

Best practices for moving from correlation to causation in ecological research

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ABSTRACT

In ecology, causal questions are ubiquitous, yet the literature describing systematic approaches to answering these questions is vast and fragmented across different traditions (e.g., randomization, structural equation modeling, convergent cross mapping). In our Perspective, we connect the causal assumptions, tasks, frameworks, and methods across these traditions, thereby providing a synthesis of the concepts and methodological advances for detecting and quantifying causal relationships in ecological systems. Through a newly developed workflow, we emphasize how ecologists' choices among empirical approaches are guided by the pre-existing knowledge that ecologists have and the causal assumptions that ecologists are willing to make.

1 CAUSALITY IN ECOLOGICAL STUDIES

Ecology is centered around investigating causal relationships between living organisms and their environments. In ecology, as in many other scientific fields, causality is understood as a phenomenon where change in one variable (the “cause”) induces change (the “effect”) in another variable^{1–4}. Thus, a causal relationship between X and Y exists if a perturbation in the cause X produces a change in the responding variable Y ^{4,5}, potentially through the perturbations of intermediary variables^{6,7}. This “perturbation-based” definition of causality is the definition most familiar to scientists and philosophers^{4,8}.

Because of a strong tradition of using manipulative experiments to establish causation, ecology has been shaped by two aphorisms: “correlation does not equal causation” and “causal claims can only be made from experiments.” The first aphorism oversimplifies the complexity of causal relationships and has been critiqued in the literature^{5,9,10} – correlation does not *always*

equal causation, but correlation can suggest a causal relationship (see Section 2). More importantly, the first aphorism does not imply the second: imperfectly designed experimental studies can mistakenly suggest causal relationships where none exist, and causation can, in fact, be established through well-designed observational studies^{11–13}. Natural history approaches, for instance, have long been used to establish credible causal claims (e.g., sea otters driving trophic cascades in subtidal communities^{14,15}). Recently, interest in observational approaches has grown^{16,17} due to the economic, ethical, and logistical challenges of manipulating ecological variables¹⁸ and the limitations of experiments in capturing complex, large-scale causal relationships in nature¹⁹. Observational data, particularly from multiple locations and time points, are increasingly valued for complementing experiments and supporting more generalizable causal claims^{19–21}.

To formalize the requirements for making causal claims from experimental and observational data, scholars in various fields have made substantial advances in mathematical and statistical tools over the past 50 years^{12,22–28}. Applications of these advances have changed how we think about scientific topics such as environmental and genetic causes of disease^{29–31}, military veterans' health³², criminology^{33,34}, and education^{35,36}, and have influenced policies on air pollution^{37,38} and carcinogens³⁹. These same advances are increasingly being proposed by ecologists to investigate causal questions using observational^{9,27,40–49} and experimental data^{50–52}. Yet the way in which these advances relate to each other is not readily apparent from the published literature. For example, what are the conceptual connections between studies that use experimental designs and studies that use convergent cross mapping algorithms? Published reviews typically focus on one set of approaches at a time (e.g. quasi-experimental designs,

structural causal models, dynamical systems)^{27,41,44,53,54}, which makes it difficult for ecologists to understand how, or if, the seemingly disparate approaches are related.

In this Perspective, we connection the assumptions, tasks, frameworks, and methods across these approaches, thereby providing a synthesis of the concepts and methodological advances for detecting and quantifying causal relationships in ecological systems. When answering a causal question, we must first identify the appropriate causal task: either causal discovery, which focuses on detecting whether causal relationships are likely to exist between variables in a system, or causal inference, which focuses on quantifying the direction and magnitude of causal relationships without bias. To accomplish these tasks, we employ causal frameworks, such as the structural causal model framework¹², the potential outcomes framework²⁵, or the dynamical systems causality framework^{55,56}, which formally define causal relationships and specify the assumptions that must be satisfied to accurately detect or quantify causal relationships from data. These frameworks then guide the selection of causal methods, that is, study designs and algorithms, which are used to operationalize these assumptions and establish the conditions necessary to make causal claims. To outline the process of navigating tasks, frameworks, and methods, we created a workflow for answering causal questions in ecological research. To provide further readings and software to implement the ideas in the Perspective, we provide comprehensive Supplemental Information (SI).

Throughout our Perspective, we highlight how well-articulated causal assumptions are the “glue” that unifies the myriad approaches to answering causal questions in ecology. These assumptions facilitate transparent discussions about the adequacy of study designs and algorithms that help scholars move from observations of statistical dependence in data to claims about causal relationships in ecological systems.

2 USING ASSUMPTIONS TO MOVE FROM CORRELATION TO CAUSATION

Data never “speak” by themselves. To derive meaningful causal insights from data, we must rely on well-defined hypotheses, statistical models grounded in ecological theory, and both testable and untestable assumptions^{57–59}. The importance of hypotheses, appropriate statistical models, and statistical assumptions is well known in ecology.

Less well known is the importance of causal assumptions that allow researchers to go from making claims about correlations to making claims about causation. Unlike most statistical assumptions, causal assumptions are typically untestable; that is, causal assumptions cannot be verified from data, even unlimited data. For example, experimentalists assume that randomization of a treatment ensures that any differences in outcomes across the randomized groups can only be attributed to either the treatment or sampling variability⁵⁰. Yet, experimentalists cannot verify this assumption. Causal assumptions, when combined with principles of probability theory and statistical dependence, allow us to make causal claims from data. The formalization of these assumptions is one of the most important scientific advances for answering causal research questions^{26,28,58}. For more details on the contrast between statistical and causal assumptions, see SI Section 1.

Causal assumptions, in tandem with statistical assumptions about the data structure, establish when statistical dependence can be interpreted as evidence for the perturbation-based notion of causality^{12,25,27,60}. In ecology, a commonly used measure of statistical dependence is correlation, which describes the linear similarity between two sets of observations. Consider a scenario in which we seek to determine whether, or by how much, variation in abundance of aphid predators (e.g., ladybird beetles) (X) changes the abundance of aphids (Y). If our knowledge about the probability of aphid abundance changes after learning something about

ladybird beetle abundance, then ladybird beetle abundance and aphid abundance are statistically dependent. This dependence forms the starting point for investigating potential causal relationships between two variables.

Statistical dependence is linked to causality through the Common Cause Principle⁶¹, which states that if a statistical dependence exists between two variables X and Y , then at least one of the following is true: X causes Y , Y causes X , or X and Y are both caused by a third variable C (Fig. 1). The presence of correlation can thus be mapped to the potential presence of a causal relationship. The lack of correlation, however, does not necessarily rule out statistical dependence or causality, as correlation is just one possible measure of dependence between two variables.

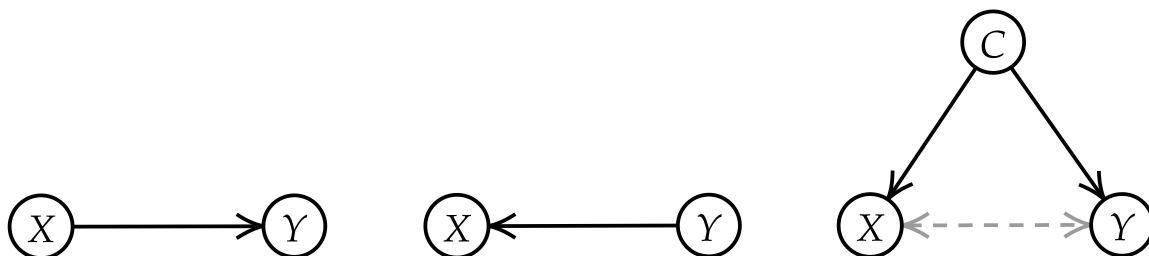


Fig. 1. Statistical dependence implies three possible causal relationships: X causes Y , Y causes X , or X and Y are caused by a common variable C . All three relationships can exist simultaneously in many contexts (indicated by the dashed grey arrows). Causal assumptions aim to eliminate the third possibility because the presence of C introduces additional statistical dependence between X and Y that is not due to any direct causal relationship.

132 In many causal analyses, eliminating the possibility that a third variable C causes both X
133 and Y is a priority, because we wish to distinguish variables with direct causal links from those
134 that are not causally influencing each other (i.e., we seek to eliminate non-causal, rival
135 explanations for statistical dependencies). For example, in Fig. 2 broad-spectrum pesticide use
136 (C) affects ladybird beetle abundance (X) and earthworm abundance (Y_2). However, ladybird
137 beetle abundance does not influence earthworm abundance, nor vice versa. In this case, any
138 observed statistical dependence between X and Y_2 is entirely attributable to their common cause
139 C .

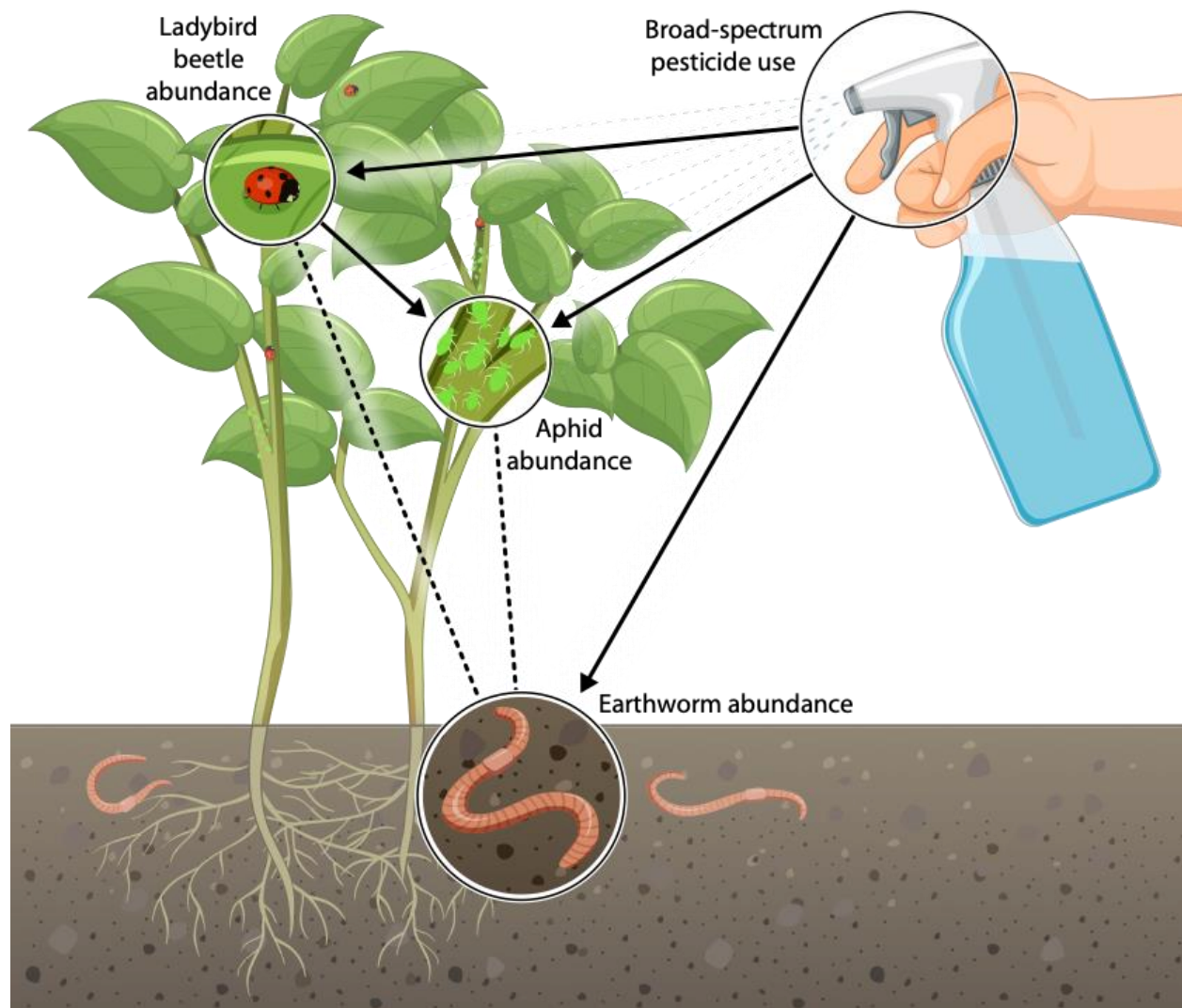


Fig. 2. Illustration of the Common Cause Principle in an ecological system where abundance of ladybird beetles, aphids, and earthworms are statistically dependent but not necessarily causally related. Blue arrows represent directional causal relationships, and red dashed lines represent statistical dependence but not causal relationships.

