

The insight of why: Causal inference in Earth system science

Jianbin SU¹, Duxin CHEN², Donghai ZHENG¹, Yang SU³ & Xin LI^{1*}

¹ National Tibetan Plateau Data Center, State Key Laboratory of Tibetan Plateau Earth System, Environment and Resources (TPESER),
Institute of Tibetan Plateau Research, Chinese Academy of Sciences, Beijing 100101, China;

² School of Mathematics, Southeast University, Nanjing 210096, China;

³ Northwest Institute of Eco-Environment and Resources, University of Chinese Academy of Sciences, Lanzhou 730000, China

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Abstract The utilization of big Earth data has provided insights into the planet we inhabit in unprecedented dimensions and scales. Unraveling the concealed causal connections within intricate data holds paramount importance for attaining a profound comprehension of the Earth system. Statistical methods founded on correlation have predominated in Earth system science (ESS) for a long time. Nevertheless, correlation does not imply causation, especially when confronted with spurious correlations resulting from big data. Consequently, traditional correlation and regression methods are inadequate for addressing causation related problems in the Earth system. In recent years, propelled by advancements in causal theory and inference methods, particularly the maturity of causal discovery and causal graphical models, causal inference has demonstrated vigorous vitality in various research directions in the Earth system, such as regularities revealing, processes understanding, hypothesis testing, and physical models improving. This paper commences by delving into the origins, connotations, and development of causality, subsequently outlining the principal frameworks of causal inference and the commonly used methods in ESS. Additionally, it reviews the applications of causal inference in the main branches of the Earth system and summarizes the challenges and development directions of causal inference in ESS. In the big Earth data era, as an important method of big data analysis, causal inference, along with physical model and machine learning, can assist the paradigm transformation of ESS from a model-driven paradigm to a paradigm of integration of both mechanism and data. Looking forward, the establishment of a meticulously structured and normalized causal theory can act as a foundational cornerstone for fostering causal cognition in ESS and propel the leap from fragmented research towards a comprehensive understanding of the Earth system.

Keywords Causal inference, Machine learning, Earth system science, Causal discovery, Artificial Intelligence

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1. Introduction

The Earth system encompasses integral components of the atmosphere, hydrosphere, lithosphere (including the crust, mantle, and core), and biosphere (including human beings). Earth system science (ESS) adopts a comprehensive, global, and systematic perspective to explore the interrelationships and interactions among these subsystems across various spatial and temporal scales. This methodology significantly

enhances our understanding of the environment in which we inhabit (Reichstein et al., 2019; Steffen et al., 2020). The coexistence and game between correlation and causation have never cease in the study of Earth system interactions. Initially, causality was regarded as the theoretical embodiment of objective law. Under the premise of “real-world simplicity”, causal relationships can be extracted from the interactions of key Earth system variables through numerically controlled experiments. These endeavors have propelled the advancement of ESS theory and have served as the

* Corresponding author (email: xinli@itpcas.ac.cn)

foundation for constructing diverse geophysical models. Influenced by modern control theory and information theory, statistical analyses centered on correlation (e.g., regression and machine learning) have gradually become mainstream methods in ESS research and have partly addressed the challenge of quantitative prediction (Shen and Zhang, 2023). In 2008, Anderson (2008) proposed the notion of “correlation replacing causality”, which brought the game between correlation and causation to the forefront and ignited intense debates on their relationship in the era of big data (Succi and Coveney, 2019).

In fact, prior to the establishment of a clear definition of causality, correlation and causation were historically used interchangeably, despite the essential differences between the two concepts. Correlation generally represents a general association, whereas causality implies a dependence relationship (Altman and Krzywinski, 2015). While variables with a causal relationship must be correlated, correlation alone does not necessarily imply causation (Aslam, 2015). The emergence of the big data era has greatly facilitated scientific research, but it has also led to the proliferation of “spurious correlations” (Calude and Longo, 2017). This issue is particularly prominent in high-dimensional and strongly nonlinear Earth systems, where “spurious correlations” are quite prevalent (Runge et al., 2019a), potentially posing risks for research based on traditional correlation methods (Nearing et al., 2020). Furthermore, impacted by confounding factors and potential hidden variables, it becomes challenging to provide a reasonable explanation for inference results based on correlation (Peng and Susan, 2022). For instance, in ESS research, the underlying logic and interpretability of results from correlation based machine learning models have consistently hindered their further advancement (Shen and Zhang, 2023). Undoubtedly, correlation-based methods have achieved a series of successes in ESS research. However, as a fundamental scientific concept, causality has the potential to expand the scope of traditional correlation research and play a crucial role in explanation, prediction, control, and decision-making (Zhang et al., 2018). Therefore, we argue that the assertion that “correlation replaces causality” is not appropriate for ESS research. The theoretical development of ESS still relies on a deep interpretation of causality among geophysical variables.

While simple causal associations can be recognized based on common sense and personal experience, establishing causal relationships becomes increasingly difficult within complex systems. In practice, the identification of causal associations and quantification of causal effects pose significant challenges in analyzing complex dynamical systems, particularly in the context of systems with multiple variables (Pearl and Mackenzie, 2018). Traditional randomized controlled experiments are the most effective method for inferring causal association (Wang and Chen, 2022), but they

are often impractical when studying large-scale complex dynamical systems like the Earth system. Simulation experiments have emerged as a prevalent approach in studying causal association in ESS, but they often require substantial time, resources, and expertise (Stocker, 2014). In recent decades, the rapid growth of observations, including ground-based and remote sensing data, as well as outputs from Earth system models, has prompted a paradigm shift in ESS towards data-intensive scientific discoveries (Guo et al., 2017). The data-driven causal inference has consequently garnered increasing attention. By establishing causal associations between phenomena and confounding factors, causal inference enables the identification of independent and actual effects of specific components within complex Earth systems (Li et al., 2023). Compared to classical statistical techniques, causal inference can discern direct and indirect pathway, as well as common driving factors, from data, making it a more viable and applicable in ESS research (Runge et al., 2019a). In the field of ESS, research causal inference has been conducted to address various important questions, including how to identify interactions and pathways among different components of the Earth system; how to quantify the driving-response relationships form diverse geophysical variables within complex Earth system; how to assess and quantify the impact and contribution of subsystems/variables on extreme events; and how to objectively evaluate the direct and indirect factors influencing climate change, and thus robustly predicting future climate change trends? To tackle these inquiries, it is essential to decipher causal associations between different components of the Earth system, analyze causal effects among different variables, and accurately identify causal pathways.

Therefore, this paper sets out to explore the origins and intension of causal association and provides a comprehensive overview of the theoretical framework and common methodologies utilized in causal inference. Furthermore, it reviews the applications of causal inference in the main fields of ESS and analyzes the challenges and future trends of causal inference in ESS.

2. The origin, content and development of causal association

2.1 The philosophical origin of causality

The discourse on causality in the history of philosophy has spanned thousands of years, as depicted in Figure 1. The earliest definition of “cause” can be traced back to the ancient Greek philosopher Aristotle, who emphasized that cause is employed to address the question of “why”. Aristotle’s renowned “four-cause hypothesis” theory logically categorized the “form-formal causes” as the “first causes” and argued that the necessary conditions for the manifesta-

