101,102</sup>. A rapidly expanding body of work further examines citations to scientific articles from other domains (for example, patents, clinical drug trials and policy documents) to understand the applied value of science<sup>10,12,65,66,103–105</sup>.

### Individuals

Analysing individual careers allows researchers to answer questions such as: How do we quantify individual scientific productivity? What is a typical career lifecycle? How are resources and credits allocated across individuals and careers? A scholar's career can be examined through the papers they publish<sup>30,31,106–108</sup>, with attention to career progression and mobility, publication counts and citation impact, as well as grant funding<sup>24,109,110</sup> and prizes<sup>111–113</sup>.

Studies of individual impact focus on output, typically approximated by the number of papers a researcher publishes and citation indicators. A popular measure for individual impact is the *h*-index<sup>114</sup>, which takes both volume and per-paper impact into consideration. Specifically, a scientist is assigned the largest value *h* such that they have *h* papers that were each cited at least *h* times. Later studies build on the idea of the *h*-index and propose variants to address limitations<sup>115</sup>, these variants ranging from emphasizing highly cited papers in a career<sup>116</sup>, to field differences<sup>117</sup> and normalizations<sup>118</sup>, to the relative contribution of an individual in collaborative works<sup>119</sup>.

To study dynamics in output over the lifecycle, individuals can be studied according to age, career age or the sequence of publications. A long-standing literature has investigated the relationship between age and the likelihood of outstanding achievement<sup>28,106,111,120,121</sup>. Recent studies further decouple the relationship between age, publication volume and per-paper citation, and measure the likelihood of producing highly cited papers in the sequence of works one produces<sup>30,31</sup>.

As simple as it sounds, representing careers using publication records is difficult. Collecting the full publication list of a researcher is the foundation to study individuals yet remains a key challenge, requiring name disambiguation techniques to match specific works to specific researchers. Although algorithms are increasingly capable at identifying millions of career profiles<sup>122</sup>, they vary in accuracy and robustness. ORCID can help to alleviate the problem by offering researchers the opportunity to create, maintain and update individual profiles themselves, and it goes beyond publications to collect broader outputs and activities<sup>123</sup>. A second challenge is survivorship bias. Empirical studies tend to focus on careers that are long enough to afford statistical analyses, which limits the applicability of the findings to scientific careers as a whole. A third challenge is the breadth of scientists' activities, where focusing on publications ignores other important contributions such as mentorship and teaching, service (for example, refereeing papers, reviewing grant proposals and editing journals) or leadership within their organizations. Although researchers have begun exploring these dimensions by linking individual publication profiles with genealogical databases<sup>61,124</sup>, dissertations<sup>34</sup>, grants<sup>109</sup>, curriculum vitae<sup>21</sup> and acknowledgements<sup>125</sup>, scientific careers beyond publication records remain under-studied<sup>126,127</sup>. Lastly, citation-based indicators only serve as an approximation of individual performance with similar limitations as discussed above. The scientific community has called for more appropriate practices<sup>85,128</sup>, ranging from incorporating expert assessment of research contributions to broadening the measures of impact beyond publications.

Teams

Over many decades, science has exhibited a substantial and steady shift away from solo authorship towards coauthorship, especially among highly cited works<sup>18,129,130</sup>. In light of this shift, a research field, the science of team science<sup>131,132</sup>, has emerged to study the mechanisms that facilitate or hinder the effectiveness of teams. Team size can be proxied by the number of coauthors on a paper, which has been shown to predict distinctive types of advance: whereas larger teams tend to develop ideas, smaller teams tend to disrupt current ways of thinking<sup>17</sup>. Team characteristics can be inferred from coauthors' backgrounds<sup>133–135</sup>, allowing quantification of a team's diversity in terms of field, age, gender or ethnicity. Collaboration networks based on coauthorship<sup>130,136–139</sup> offer nuanced network-based indicators to understand individual and institutional collaborations.