To eliminate these “common causes” (a.k.a., “confounding variables” or “confounders”), researchers make three assumptions: the Causal Sufficiency Assumption²⁸, the Causal Markov

Condition^{61–63}, and the Causal Faithfulness Assumption²⁸ (Box 1). The combination of these three untestable assumptions allows us to distinguish direct causal relationships between variables from dependence between variables induced by a common cause. By including all common causes in a model describing the relationship between X and Y (A1 in Box 1), we can eliminate the portion of the dependence attributable to shared causes C (A2). We can then interpret the remaining statistical independencies as evidence of no causal relationship between the variables (A3), while any remaining statistical dependence implies the possibility of a direct causal relationship.

For example, if pesticide use (C) is a common cause of both ladybird beetle abundance (X) and aphid abundance (Y), then we should include pesticide use in a model of the relationship between ladybird beetle abundance and aphid abundance (Fig. 2). If pesticide use is the only common cause and, after conditioning on it, ladybird beetle abundance is statistically independent of aphid abundance (i.e., they are conditionally independent), then, under the three causal assumptions, we can infer that no causal relationship between ladybird beetle abundance and aphid abundance exists. Conversely, if ladybird beetle abundance and aphid abundance are *not* independent conditional on pesticide use, then a causal relationship between ladybird beetle abundance and aphid abundance may exist (i.e., a lack of conditional independence simply means we cannot rule out a causal relationship, but it does not provide definitive evidence of causation).

The three causal assumptions required to connect statistical dependence to causal dependence – the Causal Sufficiency Assumption, Causal Markov Assumption, and Causal Faithfulness Assumption – are the foundation upon which causal claims are made from experimental and observational data. These causal assumptions allow us to differentiate the

171 causal dependencies between two variables from the non-causal dependencies created by
172 confounding variables.

Box 1. Three fundamental causal assumptions

For these assumptions, we define two variables X and Y as statistically dependent if the probability that Y takes a specific value given that X has taken a specific value is different from the probability that Y takes a specific value without any information about the value that X has taken. In other words, if X and Y are statistically dependent, knowing something about X changes what is known about the probability of Y .

- A1. **Causal Sufficiency**⁵² (a.k.a., the “no unmeasured confounding” assumption^{55–57}), requires that we observe all variables in a set $\mathcal{C}$ that causally influence any pairs of variables X and Y , and we include $\mathcal{C}$ in our model that describes the relationship between X and Y , thus ensuring that no confounding variables are unobserved.
- A2. The **Causal Markov Condition**^{54,58,59} states that if a pair of variables X and Y are statistically dependent solely because both are caused by a common variable C , and if we control for C by including it in our model, then X and Y become conditionally independent given C .
- A3. **Causal Faithfulness**⁵², stated very loosely, declares that statistical independence (conditional or unconditional) between a pair of variables X and Y indicates the absence of a causal relationship between those variables.

The combination of the **Causal Markov Assumption** (A2) and the **Causal Faithfulness Assumption** (A3) allows us to claim that if two variables, X and Y , are conditionally independent when C is included in the model, then X and Y are not causally related but instead are caused by a third common variable C . The **Causal Sufficiency Assumption** (A1) then ensures that we can distinguish causal relationships from dependence induced by a common cause if we include all possible confounders between variables in a model that describes the relationship between X and Y .

The Causal Markov and Causal Faithfulness assumptions have formal definitions requiring technical notation that are beyond the scope of this article. For a full discussion of these assumptions, we refer the reader to Pearl (2000)²³ and Spirtes and Zhang (2016)⁶⁰.

3 SATISFYING CAUSAL ASSUMPTIONS WITH PRE-EXISTING KNOWLEDGE, STUDY DESIGNS, AND ALGORITHMS

Given the restrictive and untestable nature of the three causal assumptions introduced in Section 2, ecologists may wonder whether causal claims can realistically be made from ecological data, since satisfying these assumptions requires building models that account for all confounders. Unlike models built for prediction or description, models built to make causal claims cannot be validated using goodness-of-fit or predictive accuracy metrics, as these metrics assess how well a model describes the observed data but do not evaluate how well the model satisfies the untestable assumptions required for making causal claims^{64,65} (for more details, see SI Section 2). In the following subsections, we describe how the foundations for satisfying causal assumptions are provided by pre-existing knowledge, study designs, and algorithms.

3.1 Pre-existing knowledge

To satisfy the three causal assumptions, pre-existing knowledge is essential⁵⁹. We use pre-existing knowledge to hypothesize causal relationships between variables by specifying the outcome(s) of interest (Y) and identifying potential causes (X). We also use pre-existing knowledge to identify potential confounders and determine which confounders can be measured in a study^{43,66,67}. The more pre-existing knowledge that we can apply towards satisfying causal assumptions, the more sophisticated the causal questions we can answer.

Pre-existing knowledge can include general and domain-specific ecological theory, subject matter expertise, field experience, and findings from previous studies, including studies that use empirical approaches lacking causal interpretations (see SI Section 2). Because pre-

existing knowledge is often complex and wide-ranging, we need succinct and straightforward ways to summarize it. In Section 5, we describe two common tools for organizing our understanding of an ecological system (i.e., our ‘mechanistic knowledge’⁶⁶).

3.2 Study designs and algorithms

Pre-existing knowledge is typically not sufficient to satisfy causal assumptions. For instance, even if we can identify all confounders with pre-existing knowledge, we are unlikely to be able to measure them all, which would be necessary to satisfy the Causal Sufficiency Assumption. However, study designs and algorithms provide us with the opportunity to address such challenges by relaxing one or more of the three causal assumptions in Section 2 in favor of equally untestable but (hopefully) more plausible causal assumptions.

Experimental designs, for example, substitute the Causal Sufficiency Assumption with the assumption that treatment randomization eliminates the effects of unmeasured confounding variables^{25,68}. Confounders are thus addressed through design rather than measurement. In non-experimental studies, observational designs often relax the Causal Sufficiency Assumption through statistical techniques that define the minimum set of confounding variables that need to be observed to accomplish the desired causal task^{57,58,69}, or through statistical techniques that allow researchers to pursue alternative research goals that reduce the number of confounders that must be measured (e.g., by defining alternative causal effects^{70,71}). These statistical techniques and redefined research goals can also be used with experimental designs that face implementation challenges, such as when the experimental manipulation affects the outcome variable through other pathways (i.e., randomization is a confounder), or when post-randomization observations are missing (i.e., attrition). We provide more details on both

experimental and observational study designs and algorithms for each of the causal tasks in Section 8.

4 A WORKFLOW FOR ANSWERING CAUSAL QUESTIONS IN ECOLOGY

We now present a comprehensive workflow that summarizes the key steps for conducting causal analyses (Fig. 3), with examples for each of the steps using two hypothetical ecological studies (Box 2). Our workflow illustrates how to systematically address causal questions in ecology.

The workflow serves as a roadmap, starting with the description of the causal question and ending with the interpretation and validation of the results. Each step in the workflow represents a decision point where we take action to ensure our causal analysis is robust, transparent, and aligned with the assumptions necessary to make causal claims from statistical analyses of ecological data. The workflow is designed to be flexible, allowing ecologists to tailor their approach based on their pre-existing knowledge, data, and methodological preferences.

To illustrate the workflow's application to real-world ecological research, we use two example ecologists, an intertidal ecologist and a tiger ecologist. In Box 2, we summarize how each ecologist navigates the workflow. In Sections 5 through 8, we elaborate on each of the following workflow steps:

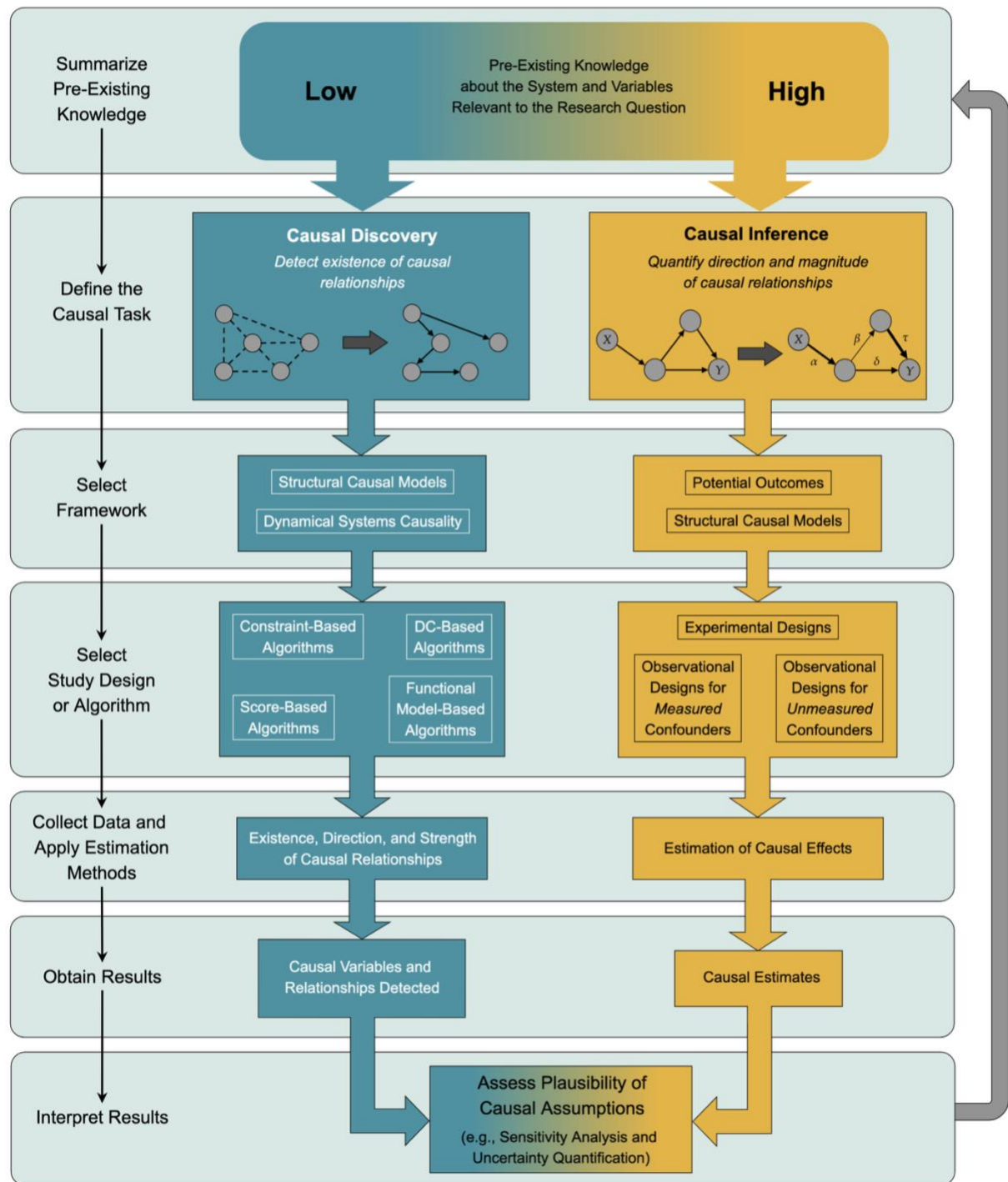
1. **Define the Causal Question and Summarize Pre-Existing Knowledge** (Section 5): We must first define the causal research question with at least one outcome variable (Y) and one or more hypothesized causal variables (X) (see SI Section 2 for differences between causal and non-causal questions in ecology). Then, to identify all confounding variables,

we must assess the corpus of pre-existing knowledge on the causes and outcomes of interest. We can summarize this knowledge using causal diagrams or thought experiments.