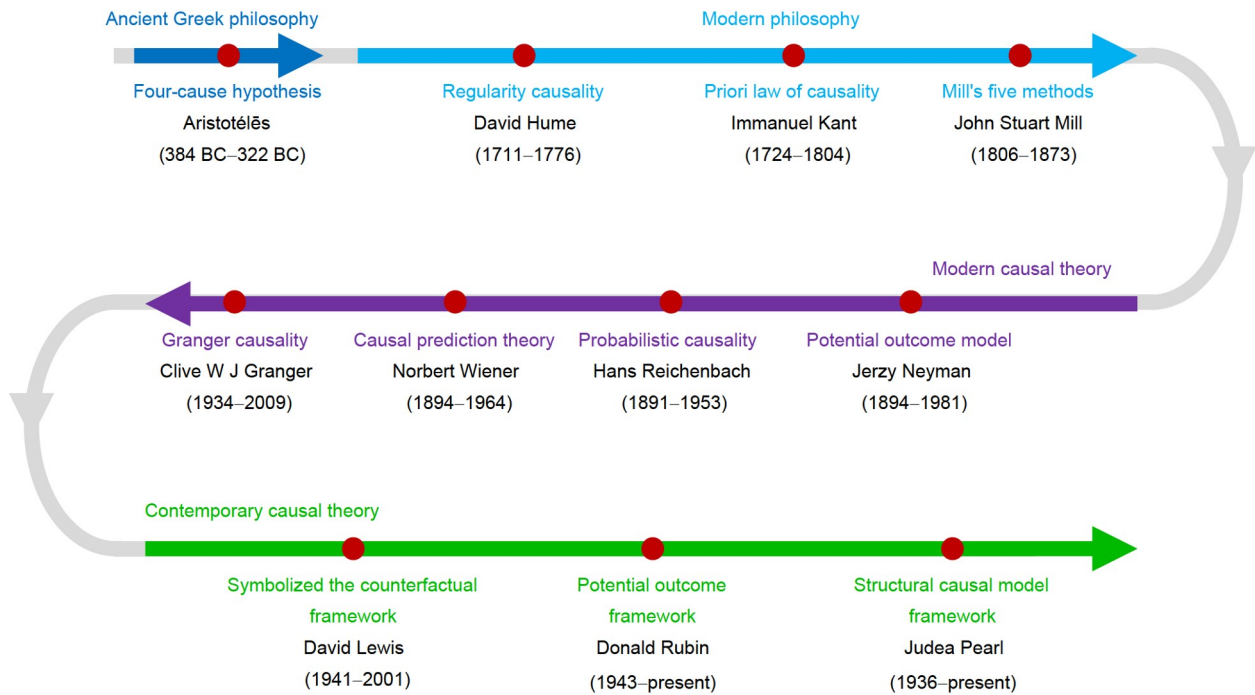


Figure 1 Overview of causal origin.

tion of phenomena should be regarded as causes (Sabine and Russell, 1946). Aristotle's theory aimed to uncover the enduring essence underlying transient phenomena and exerted a profound influence on modern Western philosophical and natural science. In the realm of modern philosophical epistemology, David Hume extensively examined causality from an empiricist perspective and proposed a theory of regularity causality (Hume, 2003). Methodologically, Hume not only provided insights into "what is the cause" but also addressed "how to identify a cause", thereby establishing the basis for causal thinking and causal inference (Kleinberg, 2015). Immanuel Kant, on the other hand, critically analyzed the empirical view of causality and reinterpreted it from a subjective and teleological standpoint, proposing the "a priori solution" to causality. Kant maintained that every phenomenon must have a cause, while the analysis of causality should rely on empirical experience. Kant's theory bridged the gap between empirical understanding and the rationalist notion of the innate existence of causality, harmonizing intuitive experience and rational thinking. John Stuart Mill endorsed the theory of regularity causality and proposed the "Mill's Method" as fundamental tools for causal induction and inference (Mill, 1874). Among these methods, the "Method of Differentiation" determined causality through individual control and comparison, laying the groundwork for modern causal thought. In summary, the understanding of cause and effect during this period primarily revolved around the concepts of "cause" and the general "law of causality".

In the 20th century, with the advancement of positivism, the study of causality underwent a transformation, shifting from the focus on "causal laws" to the exploration of probabilistic causality. This shift marked a pivotal "technical turn" in causal theory, moving it away from its purely philosophical origins. In this process, Jerzy Neyman illustrated the integration of random experiments and statistical inference using agricultural experiments and introduced the "potential outcome" model (Splawa-Neyman et al., 1990). While this model successfully mathematized causal inference in randomized experiments, it did not address the challenges posed by non-experimental observational studies due to the absence of randomization. Subsequently, Hans Reichenbach proposed the theory of probability causality, which provided a framework for the investigation of probabilistic causality (Reichenbach, 1956). Meanwhile, Norbert Wiener, widely acknowledged as the father of cybernetics, approached causality from a predictive perspective and introduced the theory of causal prediction (Wiener and Masani, 1958). He argued that, in a time series model, if variable X is the cause of variable Y , historical information about X can enhance the prediction accuracy of Y . However, this theory did not lead further breakthroughs in causal related data analysis. Later, Clive W J Granger, a Nobel laureate in economics, refined Wiener's causal prediction theory by utilizing linear autoregressive models of stochastic processes and introduced the Granger causality model, which ushered in a new era of time-series causal inference (Granger, 1969).

Benefited from the enlightenment on counterfactual

causality by Hume and Kant in philosophy, David Lewis symbolized the counterfactual framework and proposed a complete logical chain for counterfactual causality (Lewis, 1974), which elevated the theoretical study of causal inference to a higher stage and pointed out the direction of progress for the study of causal inference. Building upon the counterfactual theory, Donald Rubin recognized the potential outcomes as a powerful tool for understanding causal association and successfully applied them to non-experimental observational studies (Rubin, 1974), thus creating the widely accepted potential outcome framework (POF) in causal inference (Imbens and Rubin, 2015). Subsequently, Turing Award laureate Judea Pearl proposed an innovatively formalized theory of causality that incorporated graphical models, structural equations, and counterfactual analysis. This groundbreaking work established the widely embraced framework of the structural causal model (SCM) (Pearl and Mackenzie, 2018) and greatly promoted the process of integration of causal inference and machine learning (Zhang et al., 2018). Although the POF and SCM represent distinct perspectives in the development of causal theory, they share a common essence and fundamental consistency. Based on the causal system established by Pearl, the following sections will review the three levels of causation and delve into the profound nature of causality.

2.2 The ladder of causation

The causal analysis framework developed by Pearl is renowned for its clear mathematical concepts and algorithmic feasibility, establishing it as a rigorous and systematic methodology that has been acclaimed as a “causal revolution” (Pearl, 2000; Schölkopf, 2022). By deconstructing the process of causal thinking, Pearl classifies human cognitive abilities into three distinct levels: observation ability (Seeing), practical ability (Doing), and Imagination ability (Imagining). Building upon this foundation, he introduces the concept of the “ladder of causation” (Figure 2), which categorizes the deconstruction of causal relationships into three levels: association, intervention, and counterfactual, aligning with the three cognitive abilities, respectively (Pearl and Mackenzie, 2018). The first level, association, involves passive observation and the identification of objective regularities to establish a foundational understanding of causality. In practical terms, the association can be expressed as “What if I see ...?” and is known as conditional probability in statistics (i.e., $P(Y|X)$). Recent machine learning models widely employed in ESS research rely on the utilization of interrelationships among variables for prediction (Shen and Zhang, 2023). The second level, intervention, combines passive observation with active manipulation, leading to an

