



The application of machine learning to air pollution research: A bibliometric analysis

Yunzhe Li^a, Zhipeng Sha^a, Aohan Tang^{a,*}, Keith Goulding^b, Xuejun Liu^a

^a Beijing Key Laboratory of Farmland Soil Pollution Prevention and Remediation, College of Resources and Environmental Science, China Agricultural University, Beijing 100193, China

^b Sustainable Soils and Crops, Rothamsted Research, Harpenden AL5 2JQ, UK

ARTICLE INFO

Edited by HAO ZHU

Keywords:

Air pollution
Machine learning
Bibliometric analysis
Research focuses
Development

ABSTRACT

Machine learning (ML) is an advanced computer algorithm that simulates the human learning process to solve problems. With an explosion of monitoring data and the increasing demand for fast and accurate prediction, ML models have been rapidly developed and applied in air pollution research. In order to explore the status of ML applications in air pollution research, a bibliometric analysis was made based on 2962 articles published from 1990 to 2021. The number of publications increased sharply after 2017, comprising approximately 75% of the total. Institutions in China and United States contributed half of all publications with most research being conducted by individual groups rather than global collaborations. Cluster analysis revealed four main research topics for the application of ML: chemical characterization of pollutants, short-term forecasting, detection improvement and optimizing emission control. The rapid development of ML algorithms has increased the capability to explore the chemical characteristics of multiple pollutants, analyze chemical reactions and their driving factors, and simulate scenarios. Combined with multi-field data, ML models are a powerful tool for analyzing atmospheric chemical processes and evaluating the management of air quality and deserve greater attention in future.

1. Introduction

Air pollution is harmful to human health and ecosystem stability, causing 7 million premature deaths and a \$2.9 trillion global economic loss every year (IQAir, 2020). The global premature mortality burden resulting from ambient PM_{2.5} and ozone exposure continues to increase (Chowdhury et al., 2020). In response to mounting risks, ground monitoring and remote sensing of pollutant emissions, transformation and deposition have played an important role in revealing the dynamic changes in air pollution (Cetin et al., 2018; Elsunousi et al., 2021; Hu et al., 2017; Kuerban et al., 2020; Li et al., 2023; Sevik et al., 2019; Wen et al., 2022; Xu et al., 2022a), and there has been a resultant explosion in monitoring data. Making full use of these data could provide a sound scientific basis for effective control of air pollution and policymaking.

The atmosphere is a changeable and open environmental system containing a range of pollutants and complex chemical processes, in which the relationships between components and controlling factors are not simply linear. Traditional statistical regressions models, such as parametric regression models, have limitations for fitting nonlinear

relationships when dealing with the large and growing quantity of data in atmospheric science, including poor prediction accuracy for nonlinear problems analyzed using 'Big Data' (Feng et al., 2011). Some regression models are also complicated with too many explanatory variables, and their requirements for variable distribution are strict. These disadvantages are obstacles when trying to dig deeper into complex data and obtaining more valuable information. More convenient and accurate methods are urgently required for effective data analysis.

As artificial intelligence rapidly develops, machine learning (ML) is playing an increasingly important role in dealing with very large data sets. To date, commonly used ML algorithms are supervised learning algorithms such as artificial neural networks (ANN), random forest (RF) and support vector machine (SVM). These are mainly based on sample data for computer modeling for classification and regression (Zhong et al., 2021). ML models can establish direct relationships between data and weaken the impact of outliers (Ucun Ozel et al., 2020), delivering a higher prediction accuracy and robustness when dealing with large data sets (Chen et al., 2022; Yuchi et al., 2019). They produce a better fit to the data with a smaller root mean square error (RMSE), especially in

* Correspondence to: No. 2 Yuanmingyuan West Road, Beijing 100193, China.
E-mail address: aohantang@cau.edu.cn (A. Tang).