2. **Define the Causal Task** (Section 6): When answering causal questions, we use pre-existing knowledge to determine whether to pursue causal discovery or causal inference. Causal inference, which seeks to quantify the magnitudes of causal relationships, is feasible when we have sufficient pre-existing knowledge to be confident of the causal, outcome, and confounding variables and the directions of the causal relationships. If this knowledge is insufficient, we can instead pursue causal discovery, which aims to detect the existence of causal relationships.
3. **Select Framework** (Section 7): To clearly articulate the causal and statistical assumptions that must be satisfied for valid claims in either causal task, we can use one or more causal frameworks. The potential outcomes framework and the structural causal model framework are two common frameworks used for causal inference. For causal discovery, the structural causal model and dynamical systems causality frameworks are frequently used.
4. **Select Study Design or Algorithm, Collect Data and Apply Estimation Methods, Obtain Results, and Interpret Results** (Section 8): For causal inference, study designs can be grouped into three categories: experimental designs, observational designs for measured confounders, and observational designs for unmeasured confounders. Within each of these categories, many methods exist, some of which are described in SI Table S6 (e.g., regression adjustment⁷², propensity score matching^{45,73}, and structural equation modeling⁹). For causal discovery, algorithms are used instead of study designs. These fall

into four categories: constraint-based, score-based, functional model-based, and dynamical systems causality-based. Some of the algorithms are described in SI Table S7 (e.g., convergent cross mapping²⁷, fast causal inference²⁸, and greedy equivalency search⁷⁴). Based on the requirements of the study design or algorithm, we then collect data and apply estimation methods to detect causal relationships or quantify causal effect(s). Afterwards, we interrogate the plausibility of the causal and statistical assumptions by identifying potential violations to the assumptions and exploring the implications of those violations for the conclusions.

Although we present the workflow in a linear fashion, researchers will use it iteratively in two ways: (i) the results from one causal analysis will feed into future analyses in the form of pre-existing knowledge⁶⁶ (grey arrow in Fig. 3); and (ii) after taking actions at one step, researchers may need to return to previous steps before advancing in the workflow (e.g., reassessing the study design if data collection did not go as planned).



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279 Fig. 3. A workflow that outlines the key steps and decisions for answering causal questions in

280 ecological research.

Box 2. Ecologists conducting causal analyses using the workflow in Fig. 3.

“Define the Causal Question and Summarize Pre-Existing Knowledge”

An intertidal ecologist seeks to quantify the change in bivalve abundance (Y) caused by floods (X) through changes in nitrogen (M_1) and salinity (M_2) in intertidal zones at the mouth of an estuary. The ecologist summarizes knowledge about all confounders for each of the causal relationships of interest (i.e., floods on bivalves, floods on nitrogen, floods on salinity, nitrogen on bivalves, and salinity on bivalves).

A tiger ecologist seeks to determine the ecological factors (X) that encourage more visits or longer time (Y) spent in certain locations by tigers. The ecologist summarizes knowledge about confounders of the causal relationship between ecological factors and tiger occupancy (e.g., geographic and human factors).

“Define the Causal Task”

The intertidal ecologist has robust ecological theory and a significant collection of prior studies that identified the set of all confounding variables that could bias estimation of any one of the causal relationships of interest. Thus, the ecologist pursues causal inference.

The tiger ecologist has theory and field observations to identify certain ecological factors that may influence tiger occupancy, but they do not have sufficient knowledge to identify all human and geographic confounding variables. Thus, the ecologist pursues causal discovery.

“Select Framework”

The intertidal ecologist prefers the structural causal model framework for its structural approach to reasoning about multiple causes jointly.

The tiger ecologist prefers the dynamical systems causality (DC) framework for its focus on complex, evolving systems.

“Select a Study Design or Algorithm”

The intertidal ecologist selects an observational study design in which they measure and condition on all confounding variables.

The tiger ecologist selects a DC-based algorithm.

“Collect Data and Apply Estimation Methods”

The intertidal ecologist collects observational cross-sectional data on all causal, outcome, and confounding variables related to the causal relationships of interest and then fits a structural equation model.

The tiger ecologist collects observational time series data for tiger occurrence, abundance of several prey species, poaching activity, and weather conditions at a series of locations and uses convergent cross mapping (CCM) to detect causal relationships between pairs of variables.

“Obtain and Interpret Results”

The intertidal ecologist obtains estimates of the causal effects of floods on bivalve abundance that arise through the changes in nitrogen and salinity. They perform a causal sensitivity analysis that quantifies how much the estimates change in the presence of an unmeasured confounding variable.

The tiger ecologist obtains a network with detected causal relationships between pairs of variables. They perform a sensitivity analysis that shows how the detected causal relationships change when the CCM hyperparameter settings are changed.

5 SUMMARIZE PRE-EXISTING KNOWLEDGE

One common conceptual tool for summarizing pre-existing knowledge is a causal diagram. Causal diagrams help us organize our pre-existing knowledge by visually mapping the presumed causal relationships among causes (X), their outcomes (Y), and confounding variables (C). The most widely-used type of causal diagram is the causal directed acyclic graph (causal DAG), which follows a set of formal rules that define how causal relationships must be encoded⁷⁵. A causal DAG includes the focal variables of a study (i.e., the “cause” and the “outcome” variables), along with all suspected common causes (i.e. confounders) between the focal variables. Directed edges (arrows) between variables indicate that unidirectional causal relationships are presumed to exist, and the absence of an arrow between two variables reflects a strong assumption that a causal relationship does not exist¹². Causal DAGs, which must include all potential confounders of presumed causal relationships, enable us to identify the confounding variables we need to address with an experimental or statistical technique. Thus, causal DAGs should be constructed at the beginning of a study, before data are collected and the specific study design or algorithm is chosen.

Some ecologists will be familiar with the structural equation model (SEM) diagram⁹, which can be interpreted as a causal DAG when its structure represents only unidirectional relationships and explicitly encodes assumptions about causal relationships, including all relevant confounders^{76,77}. SEM diagrams also include additional parametric assumptions and are purpose-built for SEM analyses⁷⁶, whereas causal DAGs, which require no assumptions about the functional forms of causal relationships between variables, can be used in any type of causal analysis.

Another conceptual tool for summarizing pre-existing knowledge is a thought experiment in which researchers consider how a hypothetical ideal randomized controlled trial (RCT) – often termed a “target trial”^{78,79} – would be designed to answer their causal research question²⁵. By comparing the ideal (target) trial with the actual data generating process, we can identify discrepancies that may lead to bias through confounding variables that distort the observed relationship between the causal variable and the outcome. Formulating such a target trial forces us to articulate all the key components of an ideal RCT and then systematically determine which of these components may be absent or imperfect in our study. In doing so, it becomes clearer which variables, including potential confounders, should be adjusted for to emulate the conditions of an ideal experiment. Just as drawing causal DAGs helps visualize the network of causal relationships and identify confounders, formulating these thought experiments provides a concrete tool for planning rigorous study designs (i.e., the thought experiment forces us to ask the question, “Where does the variation in the causal variable come from?” a.k.a., “What is the treatment assignment mechanism?”). For resources that describe how to draw causal DAGs or develop thought experiments for studies, see SI Section 3.

6 DEFINE THE CAUSAL TASK – CAUSAL DISCOVERY OR CAUSAL INFERENCE

In deciding the most appropriate causal task for a research question, we must carefully consider the gap between available knowledge and the knowledge that would be required to plausibly satisfy causal assumptions. When pre-existing knowledge is extensive, we may pursue the task of causal inference. When pre-existing knowledge is limited, we may instead pursue causal discovery. Although the dividing lines between these two tasks is not as clearcut as

implied in our workflow (i.e., causal research lies on a continuum rather than in one of two camps), the contrast between their goals is illuminating for understanding how each task draws on pre-existing knowledge.

The goal of **causal inference** is to quantify the magnitudes of causal effects, either under a range of typical conditions or under specific interventions (e.g., new management policies, abrupt ecological changes). Causal inference requires substantial pre-existing knowledge about which variables act as causes, outcomes, and confounders, as well as the directions of causal processes (“high” pre-existing knowledge in Fig. 3). Quantifying multiple causal effects within an ecological system is even more challenging because sufficient pre-existing knowledge must exist to satisfy the required causal assumptions for every pair of cause-outcome variables.

When quantifying causal effects, defining the specific effect(s) of interest is important for connecting theoretical quantities to data. Different causal effects require different variations of the causal assumptions⁸⁰. Ecologists are often interested in the average effect of X on Y across all observations, that is, the average change in the outcome Y per unit change in X . However, other effects may also be relevant, such as mediation effects⁸¹ (effects of intermediary variables between a cause and its outcome) or effects for subgroups⁸² (e.g., the average effect of X on Y only for observations which experienced specific values of X). Moreover, some causal effects may be preferred because the causal assumptions for these effects can be more plausibly satisfied for a study (e.g., complier average causal effects, local average treatment effects, etc.).

In contrast to causal inference, **causal discovery** aims to detect or “learn” causal relationships among measured variables. Although causal discovery requires causal assumptions, they are less restrictive than they are in causal inference, and thus, less pre-existing knowledge is required (“low” pre-existing knowledge in Fig. 3). While causal discovery methods offer

flexibility in investigating causal questions with limited pre-existing knowledge, this advantage comes with the trade-off of potentially less precise or less certain conclusions about causal relationships. Causal discovery is therefore primarily valuable for generating more knowledge to guide subsequent studies.

To detect causal relationships, causal discovery involves defining an initial causal diagram (see Section 5) and refining it with statistical evidence from data. One strategy begins with a causal diagram that assumes causal relationships exist among all variables. Statistical independence tests are then systematically applied to eliminate connections between variables where evidence of a causal relationship is not supported by the data⁵³. Another strategy starts with a causal diagram that assumes no causal connections among variables and iteratively adds them where statistical evidence suggests a potential causal relationship⁸³. This second strategy is particularly amenable to incorporating pre-existing knowledge by allowing researchers to specify relationships that should be included or excluded from the outset. Both strategies rely on variations of the three causal assumptions introduced in Section 2 and aim to produce a refined causal diagram that reflects only the causal relationships consistent with the observed data and the underlying assumptions.

7 SELECT A CAUSAL FRAMEWORK

Causal frameworks structure how causal assumptions are represented for a given task, ensuring consistency between study design/algorithm, data collection, and estimation procedures.

7.1 Causal frameworks for causal inference

For causal inference, assumptions and estimation procedures are expressed using one of three causal frameworks: the structural causal model (SCM) framework; the Neyman-Rubin causal model, also commonly known as the potential outcomes (PO) framework; and the decision-theoretic framework²². While we focus on the SCM and PO frameworks, readers interested in the decision-theoretic framework can refer to Dawid (2000)²² and Dawid (2012)⁸⁴.

The choice of framework is primarily based on researcher preferences, as the PO and SCM frameworks have been shown to be logically and mathematically equivalent^{85–87}. The PO framework may appeal to experimentalists because it expresses causal assumptions by approximating the conditions that most accurately represent an idealized “gold standard” randomized controlled experiment. Alternatively, researchers who primarily model ecological systems as collections of simultaneously interacting variables may prefer the SCM framework, which represents systems as causal DAGs. Structural equation modeling, when used to make causal claims under the necessary causal assumptions^{9,46}, is a subset of the SCM framework^{77,88}.

Formalizations of the causal assumptions for causal inference as expressed using the PO framework and the SCM framework are described in SI Section 4 and Box S1. Resources for learning more about the core concepts of the PO and SCM frameworks can be found in SI Section 5.

7.2 Causal frameworks for causal discovery

For causal discovery, the assumptions and estimation procedures are expressed using either the SCM framework or the dynamical systems causality (DC) framework^{55,56}. Causal

discovery using the SCM framework is well-suited for ecological systems with multiple interacting variables, where causal relationships are expected to be stable across observations. SCM-based causal discovery algorithms also allow researchers to incorporate pre-existing knowledge by specifying constraints on potential causal relationships, making them particularly useful for exploratory studies where some causal relationships are known or hypothesized. In contrast, the DC framework may be more suitable for complex dynamic systems where causal effects unfold over time and cannot be represented as static combinations of causative factors. DC-based algorithms typically use time series data to infer causal relationships by testing whether knowledge of one variable's past improves the ability to anticipate changes in another variable. Measures of improvement span changes in predictability or statistical dependence, including those captured by information-theoretic measures^{83,89}.