However, there are limitations to using coauthorship alone to study teams<sup>132</sup>. First, coauthorship can obscure individual roles<sup>140–142</sup>, which has prompted institutional responses to help to allocate credit, including authorship order and individual contribution statements<sup>56,143</sup>. Second, coauthorship does not reflect the complex dynamics and interactions between team members that are often instrumental for team success<sup>53,144</sup>. Third, collaborative contributions can extend beyond coauthorship in publications to include members of a research laboratory<sup>145</sup> or co-principal investigators (co-PIs) on a grant<sup>146</sup>. Initiatives such as CRediT may help to address some of these issues by recording detailed roles for each contributor<sup>147</sup>.

Institutions

Research institutions, such as departments, universities, national laboratories and firms, encompass wider groups of researchers and their corresponding outputs. Institutional membership can be inferred from affiliations listed on publications or patents<sup>148,149</sup>, and the output of an institution can be aggregated over all its affiliated researchers<sup>150</sup>. Institutional research information systems (CRIS) contain more comprehensive research outputs and activities from employees.

Some research questions consider the institution as a whole, investigating the returns to research and development investment<sup>104</sup>, inequality of resource allocation<sup>22</sup> and the flow of scientists<sup>21,148,149</sup>. Other questions focus on institutional structures as sources of research productivity by looking into the role of peer effects<sup>125,151–153</sup>, how institutional policies impact research outcomes<sup>154,155</sup> and whether interdisciplinary efforts foster innovation<sup>55</sup>. Institution-oriented measurement faces similar limitations as with analyses of individuals and teams, including name disambiguation for a given institution and the limited capacity of formal publication records to characterize the full range of relevant institutional outcomes. It is also unclear how to allocate credit among multiple institutions associated with a paper. Moreover, relevant institutional employees extend beyond publishing researchers: interns, technicians and administrators all contribute to research endeavours<sup>130</sup>.

In sum, measurements allow researchers to quantify scientific production and use across numerous dimensions, but they also raise questions of construct validity: Does the proposed metric really reflect what we want to measure? Testing the construct's validity is important, as is understanding a construct's limits. Where possible, using alternative measurement approaches, or qualitative methods such as interviews and surveys, can improve measurement accuracy and the robustness of findings.

Empirical methods

In this section, we review two broad categories of empirical approaches (Table 1), each with distinctive goals: (1) to discover, estimate and predict empirical regularities; and (2) to identify causal mechanisms. For each method, we give a concrete example to help to explain how the method works, summarize related work for interested readers, and discuss contributions and limitations.

**Table 1 | Empirical approaches in science of science research**

Category	Method	Core objectives and contributions
Descriptive and predictive approaches	Empirical regularities and generalizable facts	Establish observational regularities about science; confirm or reject existing theories or hypotheses; provide novel discoveries motivating new theory
	Classic regression	Engage formal hypothesis testing about relationships between variables and estimate their precision and magnitude
	Mechanistic models	Model fundamental data generating processes; provide falsifiable tests of formal theory
	Machine learning	Represent data with multiple levels of abstraction; provide superior predictive accuracy
Causal approaches	Matching and fixed effects	Reduce bias in regression estimation and come closer to causal inference; provide more effective controls for characteristics that may otherwise drive correlations
	Quasi-experiments	Exploit innate randomness in the data context to allow causal inference about the relationship between variables
	Experiments	Construct formal experiments in well-controlled environments to deliver causal inference and study specific mechanisms and interventions

This table provides a schematic overview for section 4, organizing empirical methods according to types of research questions and methodological goals that are commonly used in science of science research.

Descriptive and predictive approaches

**Empirical regularities and generalizable facts.** The discovery of empirical regularities in science has had a key role in driving conceptual developments and the directions of future research. By observing empirical patterns at scale, researchers unveil central facts that shape science and present core features that theories of scientific progress and practice must explain. For example, consider citation distributions. de Solla Price first proposed that citation distributions are fat-tailed<sup>39</sup>, indicating that a few papers have extremely high citations while most papers have relatively few or even no citations at all. de Solla Price proposed that citation distribution was a power law, while researchers have since refined this view to show that the distribution appears log-normal, a nearly universal regularity across time and fields<sup>156,157</sup>. The fat-tailed nature of citation distributions and its universality across the sciences has in turn sparked substantial theoretical work that seeks to explain this key empirical regularity<sup>20,156,158,159</sup>.