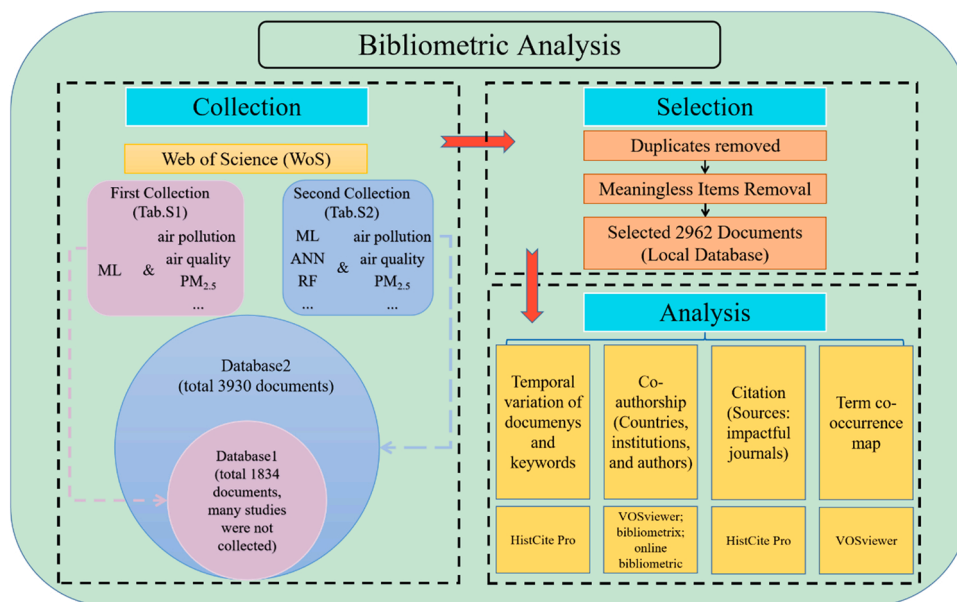


Fig. 1. Flow chart of the bibliometric analysis.

nonlinear situations (Chen et al., 2022; Feng et al., 2011; Zimmerman et al., 2018). Also, multiple types data like integers and strings can be introduced when model construction. ML models are relatively simple, less time-consuming and low-cost compared to numerical models. These advantages make ML models increasingly popular in atmospheric science research (Liao et al., 2021; Zheng et al., 2021). Combined with multiple fields of data, ML models are key components for many tasks, such as short-term forecasting (Yan et al., 2021), analysis of the chemical behavior of pollutants (Huang et al., 2021) and impact assessment (Lv et al., 2023).

Bibliometric analysis is a valuable tool for analyzing the research status of a specific field (Qin et al., 2022a; Zhang and Chen, 2020). It can not only provide an analysis of the development of themes in research (Zhang et al., 2020b), but also show interrelations between countries, institutions and authors by revealing social networks (van Eck and Waltman, 2010). With the aim of advancing the understanding of ML, we made a bibliometric analysis of its applications and the development in global air pollution research. This provides further insight into the most appropriate application of ML in atmospheric science research in the future.

2. Materials and methods

2.1. Data collection

Literature recorded in the Web of Science (WoS) core database from 1990 to 2021 was collected. The search and analysis processes are shown in Fig. 1. Keywords used for this initial selection are shown in Tab. S1, and a total of 1834 documents were collected in database1. However, some documents were missed because the names of specific ML algorithms rather than “machine learning” were used in the titles or keywords of these papers. Therefore, keywords were expanded with specific ML algorithm names such as ANN, RF, and SVM. The keywords used in the second collection together with the retrieved paper numbers are shown in Tab. S2. A total of 3930 documents were collected in database2. The percentages of research articles, conference papers and reviews were 75.4%, 23.9% and 1.3%, respectively. Peer-reviewed publications identified as “article” and “review” were selected for further analysis (Bao et al., 2021; Qin et al., 2022a; Zhang et al., 2020b). After removing duplicate documents and irrelevant items, a total of 2962 publications were selected and formed into a new database named

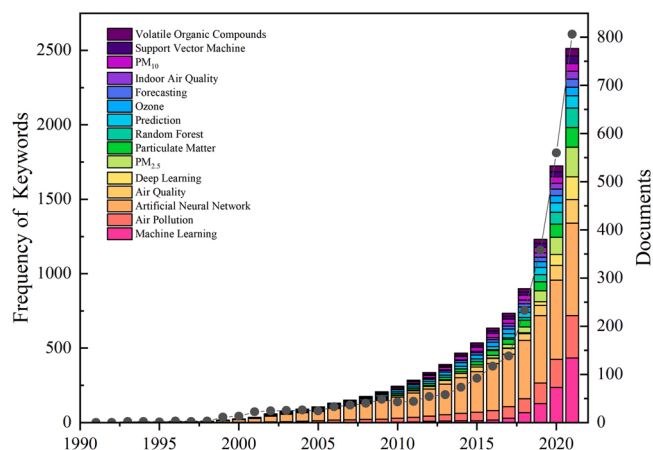


Fig. 2. Number of publications and frequency of occurrence of keywords from 1990 to 2021

“Local Database” for subsequent analysis. The required information from each document, such as keywords, abstract, authors, source, reference, etc., was downloaded in “txt” format for analysis.

2.2. Bibliometric analysis methods

Based on the Local Database, four types of analytical and visualization software were used for bibliometric analysis. Firstly, HistCite Pro (v2.1) was used to output informetric indicators, including the annual variation of publications and keyword occurrence, as well as citations of literature and journals. Then, three mature types of visualization software were introduced for social-relation analysis to reveal active groups, researchers, and their collaboration networks. The “bibliometrix” package in R, and an online bibliometric analysis software (<https://bibliometric.com/>) described the country distribution and collaboration networks. VOSviewer (v1.6) was used to construct bibliometric maps of institutions and authors. Finally, a term co-occurrence map was created from titles and abstracts for cluster analysis in VOSviewer to show the main directions and focuses of current research.