SCM-based causal discovery algorithms generally begin with a causal diagram that assumes relationships between all variables in the data, and then they iteratively test for statistical independence between pairs of variables. Edges are removed where statistical independence is found, refining the causal diagram to represent only causal relationships consistent with the statistical independencies reflected in the data⁵³. In contrast, DC-based algorithms typically start with no assumed causal relationships among variables, and test whether statistical dependence between each pair of variables in each direction ($X \rightarrow Y$ and $Y \rightarrow X$) are significantly different from white noise or null hypothesis models^{83,90}. If the dependence meets the threshold for significance (typically, $\alpha = 0.05$) in only one of the directions, say $X \rightarrow Y$, then asymmetric coupling is detected, indicating a causal information flow from X (the driving system) to Y (the response system). The strength of the causal relationship is then estimated using a distance metric^{56,83}. In both the SCM and DC frameworks, multiple causal diagrams can

be consistent with the same structure of statistical dependencies in data, but pre-existing knowledge can refine the causal diagrams by constraining what relationships are possible.

Formalizations of the causal assumptions for causal discovery as expressed using the SCM framework and the DC framework are described in SI Section 4 and Box S2. Resources for learning more about the core concepts of the SCM and DC frameworks can be found in SI Section 5.

8 SELECT A STUDY DESIGN OR ALGORITHM, APPLY ESTIMATION METHODS, OBTAIN RESULTS, AND INTERPRET RESULTS

Study designs for causal inference and algorithms for causal discovery provide structured approaches for satisfying or relaxing the untestable causal assumptions through decisions about the data and analysis (i.e., designs and algorithms operationalize causal frameworks). Designs and algorithms also lead us to appropriate methods for estimation and interpretation of the results.

This section provides an overview of key study designs for causal inference and algorithms for causal discovery. The details and applications of each approach are beyond the scope of this Perspective, but in SI Section 6 we provide resources, including guidance on implementation and relevant software packages. While we focus on foundational study designs and algorithms, we summarize in SI Section 7 some advanced methods, including those that integrate machine learning techniques into their estimation procedures, which are rapidly emerging and may offer new opportunities for ecological research.

8.1 Study designs for causal inference

Study designs for causal inference fall into three categories: (1) experimental designs that aim to minimize confounding from both measured and unmeasured variables through manipulation of the causal variable, (2) observational designs that explicitly identify and control for measured confounders, and (3) observational designs that eliminate unmeasured, and potentially unknown, confounding by leveraging external sources of variation (specific designs from these three categories are listed in SI Table S6).

Experimental designs (e.g., randomized controlled trials⁵⁰ and factorial designs⁹¹) are often well-suited for causal inference because they provide a structured approach for directly manipulating the causal variable and defining the temporal order of cause and effect. Through strategies like randomization, we aim to control or eliminate the effects of confounding variables, providing justification for causal claims. However, suboptimal decisions in the design and analysis of experiments can produce invalid causal conclusions⁹², and even well-designed experiments may face challenges⁹³, such as non-compliance or non-random dropout. Moreover, in ecology, experiments may be prohibitively expensive at the scales needed to detect causal effects, or they may distort natural ecological conditions⁹⁴, making them impractical or unrepresentative.

When experiments are infeasible, impractical, or unethical, observational designs for measured and unmeasured confounders are available. Advances in causal approaches for observational studies provide statistical techniques to satisfy causal assumptions without experimental manipulation^{12,22,25,75,95}. Observational designs for measured confounders (e.g., regression adjustment⁷², propensity score matching⁷³, and structural equation modeling⁹) rely on measuring all confounding variables. When measuring, or even knowing, all relevant

confounders is not feasible, we can use observational designs for unmeasured confounders (e.g., before-after-control-impact⁹⁶ and multilevel modeling with fixed effects⁹⁷). These designs relax the causal sufficiency assumption of no unmeasured confounders by replacing it with assumptions about the structure of unmeasured confounders, typically informed by pre-existing knowledge. These designs then use statistical techniques to represent the influence of confounders based on their assumed structure, without needing to directly measure the confounders.

Experimental and observational designs can be implemented using either cross-sectional or longitudinal data. However, strong assumptions about temporal ordering (cause must precede its outcome) and stable effects over time are required to quantify causal effects using cross-sectional data. Once data are collected, we can quantify the causal effect of interest using a range of estimation methods (“Collect Data and Apply Estimation Methods” and “Obtain Results” in Fig. 3). Many estimation methods are available to implement a chosen study design, each providing a different statistical approach for estimating the causal effect of interest^{98,99}.

After estimating a causal effect, we must then interrogate the plausibility of the causal assumptions underlying the study design and explore the implications of violations to these assumptions (“Interpret Results” in Fig. 3). One common approach for assessing the implications of violations is to perform causal sensitivity analyses, which quantify how an estimated effect would change in the presence of unaddressed confounding. Many sensitivity analysis techniques are available for a variety of causal inference methods^{100–104}, including SEM¹⁰⁵. An alternative approach to interrogating the plausibility of causal assumptions involves detecting under-adjustment of confounding variables by drawing on pre-existing knowledge to formulate tests of known effects^{11,106,107} (e.g., falsification or placebo tests). We must also consider how other

forms of bias^{108,109}, including selection bias^{110,111} and measurement bias^{112–114}, may influence the estimated effects and the robustness of our conclusions.

8.2 Algorithms for causal discovery

Algorithms for causal discovery fall into four categories: DC-based algorithms and three types of SCM-based algorithms, which are called constraint-based, score-based, and functional model-based algorithms (specific algorithms from these four categories are listed in SI Table S6). DC-based methods are suited for dynamic systems and assess causal interactions based on predictability and information flow over time. Constraint-based methods use conditional independence tests to eliminate implausible causal relationships. Score-based methods evaluate possible graphical structures using a scoring criterion that captures how well the graph fits patterns of conditional independencies in the data. Functional model-based methods assume specific functional relationships between variables (e.g., linear or non-linear equations with noise) and infer causal direction by identifying which graph configuration satisfies those assumptions.

Causal discovery algorithms have been developed to accommodate different data structures, with approaches often tailored to either longitudinal data or cross-sectional data. DC-based methods (e.g., Granger causality⁶⁰ and convergent cross mapping [CCM]²⁷) require bivariate or multivariate time-series data (i.e., regularly spaced longitudinal data) to infer causal relationships through changes over time. In contrast, SCM-based algorithms (e.g., Fast Causal Inference [FCI]²⁸, Greedy Equivalency Search [GES]⁷⁴, and Peter and Clark Momentary Conditional Independence [PCMCI]¹¹⁵) can be applied to both cross-sectional and longitudinal

data, but additional assumptions about temporal ordering (i.e., causes precede their outcomes) must be satisfied when using cross-sectional data. As with causal inference, pre-existing knowledge can enhance results from SCM-based discovery methods by explicitly specifying certain relationships that should or should not be included in the causal diagram.

Once candidate causal diagrams have been obtained (“Collect Data and Apply Estimation Methods” and “Obtain Results” in Fig. 3), we must assess whether the causal assumptions of the chosen discovery algorithm are plausible for the ecological system under study and explore the implications of violations to these assumptions (“Interpret Results” in Fig. 3). To assess the reliability of conclusions drawn from the causal discovery process and to evaluate the robustness of the inferred causal relationships, sensitivity analyses that explore the stability of results across different hyperparameter settings should be undertaken¹¹⁶.

9 CHALLENGES AND OPPORTUNITIES

Making valid causal claims from ecological data requires moving beyond analyses that use prediction- and association-focused models, which typically fail to represent the true underlying causal structures of ecological systems^{64,117,118}. It instead requires satisfying or carefully relaxing the causal assumptions that allow observed statistical dependencies to be interpreted as evidence of causal relationships. While this requirement may seem daunting, especially given the complexity of ecological systems, advances in causal methodologies have demonstrated how the quality and transparency of causal claims can be improved through clearer articulation of the causal assumptions, scrutiny of their plausibility, and attention to potential violations. For example, the intertidal ecologist who uses SEM to estimate causal effects and the

tiger ecologist who uses CCM to discover causal relationships (Box 2) would (i) clearly state all the causal assumptions required by their study design or algorithm; (ii) quantify the amount of unmeasured confounding that would be needed to overturn their causal claims, or, for discovery algorithms, report how detected causal relationships change under different hyperparameter settings; and (iii) frankly discuss potential unmeasured confounding variables or other violations to their causal assumptions that could invalidate their conclusions.

By connecting the causal assumptions, tasks, frameworks, and methods that play essential roles in causal research, our workflow (Fig. 3) provides a structured approach for investigating causal questions in ecology. The workflow emphasizes the role of pre-existing knowledge, which helps us to align the causal task with the research objective, clarify assumptions through a causal framework, and select a study design or algorithm that satisfies those assumptions and guides data collection and analysis. Studies that explicitly state and justify the assumptions underlying their causal claims allow subject matter experts to evaluate the credibility of these assumptions and build on them more effectively. Thus, our workflow not only supports ecologists in conducting rigorous and transparent causal analyses, but it also facilitates cogent discussions about the potential for unresolved confounding in prior studies, which can motivate new studies. Through an iterative application of the workflow, we can enhance the accumulation and synthesis of ecological knowledge.

As causal methods evolve, new advances focus on relaxing or probing untestable assumptions in challenging real-world settings, which expand the relevance and applicability of causal methods to the complexities of ecological systems. Ecologists are uniquely positioned not only to benefit from these advances in causal analysis, but also to contribute meaningfully to their development. Ecologists' experience with experimental study designs, multiscale complex

systems, and the integration of biotic and abiotic processes offers valuable insights into widespread challenges in causal research, such as spatial interactions, downscaling, and unit-to-unit causation. As causal approaches become more accessible and adaptable, ecologists have an opportunity to refine long-standing questions, generate new theory, and develop credible causal explanations of the natural world.

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Author Contributions Statement

H.E.C. led the paper. H.E.C, L.E.D and P.J.F co-organized, and P.J.F. funded, the workshop in which J.E.K.B., H.E.C., L.E.D., J.R.F., P.J.F., M-J.F., C.G., B.S., I.S., K.J.S., G.S., and B.vH. contributed to establishing the goals and emphases of the paper. H.E.C., L.E.D and P.J.F initiated the paper concept and framing. H.E.C. and P.J.F. wrote the main text. J.E.K.B., L.E.D., J.R.F., M-J.F., B.S., I.S., K.J.S., G.S., and B.vH. suggested edits to the drafts of the paper. H.E.C. conceived and wrote the Supplemental Information.

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Supplementary Information

1. Causal versus statistical assumptions

As noted in the main text, causal and statistical assumptions are both necessary components of deriving valid causal interpretations from observed relationships in data (Stone, 1993). Although the distinctions between these two types of assumptions are not always clear cut in casual research, we find it useful to distinguish them in the following way. Statistical assumptions are formal conditions about the data and model structure that must be satisfied for valid characterizations of relationships between variables from statistical analyses. These assumptions are often testable from data. Causal assumptions are additional conditions that are required to infer causation from statistically dependent relationships and are typically untestable (Hernán et al., 2019). By “untestable”, we mean that these assumptions cannot be verified through statistical checks of data, even unlimited data, but instead must be justified using pre-existing knowledge.

Statistical assumptions commonly include assumptions about the probability distribution of random variables or observations, the specifications of relationships between variables, and conditions about data gathering or sampling (see Table S1). For example, they include assumptions about the functional relationships among variables (e.g., linearity, additivity) and about the probability distribution of random errors or observations (e.g., normality, independent and identically distributed random variables, constant variance). Statistical assumptions are encoded in the model structure; thus, they are often not described in applied data analyses.