Empirical regularities are often surprising and can contest previous beliefs of how science works. For example, it has been shown that the age distribution of great achievements peaks in middle age across a wide range of fields<sup>107,121,160</sup>, rejecting the common belief that young scientists typically drive breakthroughs in science. A closer look at the



individual careers also indicates that productivity patterns vary widely across individuals<sup>29</sup>. Further, a scholar's highest-impact papers come at a remarkably constant rate across the sequence of their work<sup>30,31</sup>.

The discovery of empirical regularities has had important roles in shaping beliefs about the nature of science<sup>10,45,161,162</sup>, sources of breakthrough ideas<sup>15,163–165</sup>, scientific careers<sup>21,29,126,127</sup>, the network structure of ideas and scientists<sup>23,98,136–139,166</sup>, gender inequality<sup>57,108,126,135,143,167,168</sup>, and many other areas of interest to scientists and science institutions<sup>22,47,86,97,102,105,134,169–171</sup>. At the same time, care must be taken to ensure that findings are not merely artefacts due to data selection or inherent bias. To differentiate meaningful patterns from spurious ones, it is important to stress test the findings through different selection criteria or across non-overlapping data sources.

**Regression analysis.** When investigating correlations among variables, a classic method is regression, which estimates how one set of variables explains variation in an outcome of interest. Regression can be used to test explicit hypotheses or predict outcomes. For example, researchers have investigated whether a paper's novelty predicts its citation impact<sup>172</sup>. Adding additional control variables to the regression, one can further examine the robustness of the focal relationship.

Although regression analysis is useful for hypothesis testing, it bears substantial limitations. If the question one wishes to ask concerns a 'causal' rather than a correlational relationship, regression is poorly suited to the task as it is impossible to control for all the confounding factors. Failing to account for such 'omitted variables' can bias the regression coefficient estimates and lead to spurious interpretations. Further, regression models often have low goodness of fit (small  $R^2$ ), indicating that the variables considered explain little of the outcome variation. As regressions typically focus on a specific relationship in simple functional forms, regressions tend to emphasize interpretability rather than overall predictability. The advent of predictive approaches powered by large-scale datasets and novel computational techniques offers new opportunities for modelling complex relationships with stronger predictive power.

**Mechanistic models.** Mechanistic modelling is an important approach to explaining empirical regularities, drawing from methods primarily used in physics. Such models predict macro-level regularities of a system by modelling micro-level interactions among basic elements with interpretable and modifiable formulas. While theoretical by nature, mechanistic models in the science of science are often empirically grounded, and this approach has developed together with the advent of large-scale, high-resolution data.

Simplicity is the core value of a mechanistic model. Consider for example, why citations follow a fat-tailed distribution. de Solla Price modelled the citing behaviour as a cumulative advantage process on a growing citation network<sup>159</sup> and found that if the probability a paper is cited grows linearly with its existing citations, the resulting distribution would follow a power law, broadly aligned with empirical observations. The model is intentionally simplified, ignoring myriad factors. Yet the simple cumulative advantage process is by itself sufficient in explaining a power law distribution of citations. In this way, mechanistic models can help to reveal key mechanisms that can explain observed patterns.

Moreover, mechanistic models can be refined as empirical evidence evolves. For example, later investigations showed that citation distributions are better characterized as log-normal<sup>156,173</sup>, prompting researchers to introduce a fitness parameter to encapsulate the inherent differences in papers' ability to attract citations<sup>174,175</sup>. Further, older papers are less likely to be cited than expected<sup>176–178</sup>, motivating more recent models<sup>20</sup> to introduce an additional aging effect<sup>179</sup>. By combining the cumulative advantage, fitness and aging effects, one can already achieve substantial predictive power not just for the overall properties of the system but also the citation dynamics of individual papers<sup>20</sup>.