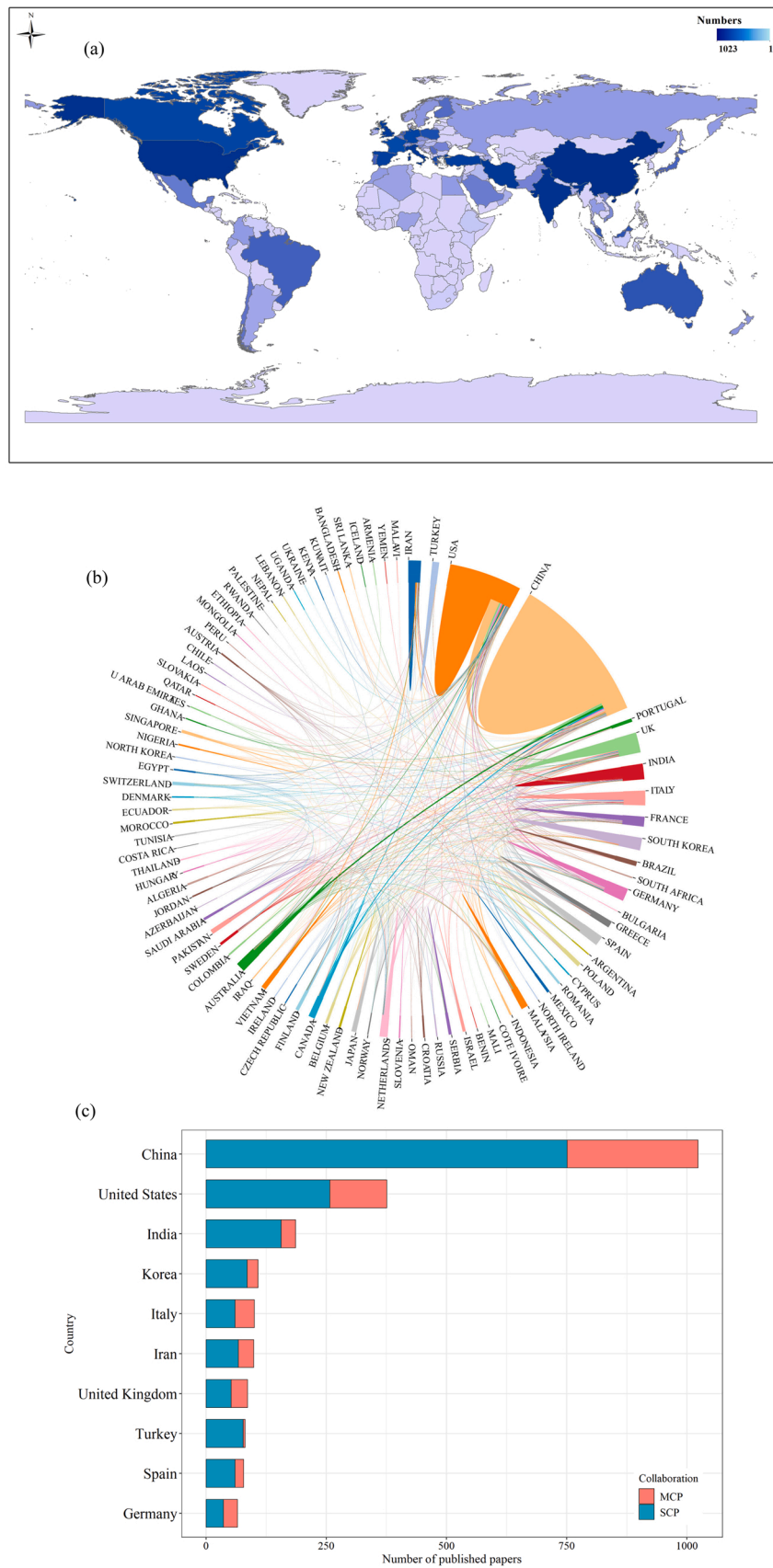


Fig. 3. (a) Distribution of publications by country; (b) Collaboration network of countries; (c) Analysis of single country publications (SCP) and multiple country publications (MCP).