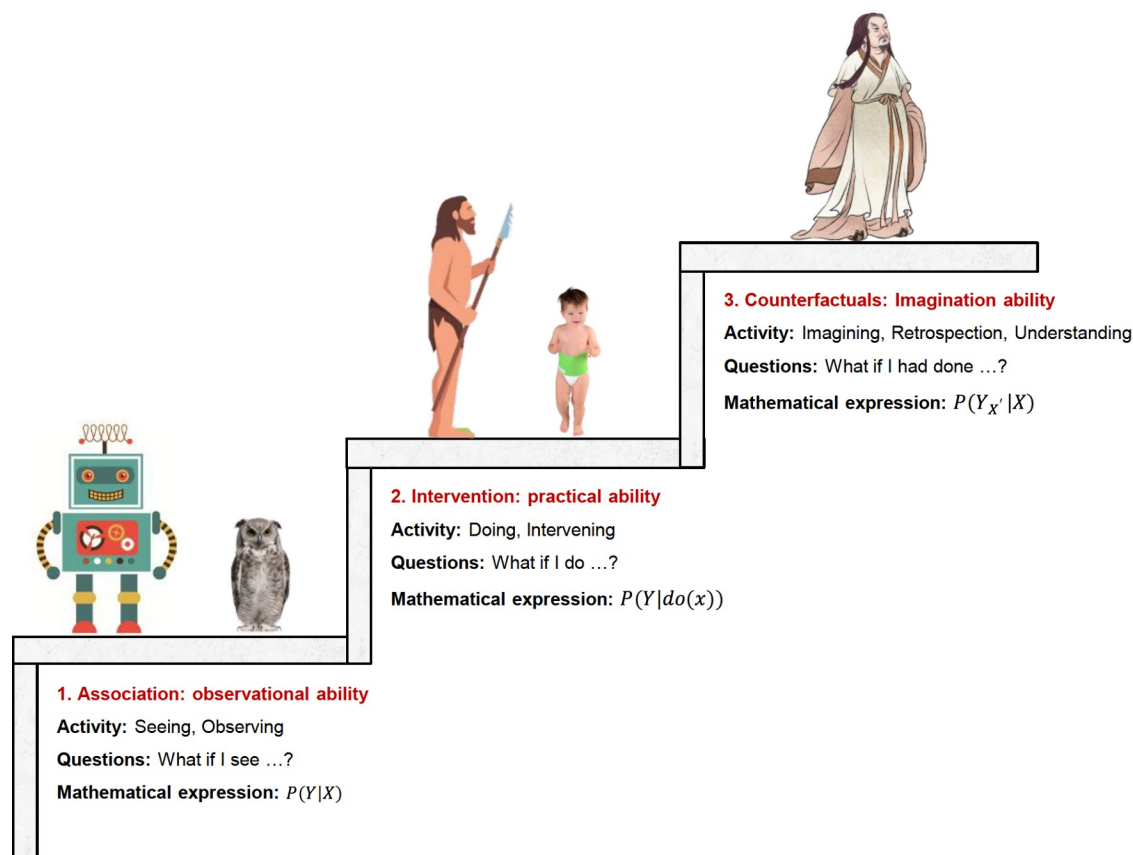


Figure 2 The Ladder of Causation, modified after Pearl and Mackenzie (2018) and permitted by Judea Pearl.

interventional understanding of causality and enabling assessments of causality's presence and direction. For instance, if intervening on X alters the distribution of Y (i.e., $P(Y|do(X))$), X is considered a cause of Y . The third level, counterfactual, involves estimating the outcome's change by modifying the conditions that contributed to the observed result (i.e., $P(Y_X|X)$). It entails retrospection and contemplation of past events, representing the highest level of causal understanding. For example, after a flood disaster, people naturally contemplate the potential outcomes had flood storage areas been activated or engineering measures implemented earlier. Although iterative counterfactual analysis cannot alter the occurrence of the disaster itself, it facilitates an exhaustive examination of its causes, offers practical recommendations for disaster prevention, and applies this knowledge to related domains, ultimately forming a comprehensive discipline.

2.3 The framework of causal inference

In recent decades, there has been a proliferation of causal inference methods in different disciplinary fields. However, many of these methods have been lacking a systematic framework and comprehensive theoretical guidance (Wang and Chen, 2022). With the development of causal theory, two prominent theoretical systems, namely the POF (Rubin, 1974; Imbens and Rubin, 2015) and the SCM framework (Pearl, 1995, 2000), have emerged as widely recognized theoretical frameworks in the field of causality. These frameworks have propelled the research of causal theory into a new stage of development.

2.3.1 The potential outcome framework

The core principle of the POF is to compare the disparities in outcomes between the intervention and non-intervention groups, attributing these differences to the impact of the intervention. However, as depicted in Figure 3, it is common to observe only one outcome for a given variable while other unobserved outcomes are potential outcomes. Taking binary intervention as an example, when $X_i(1)$ and $X_i(0)$ denote the outcomes of a given variable X_i under intervention and non-intervention, respectively, the individual causal effect (ICE) of X_i can be formulated as: $ICE(i) = X_i(1) - X_i(0)$. When considering the collective perspective, the average causal effect (ACE) can be calculated by averaging the ICEs, that is, $ACE = E(X(1)) - E(X(0))$, where $X(1)$ and $X(0)$ represent the potential outcomes under intervention and non-intervention for the population, respectively. Estimating causal effects is an important objective of causal inference within the POF. In practical applications, one of the challenges in the POF is addressing missing data. Given that observational studies cannot capture all potential outcomes for subjects, the POF seeks to estimate the absent data (i.e., potential outcomes)

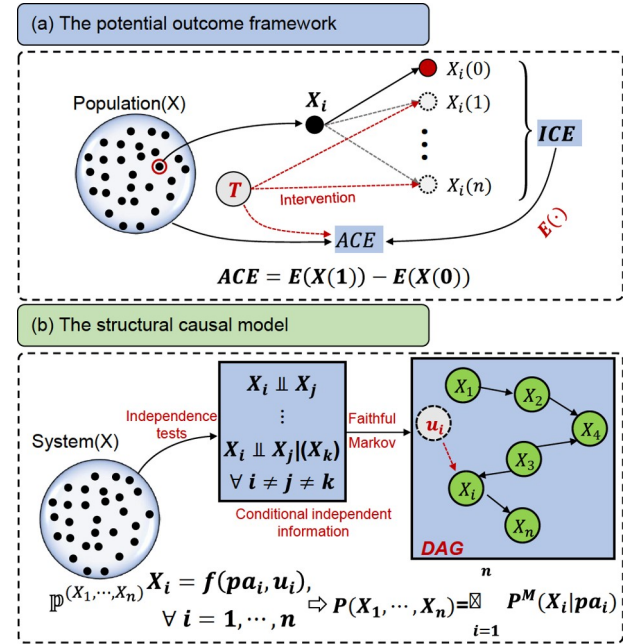


Figure 3 The Causal inference framework in the Earth system.

and infer causal effects by leveraging the distinctions between the absent data and the observed outcomes.

2.3.2 The structural causal model framework

Irrespective of its intricate theoretical foundation, the SCM framework comprises three fundamental components: graphical models, structural equations, and counterfactual interventions. The graphs serve as a visual mathematical language, encompassing nodes and edges that connect nodes (Thulasiraman and Swamy, 2011). Within the SCM framework, causal graphs typically take the form of directed acyclic graphs (DAGs), providing an intuitive representation of the specific relationships between nodes (Pearl, 2000). Structural equations act as a mathematical twin of causal graphs, enabling the quantification of the data-generating mechanisms for node variables. As depicted in Figure 3, each node variable X_i in the causal graph can be uniquely determined by its parent nodes (pa_i) and latent exogenous variables (u_i) through an equation of $X_i = f_i(pa_i, u_i)$, $\forall i = 1, 2, \dots, n$ (Pearl, 2000).

In practice applications, the core objective of the SCM framework is to discover the structure of causal graph using methodologies like conditional independence tests. Well-established criteria, including the front-door criterion, back-door criterion, are commonly employed for this purpose. It is worth noting that expert knowledge can be utilized to some extent to obtain prior causal graph structures, depending on the specific task requirements. However, it is important to acknowledge that this approach undeniably returns the trajectory of "expert systems". Within the SCM framework, the

do-operation serves as the primary method for implementing interventions, counterfactual operations, and thus conducting causal estimation. The key distinction is that the do-operator for intervention specifically targets a node variable, while the counterfactual do-operator simultaneously intervenes on both the node variable and the conditions (environmental variables) influenced by it. For instance, in the context of the current environment Z , an intervention on the node variable X_i can be represented as $do(X_i=x)$, indicating that the structural equation for node X_i is modified to $X_i=x$, eliminating the influence of its parent nodes and exogenous variables. The probability of predicting outcome Y can be denoted as $P(Y|do(X_i=x), Z)$. When a counterfactual intervention is applied to the node variable X_i , the probability of outcome Y can be expressed as $P(Y|do(X_i=x), Z')$, where Z' represents a hypothetical parallel world and all environmental factors in Z' unaffected by X_i are the same as in Z . In summary, the SCM framework provides a methodology that commences with a graph, allowing for the exploration of causal structures and the mechanisms generating the data, thereby facilitating causal estimation (Pearl and Mackenzie, 2018).