Unlike causal assumptions (see Section 2 of the main text and Table S1 below), many of the statistical assumptions underlying empirical analyses in ecology are testable – that is, the assumptions can be verified from available data – even if they are often untested by researchers conducting the analyses. There are, however, untestable statistical assumptions that are also necessary for model-based inference, and these assumptions overlap with the causal assumptions described in Section 2 and in Table S1. For example, the basis of the Causal Sufficiency Assumption is a ubiquitous statistical assumption that requires correct specification of the explanatory variables in a model, specifically the inclusion of all confounding variables and the omission of all irrelevant variables. This assumption cannot be directly verified from data (i.e., the assumption is untestable) and must be supported by background knowledge about the system being modeled. Violations to the assumption that explanatory variables have been correctly specified can result in omitted variable bias, overfitting, and simultaneity bias that negatively impact interpretability and generalizability of results.

Other statistical considerations are also important for accurate conclusions from modeled data. These can include: ensuring sufficient statistical power to detect relationships between variables (Kimmel et al., 2023), decreasing measurement error or observational noise to better detect dependent relationships (Brown et al., 1990; Hyslop & Imbens, 2001), appropriately identifying and handling patterns of missingness (Little, 2021), and using robust statistics to accommodate a wider array of probability distributions and modest departures from model assumptions. While these considerations may not be viewed as statistical assumptions *per se*,

they play an important role in determining the credibility of quantitative evidence about ecological phenomena.

The statistical and causal assumptions that are fundamental for making causal claims from ecological data are not tied to specific estimation approaches (e.g., frequentist versus Bayesian estimation). Many ecological studies emphasize the mode of estimation (mode of statistical inference) and overlook potential violations to causal and statistical assumptions that must be satisfied for valid inferences, but even minor violations can impair interpretability. Thus, extracting meaningful causal inferences from data in ecology requires both thoughtful construction of models and the scrutiny of the assumptions underlying these models (Burnham & Anderson, 2010).

Table S1. Common statistical and causal assumptions required for valid causal inference from data.

Statistical Assumptions	Causal Assumptions
<i>Correct model specification</i>	
- Model(s) include all relevant variables and no irrelevant variables. - Correctly specified functional forms of the relationships among variables (e.g., linearity, additivity).	- No unmeasured or omitted confounding variables (Causal Sufficiency Assumption). - Causal relationships follow the Causal Markov Assumption and Causal Faithfulness Assumption.
<i>Random (unit-level) error conditions</i>	
- Observations are independent and identically distributed (i.i.d.). - Random errors follow a specific probability distribution (e.g., Gaussian). - Random errors have constant variance (homoskedasticity). - Explanatory variables not correlated with random error. - Measurement error in explanatory variables is independent of the true values.	- A unit's treatment does not affect another unit's outcome (i.e., "no interference"). Related to the statistical i.i.d. assumption: i.i.d. can be violated by the presence of interference, which implies a lack of independence across units (see Zhang et al., 2023).
<i>Data-specific criteria</i>	
- For time-series: Stationarity (constant mean and variance over time). - No perfect multicollinearity among explanatory variables.	- No instantaneous causal effects ("no simultaneity"). - Every unit has a non-zero probability of receiving any level of treatment, conditional on covariates (i.e., "positivity" or "overlap").

2. Defining causal and non-causal research questions

Describing and quantifying ecological phenomena often requires a model, which is a mathematical description of how ecologists presume that variables of interest interact with each other. The form of the model is typically determined by the objective of the research question, which we divide into five categories: making causal claims, making associational claims, making predictions, summarizing data through descriptive statistics, and testing logical reasoning of hypotheses via simulations (“Define Research Question” in Figure S1).

Answering the first three types of questions requires statistical inference, which allows ecologists to learn information from observations using probability theory and use that information to make claims about relationships between variables, predict new information, and describe patterns in data (darker-shaded portion of the top box, to the left of the vertical dashed line in Figure S1). When sufficient data are not available or statistical inference is not suitable, mathematical modeling can be used to simulate hypothesized ecological interactions and check for logical fallacies (lighter-shaded portion of the top box, to the right of the vertical dashed line in Figure S1). Associational analyses, predictive models, or simulation-based approaches can also be useful for deriving knowledge that can contribute to future causal research questions (Figure S1 and Figure 3 in main text).

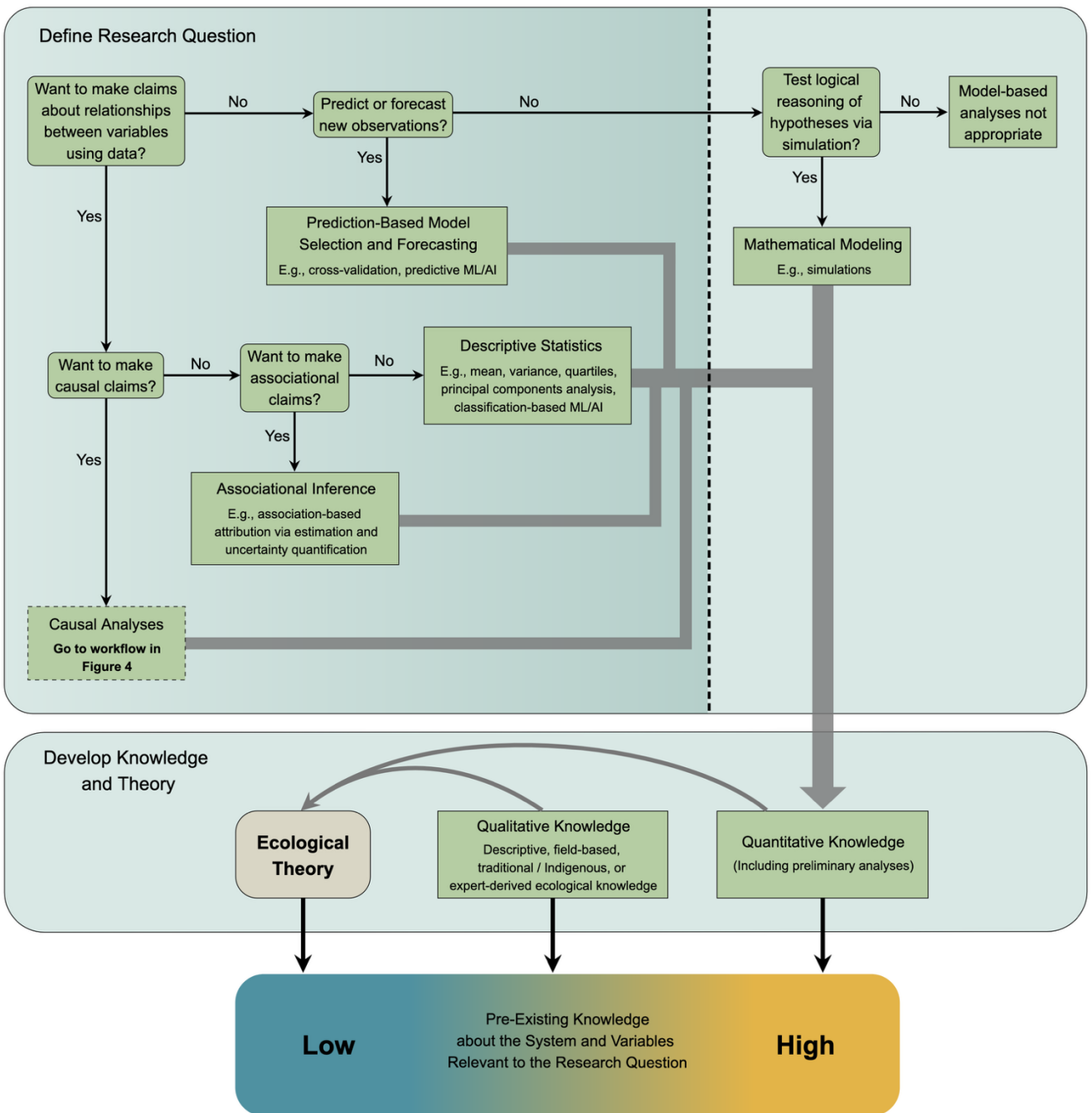


Figure S1. Decision tree for determining the type of analysis most appropriate for the research goal. Prediction-based model selection and forecasting, descriptive statistics, associational inference, and causal analyses use statistical inference, which separates them from approaches like simulation-based mathematical modeling. That separation is represented by the vertical dashed line that separates lighter and darker shaded regions of the top box. The bottom gradient box is also represented in the first box in the workflow of Fig. 3.

A. Using data to derive claims about relationships between variables

When causal interpretations of statistical models are desired, causal methodologies, a subset of statistical inference, allow ecologists to make causal claims about relationships between variables from data. However, as we make clear in Section S4, using statistical inference to make causal claims requires that the experimental or nonexperimental data collection and analyses satisfy many conditions (i.e., assumptions). We provide more details on the tasks that can be accomplished through causal studies and specific methods in Section 6.

If causal claims are not desired, ecologists can draw on classical tools from statistical inference (Efron & Hastie, 2016; Holland, 1986; Nakagawa & Cuthill, 2007). These associational studies can also shape the formulation of causal research questions for subsequent studies. Many research questions have causal goals, but researchers will usually cast these questions as associational due to perceived limitations of statistical methodologies or concerns about misuse of their findings (Hernán, 2018; Jones & Schooling, 2018; Kezios & Hayes-Larson, 2018). Researchers also commonly draw causal-sounding conclusions (e.g., using terms like “drives” or “leads to”) from predictive or associational analyses (Haber et al., 2022; Han & Guyatt, 2020; Sargeant et al., 2022; Singer, 2022), thus overstating the evidence of causality by implying that the underlying causes have been properly isolated from unrelated or spurious associations (i.e., that alternative explanations for the observed associations have been ruled out). This tendency is now heavily ingrained in the scientific culture of many fields, but we strongly encourage ecologists to principally consider the goals behind their research questions before considering the methods that may be taken to achieve those goals.

Alternatively, ecologists may instead wish to probe data for general patterns among variables by using statistical inference to explore or summarize the data (“Descriptive Statistics” in Figure S1). Approaches used to describe data are often included in studies aiming to make causal or associational claims, but descriptive statistics are not the primary source of evidence for making such claims.

B. Not deriving claims about relationships among variables from data

At times, ecologists may want to predict unobserved outcomes from new input data by using training data to optimize parameter estimation such that a set of input features predict output values that most closely match observed data output values in verification data (“Prediction-Based Model Selection and Forecasting” in Figure S1). Predictive studies rely on procedures that emphasize model evaluation and selection through predictive performance, including model averaging that derives inferences from several plausible models (i.e., multi-model inference; Burnham & Anderson, 2010). Results from models selected for high prediction accuracy are often believed to produce more meaningful parameter estimates for inference than models with low prediction accuracy (Harrison et al., 2018), which has spurred the popularity of machine learning approaches touted to provide “data-driven” understandings of complex ecological processes (Christin et al., 2019; Olden et al., 2008). However, prediction models merely need to capture the rudimentary patterns and relationships in the data to produce highly accurate

118 predictions. Thus, models with high prediction accuracy often do not accurately represent the
119 true underlying causal processes of the ecological system from which the data were generated,
120 and thus they are usually not appropriate for making associational or causal claims (Addicott et
121 al., 2022; J. Li et al., 2020; Tredennick et al., 2021).

122 In other studies, ecologists may wish to simulate hypothesized relationships between
123 variables using mathematical “proof-of-concept” models (sometimes called “mechanistic
124 models”), which play an integral role in translating ecological theories and hypotheses into
125 mathematical language (e.g., the Lotka-Volterra model; Baker et al., 2018; Marquet et al., 2014;
126 Servedio et al., 2014). Numerical analysis of mathematical models allows ecologists to explore
127 and refine hypotheses, examine a model’s internal consistency, and assess how well the model
128 represents theoretical or empirical relationships. Additionally, data collected from experiments
129 and field observations can be used to constrain model parameter values or to compare model
130 output to naturally occurring patterns (Caldararu et al., 2023; Evans et al., 2013; Levins, 1966;
131 Luo et al., 2011; Tredennick et al., 2021), but statistical inference is not the goal of such models.