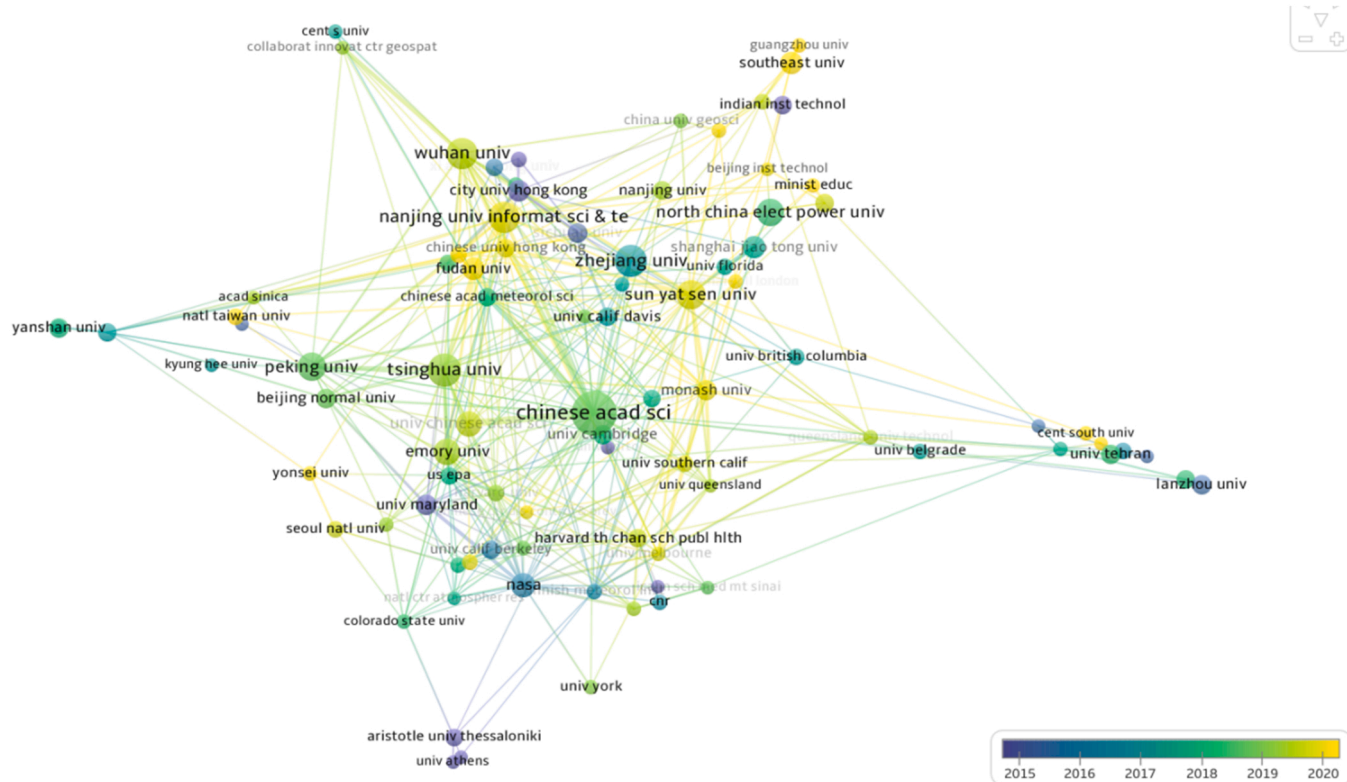


Fig. 4. Collaboration networks of the 96 institutions that each published > 10 papers. Note: The larger the marker, the more articles published; the lighter the color the more recent the publication.

3. Results and discussion

3.1. Temporal changes in the number of publications and keywords

The number of publications in the Local Database and the frequency of occurrence of the top 15 keywords are shown in Fig. 2. The publications increased from 1990 to 2021, with the first published research in 1993, applying ML to predict ambient SO_2 concentrations (Boznar et al., 1993). Research publications totaled less than 100 each year and increased slowly before 2015, with most research focusing on pollutant prediction by means of ANN. An explosive growth of publications occurred after 2017, with the total each year approaching 800 in 2021, illustrating the rapidly increasing interest in ML applications to air pollution research.

Changes in keywords are mainly reflected in two topics: ML algorithms and research targets. With the rapid increase of publications after 2015, the types of ML algorithms also increased. The phrase “machine learning” is now found in many papers, with ML algorithms such as “RF”, “SVM” and “deep learning (DL)” appearing more and more frequently in recent years. The increasing use of multiple ML algorithms probably results from the requirement for better prediction accuracy. ANN has been used to predict atmospheric pollutant concentrations at a certain point in the past (Gardner and Dorling, 1999; Yi and Prybutok, 1996). With algorithm innovation, some emerging ML models can obtain more accurate prediction with less bias. For instance, DL has the capacity to achieve hourly forecasting and grid mapping to display high spatial-temporal resolution prediction of pollutants (Brokamp et al., 2017; Najafi et al., 2016; Qin et al., 2019; Yan et al., 2021). RF supports the analysis of the relationships between target pollutants and variables and so pollution formation mechanisms (Li et al., 2022b; Ye et al., 2022).

Fine particulate matter ($\text{PM}_{2.5}$), ozone, inhalable particulate matter (PM_{10}) and volatile organic compounds (VOCs) have been the main target pollutants, among which $\text{PM}_{2.5}$ has been of the most concern, with a greatly increased frequency of ML model applications after 2017. The

application of ML models for indoor air quality control also gradually increased after 2015 (Ren and Cao, 2019; Yuchi et al., 2019). Generally, the main applications of ML were for predicting chemical characteristics of pollutants, including concentrations and their spatial and temporal variation.