In addition to citations, mechanistic models have been developed to understand the formation of collaborations<sup>136,180–183</sup>, knowledge discovery and diffusion<sup>184,185</sup>, topic selection<sup>186,187</sup>, career dynamics<sup>30,31,188,189</sup>, the growth of scientific fields<sup>190</sup> and the dynamics of failure in science and other domains<sup>178</sup>.

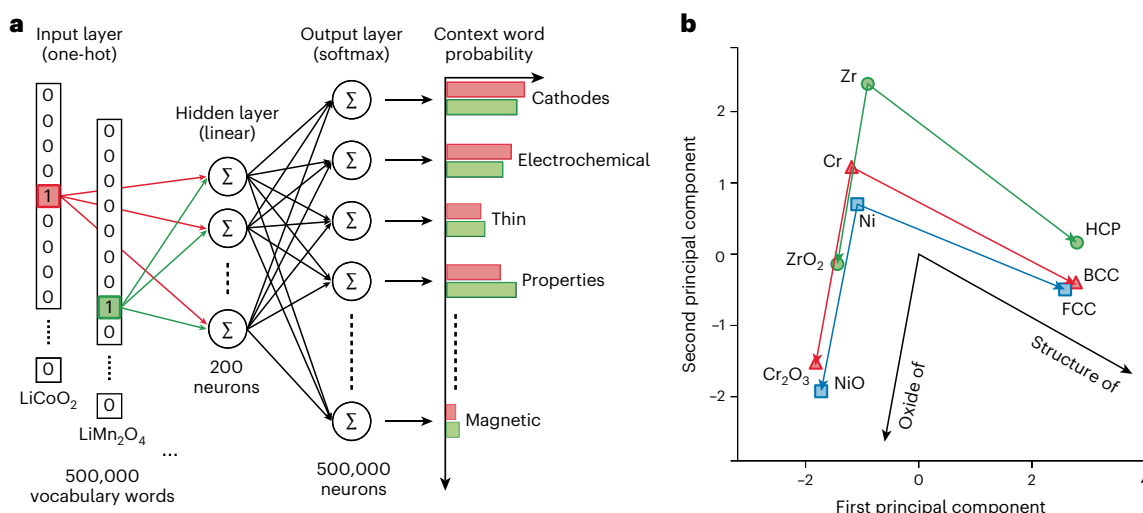
At the same time, some observers have argued that mechanistic models are too simplistic to capture the essence of complex real-world problems<sup>191</sup>. While it has been a cornerstone for the natural sciences, representing social phenomena in a limited set of mathematical equations may miss complexities and heterogeneities that make social phenomena interesting in the first place. Such concerns are not unique to the science of science, as they represent a broader theme in computational social sciences<sup>192,193</sup>, ranging from social networks<sup>194,195</sup> to human mobility<sup>196,197</sup> to epidemics<sup>198,199</sup>. Other observers have questioned the practical utility of mechanistic models and whether they can be used to guide decisions and devise actionable policies. Nevertheless, despite these limitations, several complex phenomena in the science of science are well captured by simple mechanistic models, showing a high degree of regularity beneath complex interacting systems and providing powerful insights about the nature of science. Mixing such modelling with other methods could be particularly fruitful in future investigations.

**Machine learning.** The science of science seeks in part to forecast promising directions for scientific research<sup>7,44</sup>. In recent years, machine learning methods have substantially advanced predictive capabilities<sup>200,201</sup> and are playing increasingly important parts in the science of science. In contrast to the previous methods, machine learning does not emphasize hypotheses or theories. Rather, it leverages complex relationships in data and optimizes goodness of fit to make predictions and categorizations.