132 Although mathematical models, predictive models, associational studies, and descriptive
133 statistics can all contribute to quantitative ecological knowledge and pre-existing knowledge for
134 developing causal research questions (“Develop Knowledge and Theory” in Figure S1), current
135 methodologies for making causal claims from data require principles of probability theory and
136 statistical inference to be combined with the rigorous conditions for experimental and
137 observational data collection and analysis defined by causal assumptions. Some researchers have
138 argued that, under certain conditions, predictive models may also contribute to refining or
139 corroborating causal hypotheses when results from predictive studies align with theoretical
140 expectations (Nichols & Cooch, 2025). While consistent findings from predictive models may
141 contribute to pre-existing or “mechanistic” ecological knowledge (Grace, 2024), particularly
142 when supported by ecological theory and expert understanding, predictive performance alone is
143 insufficient to justify causal claims.

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3. Formally summarizing pre-existing knowledge

Establishing the conditions for making valid causal claims from data is achieved by satisfying the causal assumptions that permit us to detect and quantify causal relationships using statistical dependence. A central task for ecologists interested in causal relationships is to carefully consider the study design, the potential variables to be included or not included in the model, and the data collection procedures. One of the fundamental conditions for valid statistical inference and interpretability of results is that the model correctly specifies the true underlying process from which the data were generated. Developing such a correctly specified model requires pre-existing knowledge to identify potentially causative factors and potential pathways of influence through other interacting variables.

The assumptions required for causal analyses highlight how causal tasks (i.e., causal discovery and causal inference) differ from non-causal tasks (e.g., prediction or association). Unlike non-causal analyses, causal tasks depend on pre-existing knowledge to construct and justify models for causal tasks (particularly for causal inference) that satisfy these untestable causal assumptions, rather than selecting the “best” model among several plausible models based on fit metrics that evaluate prediction performance. Even causal discovery is fine-tuned with pre-existing knowledge, guiding algorithms to retain specific plausible relationships specified by the user’s pre-existing knowledge, and its results must be validated through further research.

Proper model specification is crucial for valid causal conclusions (Burnham & Anderson, 2010), thus more attention must be invested in the process of designing studies and building models using pre-existing knowledge to make causal claims from experimental and observational ecological studies. To formalizing pre-existing knowledge in causal analysis, researchers may use two widely used tools: directed acyclic graphs (DAGs) and thought experiments based on ideal randomized controlled trials (RCTs). These tools help define causal relationships and identify confounders that must be addressed to satisfy causal assumptions before any data are analyzed. Table S2 provides a guide to accessible and foundational references for learning how to apply these tools.

172 Table S2. Key concepts and accessible references for creating and applying causal DAGs and
 173 thought experiments of hypothetical ideal RCTs for summarizing pre-existing knowledge.

Concept	Suggested Readings
Basics of causal DAGs – What they are, variables to include, why they help in confounder identification	Bulbulia, 2024a; Greenland et al., 1999a; Laubach et al., 2021; Shrier & Platt, 2008
Drawing DAGs in practice – User-friendly guidelines for causal DAGs in experimental and observational settings	Arif & MacNeil, 2022; Textor et al., 2011
Using thought experiments of hypothetical ideal RCTs (i.e., “target trials”) – How to use thought experiments to simulate an ideal experiment to find confounders	Greenland, 2003; Hernán et al., 2022, 2025; Hernán & Robins, 2025, pp. 37–40; Morgan & Winship, 2015 (Ch. 1); Rubin, 1974
Distinguishing confounders vs. colliders – Ensuring we do not control for the wrong variables	Arif & Massey, 2023; Bulbulia, 2024a; Greenland, 2003

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4. Causal assumptions translated through causal frameworks

Causal inference and causal discovery both rely on untestable assumptions that allow researchers to interpret statistical patterns as evidence of causation. Three foundational assumptions are shared across major causal frameworks: Causal Sufficiency, Causal Markov, and Causal Faithfulness. However, the way these assumptions are expressed, along with the specific terminology and extensions they involve, varies across causal frameworks. In this section, we show how different frameworks formalize these assumptions and illustrate the conceptual bridges between them.

We focus on three widely used causal frameworks: the structural causal model (SCM) framework (Pearl, 2009), the potential outcomes (PO) framework (Rubin, 1974), and the dynamical systems causality (DC) framework (Harnack et al., 2017; J. Shi et al., 2022). A fourth not covered here – the decision-theoretic framework (Dawid, 2000, 2012) – also shares overlapping assumptions. Each framework uses its own notation and formalism to express the causal assumptions and structure causal reasoning. The PO and SCM frameworks are most common for causal inference, while the SCM and DC frameworks are commonly used for causal discovery.

Theoretical work has established formal correspondences among several major causal frameworks. The PO and SCM frameworks have been shown to be theoretically equivalent (Imbens, 2020; Pearl, 2009), with modern formalizations demonstrating that every Rubin Causal Model from the PO framework can be represented as an abstraction of an SCM (Ibeling & Icard, 2023). A measure-theoretic approach has also been proposed to generalize aspects of SCM and PO frameworks and address challenges like cycles, latent variables, and stochastic processes (Park et al., 2023). Causal properties of the decision-theoretic framework can be expressed through extended conditional independence assertions, aligning with the PO and SCM frameworks under specific conditions (Dawid, 2021, 2024; Pearl, 2022). Connections between the SCM and DC frameworks have also been developed, including approaches that extend SCMs to time-dependent settings and systems with feedback loops (Bongers et al., 2018, 2021) and approaches that link Granger causality (a DC-based approach) to SCMs by representing interventions and dynamic feedback processes (White et al., 2011; White & Chalak, 2009). Methods like transfer entropy, which is used in DC-based analyses, have similarly been related back to conditional independence structures central to SCMs (Runge et al., 2012). Commentaries have also highlighted key conceptual differences and areas of overlap between the PO, SCM, and DC frameworks (Lechner, 2010; Markus, 2021). While recent reviews (e.g., Vonk et al., 2023; Yuan & Shou, 2022) have discussed assumptions in causal discovery and causal inference broadly, here we systematically map how core causal assumptions translate across SCM, PO, and DC frameworks for causal inference and causal discovery.

In Box S1, we map the assumptions used for quantifying the average causal effect of X on Y in causal inference via the PO and SCM frameworks onto the three basic causal

assumptions. We also summarize two additional assumptions widely used in practice for causal inference. Together, these assumptions allow us to quantify causal effects without bias. For full details of PO assumptions for causal inference, see Hernán & Robins, 2025; for full details of SCM assumptions for causal inference, see Pearl, 2009 or Pearl, 2010.

For causal inference, the inclusion of all relevant confounding variables is necessary to satisfy the causal sufficiency assumption. However, this does not always require directly measuring every confounder. In both frameworks, design-based approaches and statistical techniques can be used to account for unmeasured confounding under certain conditions. Some frameworks, such as SCM, allow for adjustment using variables that are not direct confounders (e.g., descendants of common causes), provided that colliders and other bias-inducing paths are avoided that would otherwise introduce non-causal statistical dependencies (Pearl, 1995; Rohrer, 2018).

In Box S2, we map the assumptions used for causal discovery via the SCM and DC frameworks onto the three basic causal assumptions. We also summarize three additional assumptions commonly required in practice for causal discovery. For full details of SCM assumptions for causal discovery, see Glymour et al., 2019; for full details of DC assumptions for causal discovery, see J. Shi et al., 2022. For relationships between SCM and DC assumptions in causal discovery, see Runge, 2018.

For causal discovery, causal assumptions are used to ensure the reliability of the causal structure inferred from data. SCM-based algorithms primarily rely on the Causal Markov and Causal Faithfulness assumptions, often alongside Causal Sufficiency and additional assumptions like acyclicity and i.i.d. sampling (Glymour et al., 2019). These assumptions can often be relaxed in more advanced approaches. DC-based algorithms often implicitly rely on the causal sufficiency assumption (Paluš, 2007; Runge, 2018), where all common causes are assumed to be measured or contained within the information of the measured variables (i.e., there are no unmeasured confounders, a.k.a., “hidden common causes”), and usually require separability, which is a consequence of the causal faithfulness assumption (Eichler, 2013; Peters et al., 2017; Runge, Nowack, et al., 2019; Spirtes et al., 2000). However, some DC-based causal discovery methods have been developed for non-separable systems (e.g., J. Shi et al., 2022) and for detecting and handling the presence of unmeasured confounders (e.g., Cai et al., 2023).

Together, Boxes S1 and S2 provide a unique synthesis of how the three foundational causal assumptions are formalized and applied across diverse causal frameworks. By explicitly mapping the assumptions of each framework to these shared foundations, the Boxes serve as practical tools for clarifying how these assumptions support valid causal claims across different, and sometimes seemingly disparate, frameworks and causal tasks, thereby clarifying both their common foundations and distinct assumptions.

Box S1. Assumptions for causal inference

Choice of framework

Potential Outcomes (PO) Framework	Structural Causal Models (SCM) Framework
Useful for those familiar with randomized experimental designs. Emphasizes addressing non-causal dependencies (confounding) by leveraging specific experimental designs or imitating such scenarios via statistical techniques.	Useful for those who think about multiple causes jointly (“all-cause models”). Emphasizes defining the minimal set of conditions under which causal effects can be identified and estimated.

Causal assumptions

A1. Causal Sufficiency: All relevant confounders are measured (i.e., no unmeasured common causes).

Potential Outcomes (PO) Framework	Structural Causal Models (SCM) Framework
Terminology: “No unmeasured confounders”, “ignorability”, or “exchangeability”[†]. Key Idea: Once we adjust for all relevant confounders, the probability of receiving any given exposure level does not depend on any common causes. Therefore, we must measure and adjust for (i.e., include in the model) all variables that influence both the exposure and the outcome (and any intermediary variables; see Correia et al., 2025). Also requires <i>positivity</i> – individual units are equally likely to be exposed to a specific value of a causal factor (see below). References: Hernán & Robins, 2025; Morgan & Winship, 2015; Rosenbaum & Rubin, 1983	Terminology: “All front-door and back-door paths blocked”, or “no omitted common causes in the causal DAG”. Key Idea: All confounders identified by the front-door and back-door criteria (or additional criteria; see Maathuis & Colombo, 2015 and Shpitser & Pearl, 2008) are measured and adjusted for (e.g., included in the model). Also required <i>consistency</i> (the statistical property) – with infinite data, the estimated graph will converge to the true causal graph (see Pearl, 2009; Spirtes et al., 2000). References: Greenland et al., 1999b; Pearl, 2009
Terminology: “No interference”, “no spillover”, “no unit-to-unit causation”, or “no interactions between units” (see Cox, 1958); part of Stable Unit Treatment Value Assumption (SUTVA) (see Rubin, 1980). Key Idea: One unit’s exposure does not affect another unit’s outcome. Real-world systems often violate this assumption, requiring more complex methods (see Hudgens & Halloran 2008). References: Hudgens & Halloran, 2008; Rubin, 1978, 1980	Terminology: No spillover is implicitly assumed by SCM notation and causal DAGs. Key Idea: In a causal DAG, there are no edges from one unit’s exposure to another unit’s outcome, i.e., each unit’s outcome depends only on its own exposure. Systems that violate this assumption require multi-unit DAGs or specialized methods (see Pearl, 2009). Part of assumption that <i>units are independent and identically distributed</i> (i.i.d.) assumption; see Zhang et al., 2023. References: Pearl, 2009; Spirtes et al., 2000

A2. Causal Markov Condition: In a system with no cycles or feedback loops, any dependence between two variables that do not directly affect each other must come from a common cause influencing both. Once that common cause is accounted for, the two variables should no longer be dependent.

Potential Outcomes (PO) Framework	Structural Causal Models (SCM) Framework
Terminology: “No feedback” or “no cyclic causation” (i.e., simultaneous causation) are implied by the potential outcome notation: the outcome $Y(a)$ is measured after an exposure $A = a$. The exposure and outcome are conditionally independent once we account for all confounding variables. Key Idea: Once we measure and adjust for any shared causes, any dependence between two variables that do not share a direct causal relationship should no longer remain. This also requires that the cause precede the effect, ruling out simultaneity. References: Hernán & Robins, 2025; Morgan & Winship, 2015; Rubin, 1978	Terminology: By definition, causal DAGs are acyclic; therefore, feedback loops or bidirectional arrows (simultaneous causation) are disallowed. Sometimes referred to as <i>factorization</i> or the <i>local Markov property</i> – each node is conditionally independent of its non-descendants, given its parents. Key Idea: Once we condition on the parents (common causes), the dependence between two variables that do not directly affect each other is “blocked”. Since arrows in causal DAGs flow in one direction, it is assumed there is no cyclic causation. References: Pearl, 2009; Spirtes et al., 2000

A3. Causal Faithfulness: If two variables are statistically independent even after adjusting for confounders, then there is no causal relationship between those variables.