3.2. Influential countries and groups

A total of 101 countries have conducted air pollution research using ML. The distribution and collaborations of active groups are shown in Fig. 3. China leads with the most publications (1023), followed by the USA (376) and India (186). Fig. 3b shows the collaborations of each country, in which cooperation between China and the USA have been the most frequent (180), followed by China and the UK (59) and the USA and the UK (39). Multiple country publications (MCP) are an indicator of international collaboration. However, the proportion of MCP for the top three countries was less than 30% (Fig. 3c), which shows that most research was conducted independently.

A total of 2836 institutions contributed to the application of ML to air quality research, of which 96 published more than 10 articles. The collaborations in these 96 papers are shown in Fig. 4: the bigger the size of the label, the more publications; the lighter the color, the more recent the publication. The Chinese Academy of Sciences published the most papers with 147 documents, followed by Tsinghua University (China) (56), and Wuhan University (China) (53). Most of the affiliations with the higher numbers of publications were in China, and Chinese institutions accounted for 70% of the top 20 institutions.

Local and global citation scores are the citation number in the Local Database and global WoS core databases, respectively. The ratio between local and global citation scores ($R_{(L/G)}$) was calculated to indicate the impact of each institution. A high $R_{(L/G)}$ means that an institution has had a significant impact on air pollution research by applying ML. The results in Tab. S3 show that Emory University has the highest $R_{(L/G)}$ value of the top 20 institutions, followed by Peking University and

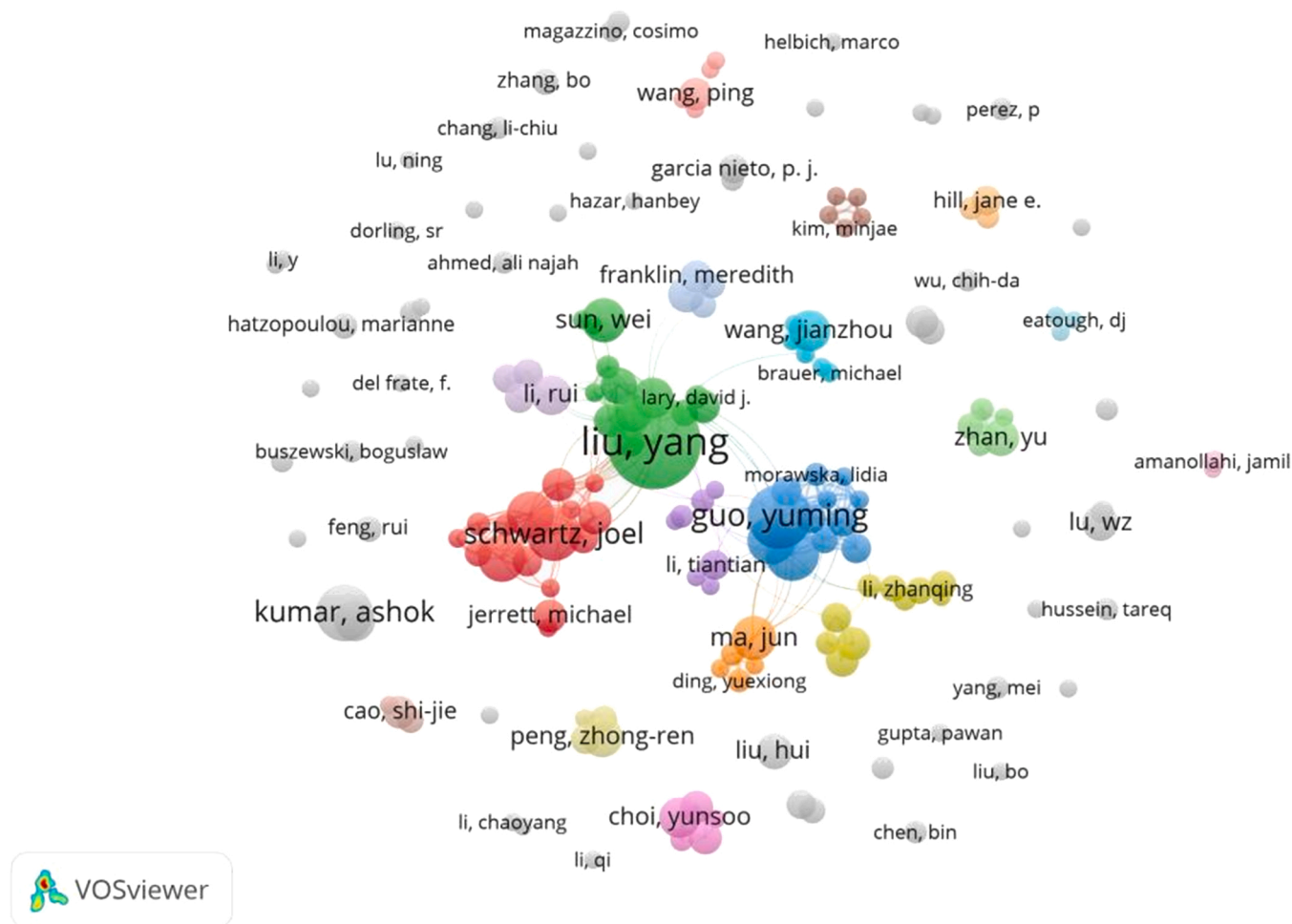


Fig. 5. Collaboration network of authors.