Traditional machine learning models include supervised, semi-supervised and unsupervised learning. The model choice depends on data availability and the research question, ranging from supervised models for citation prediction<sup>202,203</sup> to unsupervised models for community detection<sup>204</sup>. Take for example mappings of scientific knowledge<sup>94,205,206</sup>. The unsupervised method applies network clustering algorithms to map the structures of science. Related visualization tools make sense of clusters from the underlying network, allowing observers to see the organization, interactions and evolution of scientific knowledge. More recently, supervised learning, and deep neural networks in particular, have witnessed especially rapid developments<sup>207</sup>. Neural networks can generate high-dimensional representations of unstructured data such as images and texts, which encode complex properties difficult for human experts to perceive.

Take text analysis as an example. A recent study<sup>32</sup> utilizes 3.3 million paper abstracts in materials science to predict the thermoelectric properties of materials. The intuition is that the words currently used to describe a material may predict its hitherto undiscovered properties (Fig. 2). Compared with a random material, the materials predicted by the model are eight times more likely to be reported as thermoelectric in the next 5 years, suggesting that machine learning has the potential to substantially speed up knowledge discovery, especially as data continue to grow in scale and scope. Indeed, predicting the direction of new discoveries represents one of the most promising avenues for machine learning models, with neural networks being applied widely to biology<sup>208</sup>, physics<sup>209,210</sup>, mathematics<sup>211</sup>, chemistry<sup>212</sup>, medicine<sup>213</sup> and clinical applications<sup>214</sup>. Neural networks also offer a quantitative framework to probe the characteristics of creative products ranging from scientific papers<sup>53</sup>, journals<sup>215</sup>, organizations<sup>148</sup>, to paintings and movies<sup>32</sup>. Neural networks can also help to predict the reproducibility of papers from a variety of disciplines at scale<sup>53,216</sup>.

While machine learning can offer high predictive accuracy, successful applications to the science of science face challenges, particularly regarding interpretability. Researchers may value transparent and



**Fig. 2 | An example of prediction with machine learning.** This figure illustrates the word2vec skip-gram methods<sup>52</sup>, where the goal is to predict useful properties of materials using previous scientific literature. **a**, The architecture and training process of the word2vec skip-gram model, where the 3-layer, fully connected neural network learns the 200-dimensional representation (hidden layer) from

the sparse vector for each word and its context in the literature (input layer).

**b**, The top two principal components of the word embedding. Materials with similar features are close in the 2D space, allowing prediction of a material's properties. Different targeted words are shown in different colours. Reproduced with permission from ref. 52, Springer Nature Ltd.

interpretable findings for how a given feature influences an outcome, rather than a black-box model. The lack of interpretability also raises concerns about bias and fairness. In predicting reproducible patterns from data, machine learning models inevitably include and reproduce biases embedded in these data, often in non-transparent ways. The fairness of machine learning<sup>217</sup> is heavily debated in applications ranging from the criminal justice system to hiring processes. Effective and responsible use of machine learning in the science of science therefore requires thoughtful partnership between humans and machines<sup>53</sup> to build a reliable system accessible to scrutiny and modification.

### Causal approaches

The preceding methods can reveal core facts about the workings of science and develop predictive capacity. Yet, they fail to capture causal relationships, which are particularly useful in assessing policy interventions. For example, how can we test whether a science policy boosts or hinders the performance of individuals, teams or institutions? The overarching idea of causal approaches is to construct some counterfactual world where two groups are identical to each other except that one group experiences a treatment that the other group does not.

**Towards causation.** Before engaging in causal approaches, it is useful to first consider the interpretative challenges of observational data. As observational data emerge from mechanisms that are not fully known or measured, an observed correlation may be driven by underlying forces that were not accounted for in the analysis. This challenge makes causal inference fundamentally difficult in observational data. An awareness of this issue is the first step in confronting it. It further motivates intermediate empirical approaches, including the use of matching strategies and fixed effects, that can help to confront (although not fully eliminate) the inference challenge. We first consider these approaches before turning to more fully causal methods.