Although the POF and the SCM framework have different representations of causality, their understanding of causality is consistent, as both aim to determine the extent to which changing one variable can influence another variable. The SCM framework demonstrates greater expressive power and is adept at addressing complex problems, although it heavily relies on causal graphs. When confronted with intricate real-world issues, the inherent complexity makes it difficult to obtain comprehensive and accurate causal graphs, which limits the practical application of the SCM framework. Conversely, the POF provides a more concise description and requires less prior knowledge, making it more widely applicable. However, the causal interpretability of the POF is weaker than that of the SCM framework.

2.4 The Causal inference methods

2.4.1 Granger causality analysis

Granger causality analysis (GCA) is the pioneering standardized method for causal analysis that utilizes time series observations (Runge et al., 2019a). Its fundamental principle is that if the past information of time series X helps improve the predictive accuracy of time series Y , then X is considered a Granger cause of Y (Granger, 1969). Traditional GCA uses linear autoregressive models to address bivariate causal associations, providing a certain level of interpretability. However, this approach is limited to linear and stationary bivariate time series (Seth et al., 2015). To extend its applicability, numerous researchers have diversified and expanded GCA to encompass nonlinearity and multivariate scenarios, providing solutions for non-stationary time series as well (Moraffah et al., 2021). For instance, the conditional

Granger model has paved the way for studying high-dimensional causal inference (Geweke, 1982; Arize, 1993), while the kernel GCA method enhances the flexibility and adaptability of GCA in nonlinear systems. Furthermore, parameter estimation methods based on time-varying autoregressive models enable the application of GCA in non-stationary systems (Schäck et al., 2018).

2.4.2 Causal inference based on transfer entropy

With the development and refinement of information theory, the use of information metrics, especially transfer entropy (TE), for causal inference has been increasingly popularized (Schreiber, 2000). In contrast to GCA, information-based causal inference methods directly leverage the direction of information flow to infer causal associations, breaking away from the model dependency of traditional approaches (Wang and Chen, 2022). However, these information-based causal inference methods encounter significant limitations in multivariable complex systems, as they struggle to effectively identify causal pathways (Smirnov, 2013). Furthermore, information-based causal inference methods necessitate the calculation of probability density functions for variables. As the dimensionality of variables increases, they become vulnerable to the curse of dimensionality (Bellman, 1966). To address this issue, Runge et al. (2012) introduced a graph-based dimensionality decomposition method that decomposes integral TE into a combination of finite-dimensional TE, somewhat alleviating the curse of dimensionality.

Although the principles and criteria of information-based causal inference methods and GCA differ significantly, the outcomes of these two methods are equivalent when applied to variables that adhere to Gaussian distributions (Barnett et al., 2009). For example, in bivariate causal inference, causal inferences derived from pseudo TE closely correspond to the conclusions drawn from GCA across various systems, including linear, nonlinear, and chaotic systems (Silini and Masoller, 2021).

2.4.3 Nonlinear state-space methods

By utilizing state-space models, modern control theory effectively characterizes the relationships among variables in complex systems, revealing their dynamic mechanisms. The theory of state-space reconstruction, proposed by Takens (1981), provides a mathematical foundation for analyzing the dynamic mechanisms of nonlinear systems and serves as a theoretical basis for causal inference based on nonlinear state-space. Currently, nonlinear indexes of interdependence and convergent cross mapping (CCM) are the most commonly used methods for causal inference in nonlinear state-space analysis. Nonlinear indices of interdependence leverage the mapping relationships in state space to determine causal associations within the system. Commonly employed measures include the S and H indices (Arnhold et al., 1999),

the N index (Quiroga et al., 2000), the M index (Andrzejak et al., 2003), and the L index (Chicharro and Andrzejak, 2009). These indices effectively employ distance/rank statistics of the reconstructed state space to indicate the direction and strength of causal associations. On the other hand, CCM assumes that interactions occur within an underlying dynamic system and establishes causal relationships through time-delay embedding of variables (Sugihara et al., 2012; Ye et al., 2015). While sharing similarities with GCA in terms of interactions in underlying stochastic processes, CCM adopts a dynamical system perspective to analyze causal relationships, attracting widespread attention from researchers worldwide. Now, it has been widely applied in atmospheric science, ecological science, and hydrology research.

2.4.4 Causal discovery algorithm

In the framework of structural causal models, causal graphs play a crucial role, but they often remain unknown. The process of extracting causal information from observations to generate causal graphs is known as causal discovery and serves as an essential means to obtain causal structures and causal pathways. Essentially, causal discovery belongs to the realm of inverse problems as it involves inferring the data-generating mechanisms from observations. To ensure solvability, causal discovery typically relies on a set of predefined assumptions, such as the Markov condition and the faithfulness assumption (Schölkopf et al., 2021). However, even with these assumptions, causal discovery still faces challenges including Markov equivalence classes. Existing causal discovery algorithms mainly provide approximate solutions under predefined assumptions, resulting in distinctive algorithmic approaches.

Causal discovery algorithms based on combinatorial optimization are primarily employed to unveil underlying causal structures by the conditional independence of data. These methods typically commence with either an empty graph, such as the PC algorithm (Hund and Schroeder, 2020), or a fully connected graph, such as the IC algorithm (Verma and Pearl, 2022). Through an iterative process of adding or removing edges based on conditional independence information, they gradually construct a causal network. The cornerstone of combinatorial optimization algorithms lies in the test for conditional independence, which can be flexibly conducted using various types of tests. For instance, Runge et al. (2019b) proposed the PCMCI algorithm which combines the PC algorithm with the Momentary Conditional Independence (MCI) test. Such integration enables the reconstruction of large-scale causal networks from time series data. Subsequently, by separating the conditioning sets into lagged and contemporaneous sets, Runge (2020) introduced the PCMCI+ algorithm, effectively reducing spurious causal connections while maintaining high recall rates. The successful applications of causal discovery algorithms based on

combinatorial optimization have been demonstrated in diverse fields related to climate science.

Causal discovery algorithms based on combinatorial optimization face significant challenges when inferring causality from multivariate long series observations. To improve computational efficiency, causal discovery algorithms based on continuous optimization have emerged. For example, the NoTears algorithm transforms the problem of causal structure inference into a continuous optimization problem, effectively addressing the curse of dimensionality without requiring structural assumptions (Zheng et al., 2018). Expanding upon the NoTears framework, the DAG-GNN algorithm surpasses the limitations of linear models by incorporating neural network models (Yu et al., 2019). Function-based causal discovery also represents a prominent research direction in structural causal discovery. The LiNGAM method assumes that variables are linearly correlated, and the error follows a non-Gaussian distribution. Leveraging the asymmetry of causal mechanisms (Peters et al., 2017) and independent component analysis (Altman and Krzywinski, 2015), the LiNGAM method can identify causal directions (Shimizu et al., 2006). Subsequently, numerous studies have expanded upon the LiNGAM model from various perspectives (Shimizu et al., 2011; Henao and Winther, 2011), thus broadening its applicability. Notably, Hoyer et al. (2008) proposed the additive noise model (ANM) approach, which mitigates the reliance on non-Gaussian noise assumptions. For additional causal discovery algorithms, please refer to Vowels et al. (2021). Currently, the applications of continuous optimization-based and function-based causal discovery algorithms in ESS are limited. However, they hold great potential in facilitating high-dimensional and complex causal network inference, particularly in domains such as ecosystems and complex climate systems.