Sichuan University. Most Chinese institutions in the top 20 have both more publications and a higher $R_{(L/G)}$, suggesting China has had the greatest influence in this field. In Fig. 4, the lighter colors of Sun Yat-sen University (China), Fudan University (China) and Southeast University (China) show that the number of publications from these organizations has increased rapidly in recent years, suggesting that they could be important centers for ML applications in atmospheric research in the future.

Regarding authors, 11030 were recorded, but only 169 (1.5%) could be described as 'active', publishing more than 5 papers. The co-author relationships and details of active authors are shown in Fig. 5 and Tab. S4. Liu Yang ranked first with 27 publications, followed by Guo Yuming (18) and Kumar Ashok (16). Authors concentrated in the middle of Fig. 5 have multiple collaborations, but most authors have few if any collaborations. This indicates that associations between authors are generally weak and large research groupings have not yet formed. Greater collaboration should be advocated. The average publication year of each author is shown in Tab. S4, with 76% of authors was after 2019, suggesting that the application of ML to air pollution research is still a novel field.

3.3. Journals with most impact

The influence of journals can be assessed by analyzing the number of publications and citations in each, which can guide researchers as to where best to submit manuscripts. A total of 686 journals have published papers applying ML to air pollution, but only 54 journals published more than 10 papers in this field. The details of the 20 journals that published

the most papers are shown in Tab.S5. European and American journals contributed the most publications. Although papers from China dominate, Chinese journals published relatively few of these, highlighting the need for relevant and high impact journals based in China. Most journals are in the environmental science category. However, some such as *IEEE Access* and *Sensors* are not classified as environmental by the JCR, indicating that some of the research is interdisciplinary. These papers involved topics such as ML algorithm modification and efficiency improvement for chemical detection (e.g. Al-Janabi et al., 2019; Spinelle et al., 2017).

The journal *Atmospheric Environment* published by far the most papers (154), followed by *Science of the Total Environment* (97) and *Environmental Pollution* (72). $R_{(L/G)}$ and $R_{(year)}$ (the ratio of ML-related publications after 2017 to total publications in that journal) of the top journals are shown in Fig. 6. A high $R_{(year)}$ value indicates that a journal has a strong interest in air pollution research that applies ML and has received an increasing number of articles in the 5 years to 2021. The $R_{(L/G)}$ and $R_{(year)}$ values of *Environmental Pollution* and *IEEE Access* exceeded the mean values and ranked third and fourth for the number of publications. These two journals have a strong interest in air pollution research that applies ML and are regularly selected by those researching ML-related to air pollution, suggesting that they are very suitable for future research submissions. Some journals with high $R_{(L/G)}$ values were distributed in the lower right quadrant of Fig. 6. These had high citations in the Local Database, and most were classic scientific journals publishing in atmospheric science, such as *Atmospheric Environment*, *Atmospheric Pollution Research*, and *Atmospheric Chemistry and Physics*, or were influential journals in the environmental field such as *Science of the Total*