**Matching.** Matching utilizes rich information to construct a control group that is similar to the treatment group on as many observable characteristics as possible before the treatment group is exposed to the treatment. Inferences can then be made by comparing the treatment and the matched control groups. Exact matching applies to categorical values, such as country, gender, discipline or affiliation<sup>35,218</sup>. Coarsened

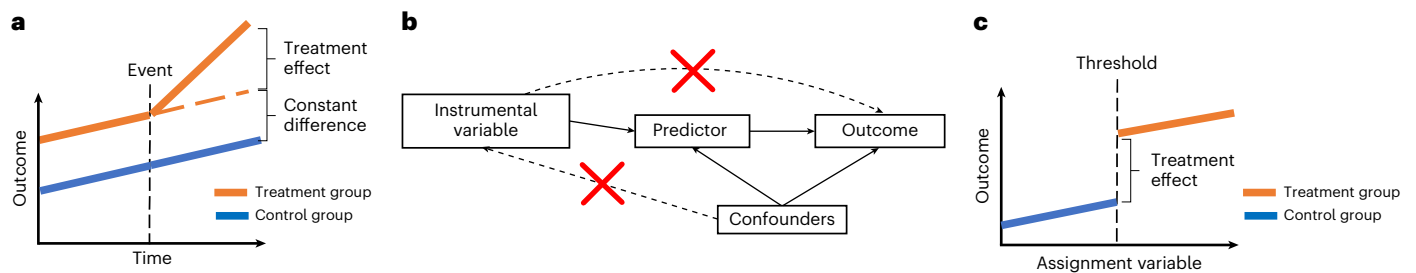
exact matching considers percentile bins of continuous variables and matches observations in the same bin<sup>133</sup>. Propensity score matching estimates the probability of receiving the 'treatment' on the basis of the controlled variables and uses the estimates to match treatment and control groups, which reduces the matching task from comparing the values of multiple covariates to comparing a single value<sup>24,219</sup>. Dynamic matching is useful for longitudinally matching variables that change over time<sup>220,221</sup>.

**Fixed effects.** Fixed effects are a powerful and now standard tool in controlling for confounders. A key requirement for using fixed effects is that there are multiple observations on the same subject or entity (person, field, institution and so on)<sup>222–224</sup>. The fixed effect works as a dummy variable that accounts for the role of any fixed characteristic of that entity. Consider the finding where gender-diverse teams produce higher-impact papers than same-gender teams do<sup>225</sup>. A confounder may be that individuals who tend to write high-impact papers may also be more likely to work in gender-diverse teams. By including individual fixed effects, one accounts for any fixed characteristics of individuals (such as IQ, cultural background or previous education) that might drive the relationship of interest.

In sum, matching and fixed effects methods reduce potential sources of bias in interpreting relationships between variables. Yet, confounders may persist in these studies. For instance, fixed effects do not control for unobserved factors that change with time within the given entity (for example, access to funding or new skills). Identifying causal effects convincingly will then typically require distinct research methods that we turn to next.

**Quasi-experiments.** Researchers in economics and other fields have developed a range of quasi-experimental methods to construct treatment and control groups. The key idea here is exploiting randomness from external events that differentially expose subjects to a particular treatment. Here we review three quasi-experimental methods: difference-in-differences, instrumental variables and regression discontinuity (Fig. 3).

**Difference-in-differences.** Difference-in-difference regression (DiD) investigates the effect of an unexpected event, comparing the affected



**Fig. 3 | Quasi-experiment methods. a–c.** This figure presents illustrations of (a) differences-in-differences, (b) instrumental variables and (c) regression discontinuity methods. The solid line in b represents causal links and the dashed line represents the relationships that are not allowed, if the IV method is to produce causal inference.

group (the treated group) with an unaffected group (the control group). The control group is intended to provide the counterfactual path—what would have happened were it not for the unexpected event. Ideally, the treated and control groups are on virtually identical paths before the treatment event, but DiD can also work if the groups are on parallel paths (Fig. 3a). For example, one study<sup>226</sup> examines how the premature death of superstar scientists affects the productivity of their previous collaborators. The control group are collaborators of superstars who did not die in the time frame. The two groups do not show significant differences in publications before a death event, yet upon the death of a star scientist, the treated collaborators on average experience a 5–8% decline in their quality-adjusted publication rates compared with the control group. DiD has wide applicability in the science of science, having been used to analyse the causal effects of grant design<sup>24</sup>, access costs to previous research<sup>155,227</sup>, university technology transfer policies<sup>154</sup>, intellectual property<sup>228</sup>, citation practices<sup>229</sup>, evolution of fields<sup>221</sup> and the impacts of paper retractions<sup>230–232</sup>. The DiD literature has grown especially rapidly in the field of economics, with substantial recent refinements<sup>233,234</sup>.