3. Causal inference and Earth system science

When studying the Earth as an open dynamic system, research methods in ESS face increased demands due to the involvement of numerous variables and strong interdependencies (Zhou et al., 2022). The progressive improvements of causal theories and inference methods provide significant opportunities to overcome the limitations of traditional correlation-based theories in ESS research. Given that multi-source observations of core variables in the Earth system are predominantly in the form of time series, the utilization of time series observations for quasi-experimental designs has long been the prevailing research direction for causal inference in the field of ESS, and it has garnered favor among numerous ESS researchers. It is important to note that time-series causal inference is fundamentally grounded in the two mainstream causal inference frameworks, serving as

proaches. Additionally, a series of challenges, including computational complexity and inference accuracy of high-dimensional time series, spurious causality in non-stationary time series, identification of latent variables and causal paths, quantification of causal strength, selection biases, and more, affect the reliability of time-series causal inference (Zeng et al., 2022). Therefore, the development of universally applicable and efficient time-series causal theories and tools is currently a focal direction in time-series causal inference research.

3.2 Application of causal inference in Earth system science

In recent years, causal inference methods have been successfully applied in various fields of ESS to address common causal-related problems. Word clouds can provide an overview of the focal research areas of causal inference in ESS. [Figure 4](#) presents a word cloud of keywords extracted from relevant studies focusing on causal inference in the Web of Science core database from 2000 to 2022. From the figure, it can be observed that the current applications of causal in-

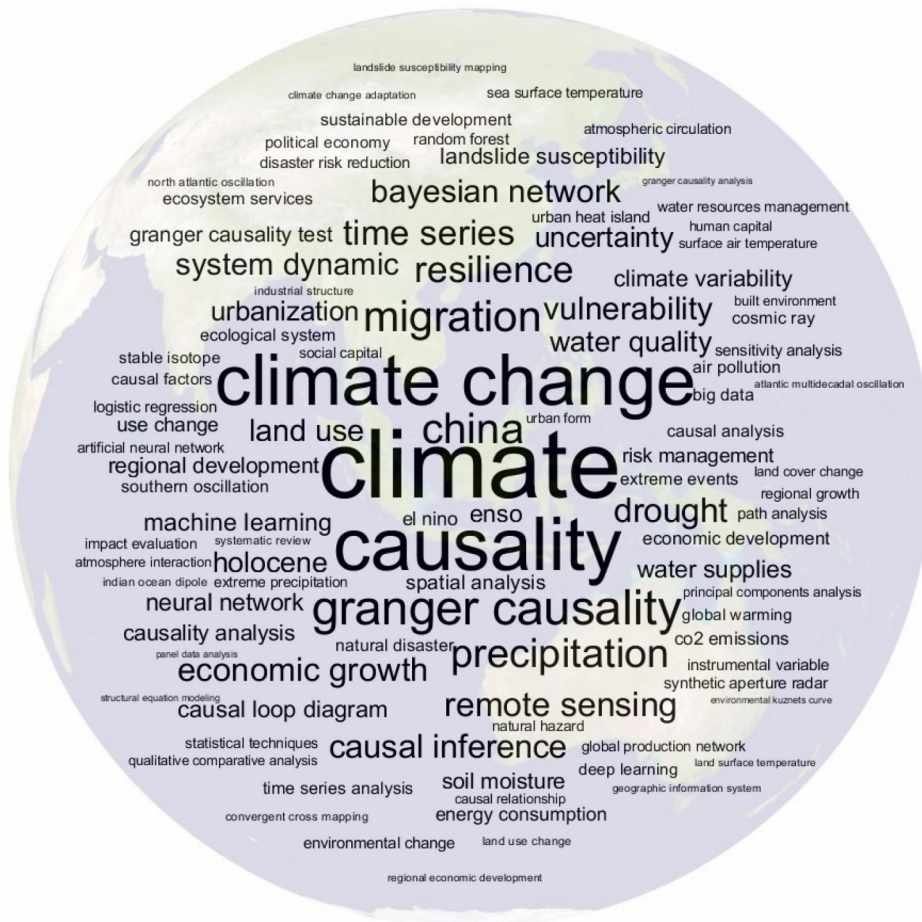


Figure 4 Word cloud map of causal inference in Earth system science, in which the size of words represents the corresponding occurrence frequency.

ference in ESS primarily revolve around atmospheric science, land surface science, ecology, and human geography. From a methodological perspective, the Granger causality method remains the mainstream approach in causal inference research. Various methods based on information entropy and nonlinear state space (e.g., CCM) have also gained significant attention from researchers. Additionally, studies within the framework of SCM, such as causal graph models and causal network discovery, have started to emerge. Figure 5 summarizes the major applications of causal inference in different branches of ESS, and the following sections will provide a brief review of the research progress of causal inference in these fields.

3.2.1 Atmospheric sciences

As a crucial component of the Earth system, the atmospheric system exhibits intricate spatiotemporal interactions among various physical processes. Interpreting these interactions from a causal perspective contributes to a deeper understanding of the operation mechanism the Earth's climate system and aids in improving climate and weather prediction models (Runge et al., 2019a). In the field of atmospheric science, causal inference is commonly used to analyze the driving factors of atmospheric circulation (Runge et al., 2014; Kretschmer et al., 2016) and plays a significant role in anomaly detection and attribution of atmospheric circulation patterns (Ebert-Uphoff and Deng, 2012). Climate teleconnections serve as the foundation for regional weather and climate forecasting, and causal inference plays a crucial role in quantifying the driving factors, causal directions, causal pathways, strength, and lag time of teleconnections (Runge et al., 2015; Nowack et al., 2020; Kretschmer et al., 2021). For instance, Kretschmer et al. (2016) used causal effect network to analyze different arctic drivers of midlatitude winter circulation, highlighting the importance of autumn sea ice concentrations in the Barents and Kara Seas as drivers of winter circulation in the midlatitudes. Ebert-Uphoff and Deng (2012) used causal graph models to deduce and validate the causal relationships between four prominent modes of atmospheric low-frequency variability in boreal winter. During the same period, Di Capua et al. (2020) evaluated the interactions between tropical convection mid-latitude summer circulation at different intra-seasonal timescales, as well as the influence of ENSO on these interactions. Through concrete examples of well-known atmospheric teleconnections, Kretschmer et al. (2021) argued that systematic causal inference methods should become a standard practice in teleconnection research. Climate and climate change have long been the focal research areas in atmospheric science (Huang et al., 2019). In the context of global climate change, causal inference has also been applied to attribution analysis of climate change (Triacca, 2005; van Nes et al., 2015) and causal evaluation of climate models (Nowack and Runge,

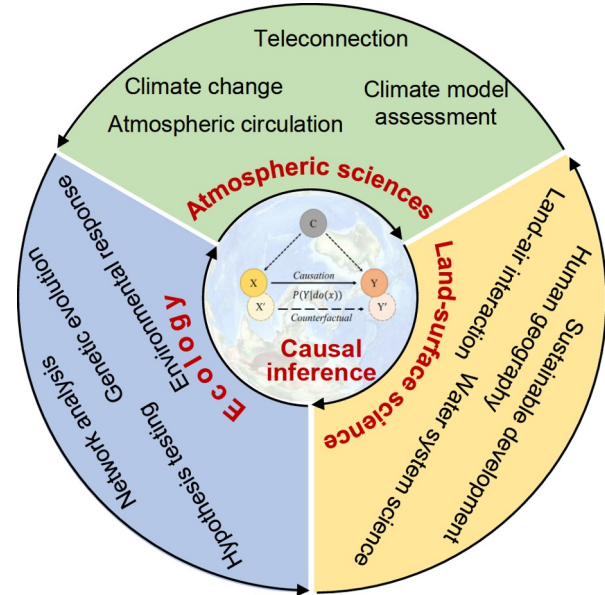


Figure 5 Application of causal inference in the main branches of ESS.

2018; Nowack et al., 2020; Vázquez-Patiño et al., 2020; Karmouche et al., 2022). Furthermore, analyzing the causal characteristics of atmospheric dynamics can aid in interpreting the impact of atmospheric circulation patterns on weather systems, thereby enhancing the attribution and understanding of extreme weather events (Hannart et al., 2015, 2016; Naveau et al., 2020) and providing valuable insights for climate policies and disaster response.