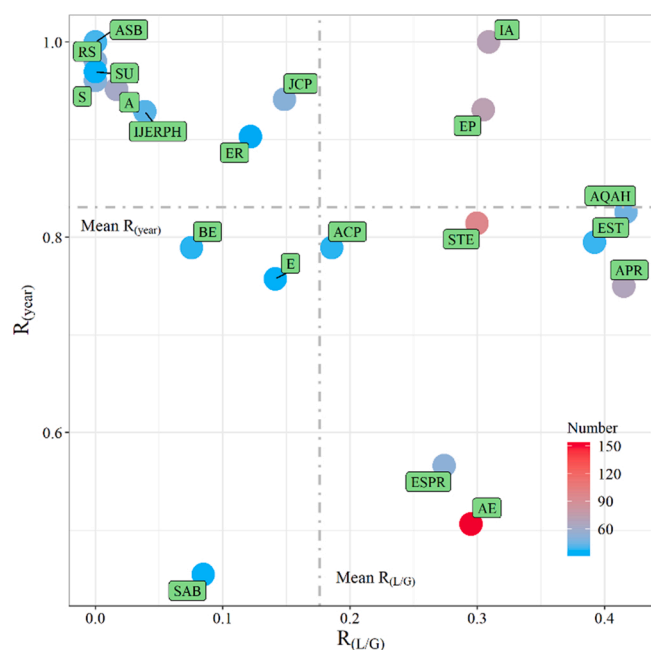


Fig. 6. Comparison of $R(L/G)$ and $R(\text{year})$ for the 20 journals publishing the most ML-related papers. (AE: Atmospheric Environment; STE: Science of the Total Environment; EP: Environmental Pollution; IA: IEEE Access; APR: Atmospheric Pollution Research; A: Atmosphere; ESPR: Environmental Science and Pollution Research; JCP: Journal of Cleaner Production; RS: Remote Sensing; S: Sensors; AQAH: Air Quality Atmosphere and Health; IJERPH: International Journal of Environmental Research and Public Health; ASB: Applied Sciences-Basel; EST: Environmental Science & Technology; ACP: Atmospheric Chemistry and Physics; BE: Building and Environment; E: Energy; SAB: Sensors and Actuators B-Chemical; SU: Sustainability; ER: Environmental Research).

Environment and Environmental Science & Technology. Most papers published in these journals were concerned with applying ML to chemical processes of air pollutants formation.

3.4. Research focuses

Cluster analysis was conducted using VOSviewer to better understand the foci of ML-related articles. As shown in Fig. 7, publications were divided into four categories. Cluster 1 contains papers reporting ‘sensors’, ‘classification’, ‘detection’, ‘VOCs,’ and similar topics. Research in Cluster 1 was mainly focused on applying ML models to identifying specific signals in software for improving the efficiency of chemical detection. ML models have been applied not only to VOC detection but also to $\text{PM}_{2.5}$, carbon monoxide (CO) and nitrogen dioxide (NO_2) monitoring (Spinelle et al., 2017; Srivastava, 2003; Wang et al., 2014; Zhang et al., 2021a; Zimmerman et al., 2018), in which ANN is the most widely used machine learning algorithm. The different sensitivities of each sensor resulted from the range of detection materials used that respond differently to the target gas (Penza and Cassano, 2003). It is difficult to meet the detection requirements with a single sensor, but the cost will increase when using multiple sensors (Lee et al., 2002). Therefore, ML algorithms are introduced in a data processing module for calibration and improving detection efficiency. Initially, unique signal values for the pure gas are recorded for each sensor and input to the data processing module with a high frequency. Then ML algorithms use the input data as “training data” for model development (Zhang et al., 2021a). The constructed models are packaged in the instrument operating software. When a gas mixture is detected, ML models can analyze the data and rapidly identify each gas with a similar signal value (Barash et al., 2012; Zhang et al., 2012).

Words such as ‘emission’, ‘ NO_x ’, ‘optimization’ and ‘engine’ are

distributed in Cluster 2. Research in this cluster focused on vehicle exhaust mitigation, where ML algorithms, especially ANN, are used to optimize parameters for reducing engine emissions (Hosamani et al., 2021; Lv et al., 2013). Typical exhaust emissions contained particulate matter (PM), nitrogen oxides (NO_x), hydrocarbons (HC) and CO (Gugulothu et al., 2021; Norouzi et al., 2020; Roy et al., 2014), which are influenced by engine type and fuel blending (Deh Kiani et al., 2010; Gugulothu et al., 2021). An effective design is critical for improving fuel efficiency and reducing emissions. To select the optimal design, ML models have been used to avoid consideration of the instantaneous combustion process and predict exhaust emissions quickly at low cost (Arcaklioglu and Çelikten, 2005). Usually, data collected from preliminary experiments can provide a rough range of parameters for model optimization. Parameters are then adjusted based on ML models for reducing emissions without having to repeat experiments.

Words such as ‘forecasting’ and ‘root mean square error’ (RMSE) are prominent in Cluster 3, while ‘particulate matter’, ‘China’, ‘observation’ and ‘estimate’ dominate in Cluster 4. These two fields of research both focused on the application of ML algorithms for fast and accurate prediction of pollutants, combined with historical meteorological, geographic and atmospheric pollutant data (Benhaddi and Ouarzazi, 2021; Hu et al., 2017). Commonly used ML methods were conventional neural network algorithms, especially DL, including convolutional neural networks (CNN) and long short-term memory (LSTM), with mean square error (MSE) and RMSE as evaluation indicators (Sun et al., 2020; Zhong et al., 2021). However, the purposes of these models are not the same. Alone or associated with atmospheric numerical models, most ML models in Cluster 3 were used to improve the accuracy of short-term forecasting for atmospheric contamination, especially $\text{PM}_{2.5}$ (Huang et al., 2021; Yan et al., 2021). In Cluster 4, most ML models were used to reveal the chemical characteristics of pollutants. Early research mainly focused on the spatiotemporal distribution of $\text{PM}_{2.5}$ (Chen et al., 2018; Gupta and Christopher, 2009; Hu et al., 2017), but gradually expanded to the chemical characterization of specific components and precursors in $\text{PM}_{2.5}$ with the development of ML models (Brokamp et al., 2017; Xu et al., 2017). Cluster 4 contained most articles (31.4%) and these had a more recent publication date (Fig. S1), indicating that applying ML for analyzing the chemical characteristics of atmospheric pollutants has become a recent focus of research.