**Instrumental variables.** Another quasi-experimental approach utilizes ‘instrumental variables’ (IV). The goal is to determine the causal influence of some feature  $X$  on some outcome  $Y$  by using a third, instrumental variable. This instrumental variable is a quasi-random event that induces variation in  $X$  and, except for its impact through  $X$ , has no other effect on the outcome  $Y$  (Fig. 3b). For example, consider a study of astronomy that seeks to understand how telescope time affects career advancement<sup>235</sup>. Here, one cannot simply look at the correlation between telescope time and career outcomes because many confounds (such as talent or grit) may influence both telescope time and career opportunities. Now consider the weather as an instrumental variable. Cloudy weather will, at random, reduce an astronomer’s observational time. Yet, the weather on particular nights is unlikely to correlate with a scientist’s innate qualities. The weather can then provide an instrumental variable to reveal a causal relationship between telescope time and career outcomes. Instrumental variables have been used to study local peer effects in research<sup>151</sup>, the impact of gender composition in scientific committees<sup>236</sup>, patents on future innovation<sup>237</sup> and taxes on inventor mobility<sup>238</sup>.

**Regression discontinuity.** In regression discontinuity, policies with an arbitrary threshold for receiving some benefit can be used to construct treatment and control groups (Fig. 3c). Take the funding paylines for grant proposals as an example. Proposals with scores increasingly close to the payline are increasingly similar in their both observable and unobservable characteristics, yet only those projects with scores above the payline receive the funding. For example, a study<sup>110</sup> examines the effect of winning an early-career grant on the probability of winning a later, mid-career grant. The probability has a discontinuous jump across the initial grant’s payline, providing the treatment and control groups needed to estimate the causal effect of receiving a

grant. This example utilizes the ‘sharp’ regression discontinuity that assumes treatment status to be fully determined by the cut-off. If we assume treatment status is only partly determined by the cut-off, we can use ‘fuzzy’ regression discontinuity designs. Here the probability of receiving a grant is used to estimate the future outcome<sup>11,110,239–241</sup>.

Although quasi-experiments are powerful tools, they face their own limitations. First, these approaches identify causal effects within a specific context and often engage small numbers of observations. How representative the samples are for broader populations or contexts is typically left as an open question. Second, the validity of the causal design is typically not ironclad. Researchers usually conduct different robustness checks to verify whether observable confounders have significant differences between the treated and control groups, before treatment. However, unobservable features may still differ between treatment and control groups. The quality of instrumental variables and the specific claim that they have no effect on the outcome except through the variable of interest, is also difficult to assess. Ultimately, researchers must rely partly on judgement to tell whether appropriate conditions are met for causal inference.

This section emphasized popular econometric approaches to causal inference. Other empirical approaches, such as graphical causal modelling<sup>242,243</sup>, also represent an important stream of work on assessing causal relationships. Such approaches usually represent causation as a directed acyclic graph, with nodes as variables and arrows between them as suspected causal relationships. In the science of science, the directed acyclic graph approach has been applied to quantify the causal effect of journal impact factor<sup>244</sup> and gender or racial bias<sup>245</sup> on citations. Graphical causal modelling has also triggered discussions on strengths and weaknesses compared to the econometrics methods<sup>246,247</sup>.

**Experiments.** In contrast to quasi-experimental approaches, laboratory and field experiments conduct direct randomization in assigning treatment and control groups. These methods engage explicitly in the data generation process, manipulating interventions to observe counterfactuals. These experiments are crafted to study mechanisms of specific interest and, by designing the experiment and formally randomizing, can produce especially rigorous causal inference.