3.2.2 Land-surface science

The land surface system is an open and complex macro-system comprising climate, topography, landforms, land, hydrology, and other elements. It serves as the primary habitat for human survival (Li, 2014; Cheng and Li, 2015). Understanding the evolutionary patterns and driving-response mechanisms of land surface system components is a pivotal research focus in the field (Chen et al., 2019). Currently, causal inference has been successfully applied in various research areas of the land surface system. In the realm of land-atmosphere interaction, causal inference has shed new insights on identifying feedback relationships between soil moisture and precipitation (Salvucci et al., 2002; Li L et al., 2020), while also investigating the potential influence of confounding factors on the feedback system (Tuttle and Salvucci, 2017). In regional climate studies, causal inference has been employed to quantify the impact of land surface vegetation changes on regional climate systems (Jiang et al., 2015; Papagiannopoulou et al., 2017; Budakoti et al., 2021). Moreover, Mosedale et al. (2006) quantitatively diagnosed the feedback of sea surface temperature on the North Atlantic Oscillation (NAO) in the Granger causality framework, providing important evidence for enhancing at-

mospheric circulation models. Within the field of hydrology and water resources, the concept of causality has been extensively discussed as part of the “unsolved problems in hydrological” proposed in 2019, and the causal associations of hydrological processes are regarded as the ultimate goal of hydrological science research (Blöschl et al., 2019). Currently, causal inference methods have been widely used in investigating interactions and feedback mechanisms in the water cycle (Wei et al., 2021; You et al., 2021; Bonotto et al., 2022). Goodwell et al. (2020) even suggest that causal analysis, particularly information theory-based approaches, has ushered in a new paradigm for water system science research.

The human-earth system is a macro-system characterized by regional, comprehensive, and complex features, and has always been at the core of research in human geography (Fan, 2019). Understanding the evolutionary patterns and feedback mechanisms of human-earth relationships at different temporal scales is crucial for comprehending the human-earth system (Chen et al., 2021). Meyfroidt (2016) proposed that structured, standardized, and explicit causal inference can benefit the study of the human-earth system and recommended strengthening case studies on causal analysis to drive theoretical development. Ferraro et al. (2019) analyzed the challenges faced by causal inference in research on the human-earth system and suggested that adversarial ensembles of high-confidence inference results are an important approach to address these challenges. In the study of human-water coupling, appropriate causal inference schemes can be used to explain certain known water resource paradoxes, such as the tragedy of the commons in groundwater, regional water conflicts, and virtual water trade, providing insights for addressing social water resource challenges (Müller and Levy, 2019). Moreover, a profound understanding of the causal relationships in human-water coupling systems can contribute to the assessment and prediction of complex human-water systems (Penny et al., 2020). The United Nations sustainable development goals (SDGs) provide a 15-year development blueprint for global sustainable development, but recent research reports indicate significant temporal challenges in achieving the SDGs (Fu et al., 2019). The complex interactions, such as synergy and antagonism, among different development goals are important factors exacerbating this challenge (Fu et al., 2020). An increasing number of researchers and practitioners believe that a comprehensive analysis of the SDGs can be accomplished through an interdependent network approach, thereby promoting genuine sustainable development. Ospina-Forero et al. (2022) systematically compare commonly used methods for SDG network analysis and suggest that graph analysis methods based on causal inference are best suited for providing policy recommendations. Taking carbon dioxide emissions as an example, economic growth is iden-

tified as a primary factor influencing carbon emissions (Zhang et al., 2014; Al-Mulali et al., 2015), while renewable energy consumption can significantly reduce carbon emissions (Kayani et al., 2020).

3.2.3 Ecology

With the intensification of extreme climate events, ecosystem services are facing significant environmental challenges, and there is a growing interest in accurately predicting complex ecosystems (Piao et al., 2019). The distribution, abundance, and flux of organisms and matter within ecosystems are controlled by interactions within and across systems and are highly sensitive to environmental changes and management policies (Addicott et al., 2022). Causal interpretation of ecosystem interaction processes is an essential approach to enhance ecological predictions. Randomized experiments have traditionally been the dominant method for causal research in ecology, and causal inference based on non-experimental observations also originated from randomized experiments (Laubach et al., 2021). Causal inference is employed to address the limitations of randomized experiments (Kimmel et al., 2021), guide experimental design (Williams and Brown, 2019), identify confounding factors (Arif and MacNeil, 2023). It has achieved initial success in various research fields, such as ecological network (Li and Convertino, 2021; Barraquand et al., 2021) and population interactions (Pacoureau et al., 2019; Schoolmaster Jr et al., 2020). In terms of environmental response, numerous researchers have attempted to establish causal associations between species and climate variables, such as the sardine-anchovy-sea surface temperature problem (Sugihara et al., 2012), the climate-induced flowering phenology problem (precipitation, temperature, and their synergistic information) (Satake et al., 2021), and the influence of climate on population connectivity and gene flow (Yang et al., 2015). In studies related to genetic evolution, data-driven causal inference provides a fresh perspective for tracing the genetic differences among populations (Dures et al., 2020; Faith et al., 2021). Furthermore, Dronova and Taddeo (2022) highlight the significant value of integrating multi-source remote sensing observations with causal inference for advancing phenology research in the new era. As multi-source data rapidly accumulates, ecological research is gradually entering the era of big data, big theory, and big science (Niu et al., 2020), and making it an opportune time to incorporate causal inference into the standard toolkit of ecology (Larsen et al., 2019).

3.3 The integration of causal inference and big data assistances a paradigm shift in Earth system science research

With the development of information technology and ob-

servational analysis techniques, the amount of data generated in various stages of scientific research has experienced exponential growth. It has become a consensus that scientific research has entered the era of “big data” (Guo et al., 2014). As an important component of scientific big data, big Earth data shares general characteristics with other scientific datasets while also exhibiting strong spatial-temporal and physical correlations. It has become a new key to understanding the Earth, providing new opportunities for Earth system scientific research (Guo et al., 2016). However, “data is just data”, and big data itself cannot directly solve problems. Data science is a collective term for the analysis of all types of data, breaking traditional statistical barriers and enabling big data to serve scientific inquiries (Hernán et al., 2019).

In ESS research, based on scientific contributions and significance, data science plays a crucial role in three primary tasks: description, prediction, and counterfactual prediction (or causal inference) (Hernán et al., 2019). Currently, the applications of data science in ESS predominantly exhibit strong predictive capabilities but lack causality. Taking machine learning/deep learning as an example, once the prediction task and scientific question are clearly delineated, users merely need to determine input and output variables based on domain knowledge and prepare the corresponding data. Machine learning algorithms can then take charge of the subsequent data analysis, providing mappings and quantifying performance measures. While the internal workings of the mapping might lack transparency, the predictive performance of machine learning is generally commendable. On the other hand, executing causal inference requires not only clear scientific questions and the preparation of relevant data but also a comprehensive understanding of the inherent causal structure of the studied system. Assisting decision-making is a fundamental objective of data science. It is commonly believed that successful prediction forms the basis for improving decision-making capabilities; however, this perspective is subject to scrutiny. For example, predictive algorithms can effectively utilize weather information for short-term flood forecasts but face challenges in providing comprehensive flood risk reduction strategies. Additionally, predictive algorithms also encounter difficulties in addressing “what if” scenarios, such as evaluating the risk-benefit profiles of various decision proposals. In the context of big data, causal inference leverages expert knowledge from traditional model paradigms to offer counterfactual prediction outcomes, naturally providing an advantage in facilitating decision-making processes. Consequently, decision analysis for complex Earth systems heavily relies on data analysis methods grounded in causal knowledge.

In summary, within the context of big data, data science holds great potential to offer critical technical tools for ad-

vancing research in Earth system science (ESS), thereby driving the transition from traditional model-based paradigms to data-driven approaches. As one of the most vital methods for big data analysis, causal inference serves as the crucial bridge connecting model-based and data-driven paradigms, consistently assuming a foundational and pioneering role in various data science tasks. Additionally, it plays a key role in facilitating the paradigm shift in ESS, potentially realizing a model-data dual-driven research paradigm.