The five most highly cited articles in the past 30 years were analyzed to provide more insight into recent research priorities (Tab. S6). Among these, Feng et al. (2015) was one of the earliest publications, in which ANN was combined with geographic models and wavelet transformation to improve the accuracy of forecasting $\text{PM}_{2.5}$ concentrations in North China. Following this, Di et al. (2016) and Hu et al. (2017) used RF and CNN, respectively, to estimate $\text{PM}_{2.5}$ concentrations with high spatial resolution across the United States, based on meteorological parameters, satellite aerosol optical depth and land-use variables. Li et al. (2017) used LSTM layers to explore the spatiotemporal correlation of pollutants for more accurate predictions in Beijing, China. Chen et al. (2018) used meteorological parameters, remote sensing data and land use information to create a $\text{PM}_{2.5}$ prediction model with RF and estimated the historical trend of $\text{PM}_{2.5}$ pollution across China. These five papers all focused on applying ML for analyzing the chemical characteristics of regional pollution, similar to the research papers that group into Cluster 4. This shows again that using ML models to analyze the chemical characteristics of atmospheric pollutants has been an important research focus.

3.5. Developments

In recent years, ML models have been applied ever more widely owing to the continuous innovation of algorithms. Analyzing articles in the impactful journals (Tab. S5) and highly cited papers (contained but not limited to Tab. S6), provides new insights for developments of ML applications in air pollution research.

concentrations in chemical transport models resulted from the underestimation of dry deposition and cloud optical depth. Further, coupled with a SHapley Additive ExPlanation (SHAP) approach, any ML model can provide a clear explanation of variable importance (evaluating contributions in physical units such as $\mu\text{g}/\text{m}^3$), which can support the dimension reduction of variables for the source apportionment of pollutants (Hou et al., 2022; Qin et al., 2022b; Zhang et al., 2022).

Scenario simulation with ML models enables researchers to evaluate control strategies. As with traditional numerical models, researchers can evaluate the effectiveness of management measures for air pollution mitigation at regional or even global scales. For example, Li et al. (2022a) predicted a decreasing trend of global aerosol pollution from 2020 to 2100, based on a number of projections in the Coupled Model Intercomparison Project Phase 6. Xu et al. (2022b) forecasted ammonia emissions and their resultant health impacts in 2030 under several scenarios in which nitrogen fertilizer was replaced by agricultural wastes. ML models are also an alternative for clarifying the factors driving air quality change over the short term. Research has simulated atmospheric pollutant variation under various emission scenarios to assess the impact of reduced anthropogenic activity during COVID-19 lockdowns periods (He et al., 2021; Shi et al., 2021). Compared to traditional numerical models, ML models are simpler and easier for new users. Moreover, data from economic, energy-related and other fields can be incorporated into ML models to further identify key driving factors, providing more comprehensive evaluations of regional or national air quality management. More scenario simulations using ML models are expected in the future.

Although ML has shown great potential in air pollution research, there are still some issues worth noting when considering its future application. Firstly, outputs of ML models are highly dependent on the quality of training data. Representativeness rather than number of variables is the basis for better model performance; pre-process variables must be carefully selected, and model users must have enough experience and patience to debug the models effectively. Secondly, outputs are merely the results of computer calculations and sometimes may contradict current understanding due to the “black box” effect if there is no good understanding and what the model does. Therefore, after model construction, the simulations should be fully verified and interpreted based on atmospheric theory.

4. Conclusion

Publications that apply ML to air pollution research have increased rapidly in the past 30 years and grew exponentially after 2017. Dominant research groups were based mainly in China and the United States, which together accounted for more than 50% of all articles. Research institutions and groups were relatively scattered, and large research collaborations have not yet formed. However, the application of ML to air pollution research has reached maturity, with a strong focus on the chemical characteristic analysis of pollutants, short-term pollutant forecasts, improving pollutant detection efficiency and optimizing design for emission reduction. Based on representative training data and effective verification, ML models supported by advanced algorithms have considerable potential to comprehensively interpret air pollution formation and control, including exploring the chemical characteristics of multiple pollutants, quantifying atmospheric chemical process and their driving factors, and simulating scenarios.

CRedit authorship contribution statement

Yunzhe Li: Data curation, Writing – original draft preparation, Visualization. **Zhipeng Sha:** Data curation, Visualization. **Aohan Tang:** Conceptualization, Methodology, Supervision. **Keith Goulding:** Writing – review & editing. **Xuejun Liu:** Writing – review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data Availability

Data will be made available on request.

Acknowledgments

This work was supported by the Key Program of the National Natural Science Foundation of China (No. 41730855), the major project of Inner Mongolian Natural Science Foundation (No. 2019ZD02), and the High-level Innovative Talent Project of China Agricultural University.

Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.ecoenv.2023.114911.

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