**Laboratory experiments.** Laboratory experiments build counterfactual worlds in well-controlled laboratory environments. Researchers randomly assign participants to the treatment or control group and then manipulate the laboratory conditions to observe different outcomes in the two groups. For example, consider laboratory experiments on team performance and gender composition<sup>144,248</sup>. The researchers randomly assign participants into groups to perform tasks such as solving puzzles or brainstorming. Teams with a higher proportion of women are found to perform better on average, offering evidence that gender diversity is causally linked to team performance. Laboratory experiments can allow researchers to test forces that are otherwise hard to observe, such as how competition influences



creativity<sup>249</sup>. Laboratory experiments have also been used to evaluate how journal impact factors shape scientists' perceptions of rewards<sup>250</sup> and gender bias in hiring<sup>251</sup>.

Laboratory experiments allow for precise control of settings and procedures to isolate causal effects of interest. However, participants may behave differently in synthetic environments than in real-world settings, raising questions about the generalizability and replicability of the results<sup>252–254</sup>. To assess causal effects in real-world settings, researchers use randomized controlled trials.

**Randomized controlled trials.** A randomized controlled trial (RCT), or field experiment, is a staple for causal inference across a wide range of disciplines. RCTs randomly assign participants into the treatment and control conditions<sup>255</sup> and can be used not only to assess mechanisms but also to test real-world interventions such as policy change. The science of science has witnessed growing use of RCTs. For instance, a field experiment<sup>146</sup> investigated whether lower search costs for collaborators increased collaboration in grant applications. The authors randomly allocated principal investigators to face-to-face sessions in a medical school, and then measured participants' chance of writing a grant proposal together. RCTs have also offered rich causal insights on peer review<sup>256–260</sup> and gender bias in science<sup>261–263</sup>.

While powerful, RCTs are difficult to conduct in the science of science, mainly for two reasons. The first concerns potential risks in a policy intervention. For instance, while randomizing funding across individuals could generate crucial causal insights for funders, it may also inadvertently harm participants' careers<sup>264</sup>. Second, key questions in the science of science often require a long-time horizon to trace outcomes, which makes RCTs costly. It also raises the difficulty of replicating findings. A relative advantage of the quasi-experimental methods discussed earlier is that one can identify causal effects over potentially long periods of time in the historical record. On the other hand, quasi-experiments must be found as opposed to designed, and they often are not available for many questions of interest. While the best approaches are context dependent, a growing community of researchers is building platforms to facilitate RCTs for the science of science, aiming to lower their costs and increase their scale. Performing RCTs in partnership with science institutions can also contribute to timely, policy-relevant research that may substantially improve science decision-making and investments.

## Outlook

Research in the science of science has been empowered by the growth of high-scale data, new measurement approaches and an expanding range of empirical methods. These tools provide enormous capacity to test conceptual frameworks about science, discover factors impacting scientific productivity, predict key scientific outcomes and design policies that better facilitate future scientific progress. A careful appreciation of empirical techniques can help researchers to choose effective tools for questions of interest and propel the field. A better and broader understanding of these methodologies may also build bridges across diverse research communities, facilitating communication and collaboration, and better leveraging the value of diverse perspectives. The science of science is about turning scientific methods on the nature of science itself. The fruits of this work, with time, can guide researchers and research institutions to greater progress in discovery and understanding across the landscape of scientific inquiry.

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## Acknowledgements

The authors thank all members of the Center for Science of Science and Innovation (CSSI) for invaluable comments. This work was supported by the Air Force Office of Scientific Research under award number FA9550-19-1-0354, National Science Foundation grant SBE 1829344, and the Alfred P. Sloan Foundation G-2019-12485.

## Competing interests

The authors declare no competing interests.

## Additional information

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**Peer review information** *Nature Human Behaviour* thanks Ludo Waltman, Erin Leahey and Sarah Bratt for their contribution to the peer review of this work.

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