4. Challenges and development trends

Causal inference, as a sophisticated data analysis method, holds an indispensable role in hypothesis validation, process understanding, pattern identification, and knowledge discovery in ESS. Nevertheless, when harnessing non-experimental Earth big data for causal inference, one must navigate the coexistence of challenges and opportunities.

4.1 Challenges

4.1.1 Causal mechanism test

The ultimate objective of causal inference is to estimate the causal effects by utilizing potential/counterfactual outcomes following interventions (Rosenbaum and Rubin, 1983). However, various causal inference frameworks have distinct definitions of causal association, resulting in significant variations in the methods used for testing causal mechanisms. Within the POF, it is assumed that the same intervention would lead to the same potential outcomes, and these potential outcomes follow the same distribution to observed observations (Rubin, 1980). Consequently, causal mechanisms can be examined by comparing the distribution of the observations and potential outcomes. On the other hand, the SCM framework employs causal graphs to simulate the inference process of counterfactual outcomes. Thus, the SCM framework solely assumes the correctness of the causal inference process, without making additional assumptions about the distribution of counterfactual outcomes (Imbens and Rubin, 2015; Peters et al., 2017). Although some researchers still employ the discrepancy between counterfactual outcomes and actual observations for causal testing (Ness et al., 2019; Pawlowski et al., 2020), it is theoretically insufficient to prove the superiority of causal models within the SCM framework based solely on a smaller discrepancy in distributions. In reality, the examination of causal mechanisms within the SCM framework still relies on the prior knowledge of the target system possessed by the algorithm designer, thus providing plausible explanations for research findings. Overall, in different causal inference frameworks, the testing of causal mechanisms either excessively depends

on assumptions or lacks theoretical examination. Therefore, discovering and testing causal mechanisms in complex systems with unknown causal structures remains a fundamental challenge and one of the main difficulties in the field of causal inference.

4.1.2 *Experimental design of causal inference*

Assuming that the data generation mechanism is a necessary condition for causal inference, these prior assumptions may be mathematically reasonable and necessary (Kretschmer et al., 2021), but caution must be exercised in their application and generalization in ESS. The selection of Earth system variables and target regions presents practical challenges in the design of causal inference experiments. Taking climate system research as an example, to accomplish specific scientific tasks, the extraction of relevant time series from gridded spatiotemporal datasets requires the utilization of reliable expert knowledge and additional reasonable assumptions. Furthermore, the temporal interactions between different variables can vary significantly, underscoring the importance of carefully selecting appropriate time scales to ensure robust causal inference results (Fernández-Loría and Provost, 2022). Spatial heterogeneity represents another significant challenge in ESS causal inference. For instance, areas with varying surface wetness conditions may exhibit distinct feedback mechanisms between soil moisture and precipitation (Taylor et al., 2012; Guillod et al., 2015). Lastly, the distributions of variables and the associated noise are crucial considerations in ESS causal inference. For example, probability distributions of precipitation often deviate from Gaussian distribution and may display long tails that represent heavy and extreme rainfall events. Consequently, the evaluation and selection of suitable causal inference methods need to be approached with care. Additionally, some causal inference methods rely on the assumption of variable stationarity, necessitating the removal of seasonal cycles and potential trends when conducting causal inference in Earth system studies.

4.1.3 *Identification of hidden variables*

As an open complex giant system, the Earth system encompasses a multitude of factors and variables that interact within a complex and temporal dynamic system. How to address the dynamic feedback of multiple variables and identify cyclic processes presents significant challenges for causal inference research within ESS. In the context of causal inference in the Earth system, latent variables typically refer to unobservable, hidden/unknown variables, or variables with substantial uncertainty. The incomplete observation of Earth system states (including time and space) inherently gives rise to latent variables, thereby introducing confounding factors (Peng and Susan, 2022). How to obtain refined and comprehensive synchronous observations of the

Earth system is a shared challenge encountered by nearly all research engaged in causal inference. In addition to confounding factors, selection bias is practically inevitable when observing Earth system variables. For instance, satellite observations are constrained by factors such as cloud cover or orbital limitations, resulting in specific time sampling, which further diminishes the robustness of inference results (Shen et al., 2020). Consequently, uncovering the local structure of latent variables and devising measurement methodologies represent significant challenges in contemporary Earth system causal inference. The advent of the big data era presents novel opportunities for research in this domain, as it enables comprehensive characterization of the structural information (causal discovery) among variables and facilitates the verification of spurious causal relationships within causal graph structures to infer latent variable structures that are challenging to observe (Vowels et al., 2021).

4.1.4 *Lack of validation data*

The development, evaluation, and comparison of causal inference algorithms require benchmark validation datasets with known causal associations. Ideally, benchmark validation datasets should originate from real data with explicitly defined causal associations or prior knowledge from randomized experiments. However, the availability of publicly accessible benchmark datasets is currently limited, which has become a recognized bottleneck in the development of causal inference algorithms (Runge et al., 2019a). The main reason for this scarcity is that in many scenarios, the underlying causal mechanisms hidden within the data are complex and unknown. Developing robust validation methods and accumulating datasets with clearly defined causal mechanisms are essential for addressing the evaluation of causal inference algorithms. Utilizing simplified Earth system models to generate synthetic data with explicit causal mechanisms is an important alternative (Ombadi et al., 2020). However, acquiring such synthetic datasets remains challenging in ESS research. In this context, the challenge for causal reasoning in the Earth system is how to select appropriate datasets and hypothesis schemes, and then customize or screen appropriate causal reasoning schemes to meet task requirements.

4.2 *Development trends*

4.2.1 *Coupling of causal inference with geophysical models*

Observation and modeling are two important approaches in Earth system research (Li X et al., 2020). Even under the assumption of “simplified reality”, the development of models still requires extensive disciplinary knowledge. Regular understanding based on data analysis, experimental cognition, and the appropriate extension and transplantation

of existing knowledge are the primary means to acquire disciplinary knowledge. These methods align precisely with the three cognitive abilities of human beings and are consistent with the three levels in the ladder of causation. Consequently, the construction of Earth system models is inherently intertwined with underlying data analysis and causal inference. With the progress of causal theory and inference methods, our scientific understanding of the Earth system has been steadily deepening, playing a vital role in identifying shortcomings in existing Earth physics models and facilitating their improvement. Causal inference based on big data can further guide the design of complex parameterization schemes in models, enhancing their accuracy (Runge et al., 2019a). Simultaneously, causal inference can unveil direct and indirect associations among Earth system variables, thereby informing model architecture. Moreover, given the high complexity of the Earth system, most existing Earth system models simplify only specific physical processes, leaving numerous physical mechanisms unclear or incompletely understood. Through quasi-experimental approaches, causal inference can utilize multi-source observations to enhance our understanding of unknown physical processes and drive novel advancements in physical models. From this perspective, causal inference contributes to the emergence of more robust Earth system models (Figure 6).

Models represent the culmination of existing disciplinary knowledge in the field of Earth system research and play a fundamental role in our understanding of Earth system processes. The construction of physical models relies on a combination of differential equations that represent known

processes and semi-empirical relationships that account for unknown processes. Through data fitting, physical models can accurately simulate the “real” Earth and even make predictions about “future” Earth (Li et al., 2022). From this perspective, the utilization of Earth system models, or further incorporating observations, enables the generation of large-scale synthetic data. This approach provides a wealth of “observational data” for causal inference and drives advancements in causal theory. Furthermore, both the theoretical knowledge derived from Earth physics models and the physical constraints of the modeling process can serve as valuable prior knowledge for causal inference. They can also guide and standardize causal inference methods and offer scientific explanations for causal inference results (Figure 6). Additionally, a well-developed and structurally robust Earth system model can facilitate causal inference by conducting counterfactual simulations, providing insights into potential outcomes under intervention scenarios (Kretschmer et al., 2021). This capability enhances the estimation of causal effects within the POF and improves the interpretability of inference results. Therefore, Earth physics models contribute to the advancement of causal theories, the refinement of causal inference frameworks, and the increased interpretability of causal inference results.