Potential Outcomes (PO) Framework	Structural Causal Models (SCM) Framework
Terminology: Implicitly assumed that any true causal effect would manifest as a dependence after all confounders are adjusted for. Key Idea: If two variables remain independent after controlling for all relevant confounders, we assume it’s not due to a coincidence but instead conclude there is no causal relationship. References: Hernán & Robins, 2025; Morgan & Winship, 2015	Terminology: Explicitly called <i>faithfulness</i> or <i>stability</i>, in which the causal DAG encodes all conditional independences. If two variables are independent, there exists no causal path (i.e., no causal relationship) between those variables in the causal DAG. Key Idea: If two variables remain independent after conditioning on the variables that block any back-door paths in a causal DAG, we assume this reflects a genuine absence of a causal relationship. References: Pearl, 2009; Spirtes et al., 2000; Wermuth & Lauritzen, 1990

Additional assumptions

B1. The exposure is well-defined (i.e., no multiple versions of the treatment, such as different strains of a disease being categorized as a single exposure). That is, there must be no ambiguity about what the cause or exposure is.

Potential Outcomes (PO) Framework	Structural Causal Models (SCM) Framework
Terminology: “Causal consistency” (not the same as the statistical property of consistency) or “well-defined treatment” †; part of SUTVA (Rubin 1978, 1980). Key Idea: No ambiguous exposure or no multiple versions of a single cause. A cause or exposure must be identically represented across all units. References: Hernán & Robins, 2025; Rubin, 1978, 1980	Terminology: A well-defined or unambiguous exposure is implied by the causal DAGs – the exposure must be unambiguous when declared as node in the causal DAG. Key Idea: The causal DAG must represent exactly one well-specified cause or exposure. If we can declare the cause or exposure as one node, we are assuming that it is well-defined. References: Pearl, 2009; Spirtes et al., 2000

B2. Among units that share the same values for the confounders, there must be some that are exposed and some that are not. In other words, the confounders must not perfectly predict the probability of exposure.*

Potential Outcomes (PO) Framework	Structural Causal Models (SCM) Framework
Terminology: “Positivity”, “overlap”, or “common support” † Key Idea: For any given combination of confounder values, there must be a nonzero chance of receiving each exposure level. References: Hernán & Robins, 2025; Morgan & Winship, 2015; Rosenbaum & Rubin, 1983	Terminology: All exposure levels are sufficiently represented in the data is implied by representing the exposure as a node in the causal DAG. Key Idea: Even if the causal DAG is correctly specified, the data must exhibit variation in exposure for every configuration of confounders. References: Pearl, 2009; Spirtes et al., 2000

†Causal consistency, positivity, and exchangeability make up the ‘identifiability conditions’ for causal effects. These conditions hold under idealized randomized experiments (see Kimmel et al., 2021).

*Positivity is a statistical assumption rather than a purely causal assumption. It requires that our data exhibit variation in exposures across all relevant confounders. See Hernán & Robins, 2025; Morgan & Winship, 2015; Rosenbaum & Rubin, 1983.

Box S2. Assumptions for causal discovery

Choice of framework

Dynamical Systems Causality (DC) Framework	Structural Causal Models (SCM) Framework
Useful for those who think about evolving states of systems over time; focuses on identifying causal relationships for dynamic or complex systems where long time series of observations are available, often under challenging scenarios (e.g., non-separability, high-dimensional nonlinearity).	Useful for those who think about multiple causes jointly (“all-cause models”). Emphasizes defining the minimal set of conditions under which causal effects can be identified and estimated.

Causal assumptions

A1. Causal Sufficiency: All relevant confounders are measured (i.e., no unmeasured common causes).

Dynamical Systems Causality (DC) Framework	Structural Causal Models (SCM) Framework
Terminology: “All variables that drive the system are embedded in the reconstructed state space”, “no missing drivers”, or “intrinsic noise is not attributable to external disturbances or measurement errors”. Key Idea: Implicitly assumes the measured variables capture the main dynamic influences. If crucial state variables are omitted, apparent causal links can be spurious. References: Ding & Toulis, 2018; Harnack et al., 2017; Orava, 1973; Sun et al., 2015	Terminology: “All relevant variables included”, or “no omitted common causes”. Key Idea: Discovery algorithms (e.g., PC, FCI) typically assume all major confounders are measured or the algorithm is adjusted to detect them. Also required <i>consistency</i> (the statistical property) – with infinite data, the estimated graph will converge to the true causal graph. References: Glymour et al., 2019; Peters et al., 2017; Spirtes et al., 2000
Terminology: The observed time series fully capture the dynamics of the unit, with no external influences (i.e., no inter-unit interference). Key Idea: The dynamics of each unit are self-contained; the time series used for discovery must reflect the complete internal state of the system. If significant spillover exists, the predictive relationships used to infer causality may be confounded by external influences. References: Harnack et al., 2017; Orava, 1973	Terminology: “No cross-unit edges” or “independence of units” in causal DAGs. Key Idea: Each unit is independent – one unit’s exposure does not affect another unit’s outcome. Part of the i.i.d. assumption – units are independent and identically distributed (see Zhang et al. 2023). References: Glymour et al., 2019; Spirtes et al., 2000

A2. Causal Markov Condition: In a system with no cycles or feedback loops, any dependence between two variables that do not directly affect each other must come from a common cause influencing both. Once that common cause is accounted for, the two variables should no longer be dependent.

Dynamical Systems Causality (DC) Framework	Structural Causal Models (SCM) Framework
Terminology: If two system components do not interact (directly or indirectly), their time series become conditionally independent (or uncorrelated) after controlling for the relevant state variables. Key Idea: In time-lagged embedding, if variable <i>A</i> does not help predict <i>B</i> once the relevant lags of <i>B</i> (and possibly other variables) are included, we treat them as causally disconnected. This also requires that the cause precede the outcome, ruling out simultaneity and cyclic causation (see below). References: Runge, Bathiany, et al., 2019; Sun et al., 2015	Terminology: Sometimes referred to as <i>factorization</i> or the <i>local Markov property</i> – each variable is conditionally independent of its confounders given its direct causes. Key Idea: If two variables are conditionally independent given some conditioning set in the data, they are not connected by any path in the DAG (or are d-separated). Implicitly assumes there is no simultaneity or cyclic causation (see below). References: Glymour et al., 2019; Peters et al., 2017; Spirtes et al., 2000

A3. Causal Faithfulness: If two variables are statistically independent even after adjusting for confounders, then there is no causal relationship between those variables.

Dynamical Systems Causality (DC) Framework	Structural Causal Models (SCM) Framework
Terminology: Referred to as <i>separability</i> – the influence of measured confounding variables can be eliminated from the information contained in the effect variable’s temporal trajectory without changing the direct relationship between the cause and effect; thus, an observed temporal dependence implies the presence of a causal relationship. Key Idea: If two variables remain independent after controlling for all relevant confounders, we assume it’s not due to a coincidence but instead conclude there is no causal relationship. References: Paluš et al., 2018; Runge, Bathiany, et al., 2019; Schreiber, 2000; Sun et al., 2015	Terminology: Explicitly called <i>faithfulness</i> or <i>stability</i>, in which the causal DAG encodes all conditional independences. If two variables are statistically independent, there exists no causal path (i.e., no causal relationship) between those variables in the causal DAG. Key Idea: If two variables remain independent after conditioning on the confounders, we assume this reflects a genuine absence of a causal relationship. References: Glymour et al., 2019; Peters et al., 2017; Spirtes et al., 2000

Additional assumptions

B1. Cause precedes effect; no simultaneity and no feedback loops.

Dynamical Systems Causality (DC) Framework	Structural Causal Models (SCM) Framework
Terminology: “Temporal ordering”, or “one variable’s state at the current time t influences the other’s state at future time $t + \ell$”. Key Idea: The future state of a system is conditionally independent of its past states, given its present state (i.e., cause precede effects in time). References: Ding & Toulis, 2018; Paluš et al., 2018	Terminology: “Acyclic”, “no bidirectional edges”, or “no feedback loops” implied in the causal DAG. Key Idea: Assumes no feedback loops or simultaneous causation exists in the data, since resultant causal DAGs are acyclic. References: Peters et al., 2017; Spirtes et al., 2000

B2. Stationarity – the system’s behavior doesn’t change dramatically over time (i.e., overall distributional patterns such as mean and variance of causes and outcomes remain relatively constant over time).

Dynamical Systems Causality (DC) Framework	Structural Causal Models (SCM) Framework
Terminology: The system's behavior does not change over time. Key Idea: Causal relationships remain consistent over time (dependencies should not fundamentally change or vanish). Also requires <i>ergodicity</i> – statistical properties (e.g., mean and variance) calculated from time series samples through the ergodic theorem do not change substantially over time. References: Harnack et al., 2017; McGoff et al., 2012; J. Shi et al., 2022	Terminology: The conditional independencies among variables are consistent over time. Key Idea: The influence of a variable’s state at a previous time $t - \ell$ on its state at the current time t remains consistent throughout the time series when controlling for the rest of the system’s state at the present time t. References: McGoff et al., 2012; Peters et al., 2017; Runge, Bathiany, et al., 2019

B3. Sufficient variability within variables in the system so that differences in exposure and outcome can be reliably detected.

Dynamical Systems Causality (DC) Framework	Structural Causal Models (SCM) Framework
Terminology: Time series provide a faithful representation of the system’s dynamics. Additionally, many approaches require that states of the system (e.g., from time series data) can be represented as a low-dimensional attractive manifold. Key Idea: There must be enough dynamic variation in the observed data to reveal causal influences, and the measured variables must adequately reflect the system’s underlying states. References: Barański et al., 2020; Deyle & Sugihara, 2011; J. Shi et al., 2022; Takens, 1981	Terminology: “Positivity” and “consistency”. Key Idea: Each variable (cause or outcome) exhibits enough variation to detect dependence (akin to <i>positivity</i> in causal inference). Also, each variable must be well-defined, so that distinct real-world processes aren’t lumped under one label (<i>consistency</i>). References: Glymour et al., 2019; Peters et al., 2017

5. Core concepts for each causal framework

While assumptions define the foundation for making valid causal claims, each causal framework also introduces a range of concepts and tools that shape how researchers think about variables, causal relationships, and estimation. To help readers navigate these differences, we provide three tables (Tables S3–S5), one for each framework (PO, SCM, and DC, respectively), that highlight foundational concepts across the frameworks, along with seminal and accessible sources for further reading. These tables are designed as navigational tools for readers seeking intuitive or technical entry points into each framework, such as ignorability and causal estimands in the PO framework, d-separation and *do*-calculus in the SCM framework, and state space reconstruction and separability in the DC framework. Familiarity with these concepts is important for understanding how causal inference and causal discovery are framed and implemented within each framework’s structure. These frameworks are not mutually exclusive and can be complementary depending on the causal task and data characteristics. Researchers should familiarize themselves with each to determine which assumptions and tools best align with their research goals.

Table S3. Key concepts and recommended references for understanding the potential outcomes (PO) framework.

Concept	Suggested Readings
Fundamentals of the PO framework	Holland, 1986; Rubin, 2005; Sobel, 2009
Stable Unit Treatment Value Assumption (SUTVA)	Sobel, 2006; VanderWeele & Hernán, 2013
Ignorability Assumption (Unconfoundedness)	Imbens, 2004; Rosenbaum & Rubin, 1983
Positivity Assumption (Overlap Condition)	Petersen et al., 2012; Westreich & Cole, 2010
Confounding variables to control for in analyses	Gelman et al., 2020; VanderWeele, 2019; VanderWeele & Shpitser, 2011
Causal estimands: average treatment effect (ATE) and others	Heiss, 2024; Imbens, 2004; Imbens & Angrist, 1994; Lipkovich et al., 2020; Wooldridge, 2010 (Ch. 21)
Multiple versions of treatment and interference	Hudgens & Halloran, 2008; Tchetgen Tchetgen & VanderWeele, 2012; VanderWeele & Hernán, 2013

306 Table S4. Key concepts and recommended references for understanding the structural causal
307 models (SCM) framework.