In conclusion, the relationship between causal inference and Earth physics models extends beyond mere coupling, demonstrating a mutualistic and synergistic nature. The collaborative development of causal inference and physical models contributes to a “better” understanding of the Earth system and represents an important direction for advancing Earth system science.

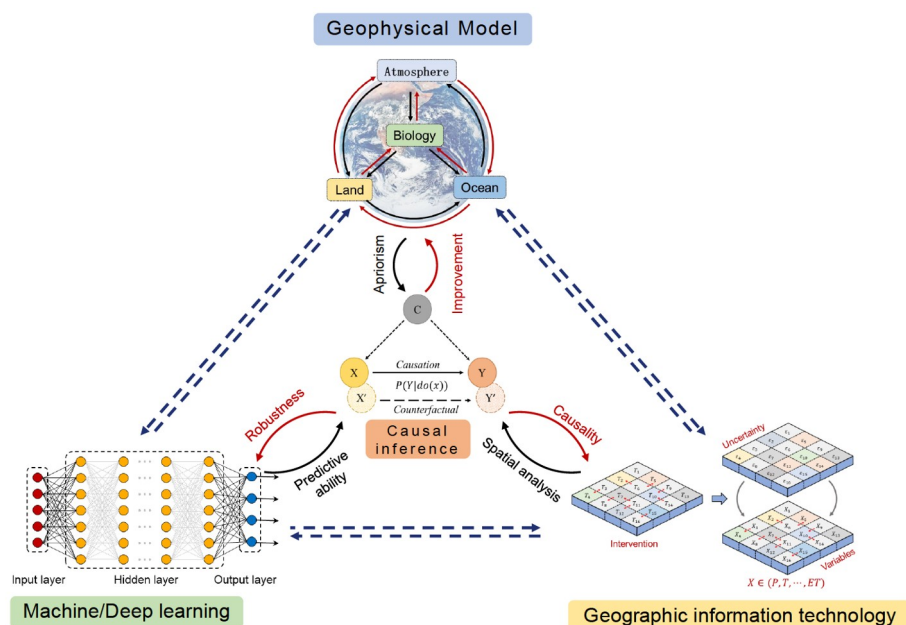


Figure 6 Development trends of causal inference in Earth system science.

4.2.2 Combination of causal reasoning and machine learning

For a significant period, both causal inference and machine learning have undergone substantial development. Since they approach their respective limitations, their intersecting synergy is rapidly emerging as a new focal point and breakthrough in the field of artificial intelligence (Schölkopf et al., 2021). Despite the notable successes of machine learning in various research domains, it still encounters significant challenges in practical applications. Firstly, machine learning models lack interpretability as they cannot explain the logic and reasoning behind their judgments. Instead, they can only unconditionally affirm or deny, making it difficult to dialectically adopt and incorporate them. Secondly, the majority of current machine learning approaches rely on the assumption of independent and identically distributed (IID) data, which implies that the data distribution of the training set and the test set is similar. However, this assumption does not guarantee the stable acquisition of prediction results (Peng and Susan, 2022). Moreover, the IID assumption further constrains the transferability of knowledge within machine learning models, limiting their applicability across different systems and data distributions (Shen and Zhang, 2023). Exploring causal relationships between variables can enhance machine learning's capacity to achieve robust predictions beyond the confines of the training distribution (Figure 6). How to bridge the gap between causal reasoning and machine learning, realizing their organic combination, has garnered considerable attention from scholars worldwide (Schölkopf et al., 2021).

Peng and Susan (2022) employed causal features to train a neural network model, thereby improving its robustness in diverse environments. Yang et al. (2021) proposed a variational autoencoder framework called CausalVAE, which includes a causal layer. The CausalVAE can partially reproduce real systems and generate counterfactual outcomes through the application of do-operations. Causal learning represents one of the forefronts of research that intimately connects causal inference and machine learning. It addresses the IID assumption within machine learning, ultimately improving its generalization capabilities and robustness. Depending on the availability of prior causal information, causal learning can be classified into two categories: those based on known causal information and those based on unknown causal information (Yao et al., 2021). Methods grounded in prior causal information typically assume knowledge of the causal structure of the target system, though latent variables may exist. Conversely, methods founded on unknown causal information necessitate additional learning of causal details, such as causal structure learning (Kalisch and Bühlmann, 2014) and causal representation learning (Schölkopf, 2022). Although some exploratory studies have been conducted (Peters et al., 2017;

Schölkopf et al., 2021; Schölkopf, 2022; Mouli and Ribeiro, 2022), the mutual benefits and synergistic collaboration between causal inference and machine learning remain in their early stages, highlighting the need for further research to fully explore their potential.

4.2.3 Spatial causal inference

With the advancement of causal theory and the improvement of inference methods, causal inference has made remarkable contributions to various branches of the Earth system. However, most applications of causal inference rely on the assumption of temporal asymmetry, while the study of spatial causal inference still faces limitations (Gao et al., 2022). The reasons for this phenomenon can be ascribed to the specificity of spatial processes, such as spatial dependence and heterogeneity, which give rise to spurious causality, thereby confounding the interpretation of inference results (Akbari et al., 2021). Furthermore, the “First Law of Geography” posits that all things are related to one another, and the strength of association increases with proximity, indicating the absence of complete spatial independence in the real world. Presently, research on spatial causal inference often relies on directly transplanting causal inference methods from non-spatial processes to spatial processes (Gao et al., 2022), lacking targeted treatment for spatial processes and struggling to meet the assumption of causal independence. Additionally, spatial spillover effects introduce a further challenge, as areas not subject to intervention can still be indirectly influenced by neighboring areas that do undergo intervention (Reich et al., 2021). To accurately infer causal associations, it is necessary to evaluate these indirect effects and filter them when feasible. Moreover, spatial spillover effects also undermine the assumption of individual independence in causal inference research, giving rise to a series of wicked problems for subsequent statistical estimation. The deep integration of causal inference algorithms and spatial statistical models offers a promising approach to address these wicked problems (Figure 6). Therefore, in order to harness the benefits of causal inference in spatial processes, it is crucial to develop targeted methods and frameworks specifically designed for spatial causal inference, thus paving the way for future advancements in this field.

5. Conclusion

Causal science originated from philosophy and has greatly benefited from modern statistics and information science. Presently, it has formed a comprehensive methodological framework. By establishing causal associations between phenomena and confounding factors, causal inference enables the discovery of hidden causal information within big data, providing a fresh perspective for gaining a deeper un-

derstanding of the Earth system. It also demonstrates vitality in various research directions of ESS, such as regularities revealing, processes understanding, hypothesis testing, and physical models improving. Meanwhile, causal inference has the ability to distinguish direct and indirect relationships, as well as identify common driving factors from data. Consequently, it transcends the limitations of traditional correlation and plays a pivotal role in interpretation, prediction, control, and decision-making. Despite notable achievements in ESS, current research on causal inference predominantly focuses on specific branches like the climate system, lacking exploration of the overarching framework and key processes that underpin the Earth system. This limitation impedes our comprehensive understanding of the Earth system. Furthermore, the personalized customization of causal inference methods by different researchers can influence the interpretation of results and undermine the fundamental understanding of physical processes within the Earth system. Therefore, there is a pressing need for a structured, standardized, and explicit top-level design, along with a universal toolkit for causal inference, to harmonize the cognitive foundation of Earth system science. Additionally, it is crucial to conduct systematic reviews of commonly employed causal inference methods in ESS, standardize assumptions related to causal inference, and establish consistent definitions and meanings of key terms (e.g., causal effects, causal mechanisms, driving factors, and causal pathways) throughout the causal inference process. In the era of abundant Earth data, causal inference presents both opportunities and challenges in its application to the Earth system. Integrating causal inference with physical models and machine learning and spatial causal inference hold great promise for the future, but it also faces challenges in experimental design, identification of latent variables, and the scarcity of reliable validation data.

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