Concept	Suggested Readings
Fundamentals of the SCM framework	Burnett & Blackwell, 2024; Cheng et al., 2024; Petersen & van der Laan, 2014; Scheines, 1997
Confounding variables to control for in analyses (d-separation; Back-door and Front-door Criteria)	Arif & Massey, 2023; Bulbulia, 2024a; Elwert, 2013; Greenland, 2003; Morgan & Winship, 2015 (Ch. 4 & 10); Pearl, 2010
Graphical rules for causal identification in graphs (<i>do</i> -calculus)	Hayduk et al., 2003; Pearl, 2009 (Ch. 1 & 11); Shpitser & Pearl, 2008; Tian & Pearl, 2002
Total and path-specific causal effects	Bulbulia, 2024b; Pearl, 2009 (Ch. 3, 4, 7); VanderWeele, 2015d
Model equivalence and Markov equivalence classes	Andersson et al., 1997; Pearl, 2009 (Ch. 5)
Causal graphs with unmeasured/latent variables	Pearl, 2009 (Ch. 12) ; Richardson & Spirtes, 2002

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310 Table S5. Key concepts and recommended references for understanding the dynamical systems
 311 causality (DC) framework.

Concept	Suggested Readings
Fundamentals of the DC framework	Deyle & Sugihara, 2011; Harnack et al., 2017; Runge, 2018; J. Shi et al., 2022; Yuan & Shou, 2022
State space reconstruction (SSR) and attractor manifolds	Cummins et al., 2015; Sauer et al., 1991; Takens, 1981
Causality via predictability	Paluš, 2007; Runge, 2018; Sugihara et al., 2012
Transfer entropy and information-theoretic causality	Schreiber, 2000; Sun et al., 2015; Sun & Bollt, 2014
Separability and causal faithfulness	Eichler, 2013; Peters et al., 2017; Runge, Nowack, et al., 2019
Confounding and hidden variables in time series	De Brouwer et al., 2021; Eichler, 2013; Sun & Bollt, 2014
Limitations in stochastic or weakly coupled systems	Cobey & Baskerville, 2016; McCracken & Weigel, 2014

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6. Study designs and algorithms for causal analyses

Selecting a study design or algorithm is a critical step in implementing a causal analysis. Different designs and algorithms offer structured ways to satisfy or relax the untestable causal assumptions and must be chosen in light of the causal task, available data, and pre-existing knowledge. Some approaches are grounded in experimental control, while others rely on statistical adjustments or algorithmic structure learning to address confounding and identify causal relationships.

To help readers explore available options, we provide a series of tables that group study designs and algorithms according to the type of causal task (inference or discovery) and whether they address measured or unmeasured confounding. Table S6 summarizes study designs for causal inference, including experimental designs, observational designs for measured confounders, and observational designs for unmeasured confounders. Table S7 summarizes algorithms for causal discovery, grouped by the causal framework and assumptions each algorithm relies on. These tables are intended to serve as a reference for researchers selecting and comparing appropriate strategies for their study goals, system knowledge, and data constraints. For additional guidance on the selection of specific causal inference study designs and causal discovery algorithms, see the flow chart in Figure 2 in Runge et al., 2023.

Causal inference requires that all confounders be addressed (see Box S1), but this does not necessarily mean every confounder must be explicitly included in a model. Instead, confounding is typically handled using a combination of design-based approaches: directly controlling for measured confounders and employing statistical designs that reduce bias from unmeasured confounders (e.g., experimental randomization or statistical approaches that mimic randomization).

If significant pre-existing knowledge is available and the goal is to obtain system-level understanding (i.e., to model the effects of all causes of an outcome), then SCM-based adjustment methods (e.g., Front-door and Back-door Criteria; see Pearl, 2009 and Arif & MacNeil, 2022) or structural equation modeling (SEM) may be appropriate approaches. While SCM-based adjustment methods typically target specific causal effects, SEM is often used to model entire systems of causal relationships simultaneously. However, this comes with tradeoffs: SEM requires more restrictive assumptions in order to support system-level inferences. These tradeoffs underscore the need to carefully align the use of SEM with the level of pre-existing knowledge and assumptions that can be plausibly justified for the ecological system under study (Grace, 2024; Pearl, 2012; Shipley, 2016). In cases where unobserved variables are present, acyclic directed mixed graphs (ADMGs) can represent the same set of conditional independencies as a DAG. ADMGs also allow for bidirectional (i.e., double-headed) arrows, enabling representation of latent confounding. These graphs rely on an extension of Pearl's *d*-separation criterion, called *m*-separation (for details, see Richardson, 2003 and Drton & Richardson, 2004).

While both SEM and SCM approaches rely on a causal graph to represent assumptions, they differ in how those assumptions are used. SCMs (Pearl, 2009) use the graph to derive conditions under which causal effects can be identified from data, often targeting specific effects of interest via tools such as the Back-door or Front-door criteria. In an SCM approach, the causal graph is used to ask, “Given this DAG, can I even estimate the causal effect of X on Y from observed data, and if so, how?” In contrast, SEMs as used in ecology (Grace et al., 2015; Shipley, 2016) typically assume the full system of causal relationships is known, and use the graph to specify a system of structural equations whose fit can be statistically tested. That is, for SEMs, the causal graph is used to ask, “Assuming this DAG is correct, do the observed data support it, and can I fit a model to estimate the effects I care about?” SEM-based causal inference does not involve formal identification theorems, and estimation is typically linear, even when nonlinear terms are used. Thus, SEMs rely more heavily on model specification and goodness-of-fit, whereas SCMs prioritize identifiability of causal effects under minimal assumptions (Pearl, 1998). SEMs can yield unbiased causal effect estimates if the model includes all relevant confounders and is correctly specified; however, unlike SCM-based methods, they do not provide formal identification criteria to assess whether these conditions are met (Bollen & Pearl, 2013; Markus, 2010; Wang & Sobel, 2013). This distinction highlights that while both approaches can be used for causal modeling, they support different inferential goals and require different standards of justification.

372 Table S6. Study designs for causal inference, grouped by category. Each study design includes a brief description, key references
 373 (including applications in ecology, where available), and links to available software and code. The resources and applications listed
 374 are not exhaustive – we prioritized accessible sources and informative, causally focused applications.

Category	Design	Resources and Applications	Software and packages ¹
Experimental designs ²	Randomized Controlled Trial (RCT): Randomly assign units to treatment or control groups, helping to balance confounders across groups.	Kim & DeVries, 2001; Kimmel et al., 2021; Pynegar et al., 2021; Tilman et al., 2006; Weigel et al., 2021; Wiik et al., 2020	experiment (R package; see https://cran.r-project.org/package=experiment) RCT (R package; see https://cran.r-project.org/package=RCT) ExpAn (Python library; see https://github.com/zalando/expan)
	Factorial Design: Randomly assign units to multiple treatment combinations to test interactions and account for confounding of multiple causal variables.	Dasgupta et al., 2015; Jayewardene, 2009; Kaspari et al., 2012; King & Tschinkel, 2008; Laube & Zotz, 2003; Nicolaisen et al., 2014; Zhao & Ding, 2022	GFD (R package; see https://cran.r-project.org/package=GFD) fullfact (R package; see https://cran.r-project.org/package=fullfact) DoE.base (R package; see https://cran.r-project.org/package=DoE.base) pyDOE2 (Python library; see https://github.com/clicumu/pyDOE2) dexpy (Python library; see https://github.com/statease/dexpy)
	Crossover Trial: Units receive multiple treatments in a random sequence, allowing each unit to serve as its own control and account for confounders that vary between units.	Díaz-Urriarte, 2002; Feinsinger et al., 1991; Fergus et al., 2023; Jaakkola, 2003; Montesanto & Cividini, 2017; Ohrens et al., 2019; Shahn et al., 2023; Treves et al., 2024	crossdes (R package; see https://cran.r-project.org/package=crossdes) CrossCarry (R package; https://cran.r-project.org/package=CrossCarry) Crossover (R package; https://cran.r-project.org/package=Crossover)
	Cluster Randomized Trial: Randomize groups instead of individual units to	Benitez et al., 2023; Branas et al., 2018; Hemming & Taljaard, 2023; Schochet, 2013	cvcrand (R package; see https://cran.r-project.org/package=cvcrand) experiment (R package; see https://cran.r-project.org/package=experiment)

¹ See also <https://cran.r-project.org/view=CausalInference>

² See also <https://cran.r-project.org/view=ExperimentalDesign>

	account for group-level confounders.		cluster_experiments (Python library; see https://github.com/david26694/cluster-experiments)
Observational designs – controlling measured confounders	Regression Adjustment: Include confounders as covariates in the regression model describing the relationship of the causal variable on the outcome.	Fieberg & Ditmer, 2012; Gelman et al., 2020; Moss et al., 2025; Nogueira et al., 2022; Simler-Williamson & Germino, 2022	R packages: Base R functions – lm(...), glm(...), etc. – or dedicated regression packages Python libraries: statsmodels, linearmodels, etc. <i>Note: No dedicated packages or libraries – standard regression functions are used when confounders are explicitly specified in models used for causal interpretation.</i>
	Stratification: Divide units into subgroups, either during study design (e.g., stratified sampling) or during analysis (e.g., subgroup comparisons), based on confounders, then compares those with similar confounders but different exposure levels.	Morgan & Winship, 2014; Oehri et al., 2020; Rosenbaum, 2002	stdReg2 (R package; see https://cran.r-project.org/package=stdReg2) stratamatch (R package; see https://cran.r-project.org/package=stratamatch)
	Inverse Probability Weighting (IPW)^a: Weight units based on their probability of exposure to create a pseudo-population where confounders are balanced.	Hernán & Robins, 2025 (Ch. 12); Nogueira et al., 2022; West et al., 2022	ipw (R package; see https://cran.r-project.org/package=ipw) twang (R package; see https://cran.r-project.org/package=twang) WeightIt (R package; see https://cran.r-project.org/package=WeightIt) CausalPy (Python library; see https://github.com/pymc-labs/CausalPy)
	Propensity Score Matching (PSM)^a: Match units with similar probabilities of exposure based on observed confounders (propensity scores) to create treatment	Butsic et al., 2017; Emmons et al., 2024; Nogueira et al., 2022; Pearson et al., 2016; Siegel, Larsen, et al., 2022; Siegel, Macaulay, et al., 2022; Simler-	Matching (R package; see https://cran.r-project.org/package=Matching) MatchIt (R package; see https://cran.r-project.org/package=MatchIt) CausalGPS (R package; see https://cran.r-project.org/package=CausalGPS) and

	and control groups with balanced covariate distributions.	Williamson & Germino, 2022; West et al., 2022; Wiik et al., 2020	pycausalgps (Python library; see https://github.com/NSAPH-Software/pycausalgps) psmpy (Python library; see https://pypi.org/project/psmpy)
	Marginal Structural Modeling (MSM)[†]: Use weighting to adjust for time-varying confounders when causal variables change over time.	Cole & Hernán, 2008; Hernán & Robins, 2025 (Ch. 12); Lei et al., 2019; Mandujano Reyes et al., 2025; Nandi et al., 2012; VanderWeele et al., 2011	bayesmsm (R package; see https://github.com/Kuan-Liu-Lab/bayesmsm) trajmsm (R package; see https://cran.r-project.org/package=trajmsm)
	Multi-level Modeling with Mixed Effects: Account for confounders from hierarchical data structures by including both fixed and random effects.	Bingenheimer & Raudenbush, 2004; Clough, 2012; Gelman, 2006; Gelman & Hill, 2006	lme4 (R package; see https://cran.r-project.org/package=lme4) brms (R package; see https://cran.r-project.org/package=brms) statsmodels (Python library; see https://www.statsmodels.org/) Bambi (Python library; see https://bambinos.github.io/bambi)
	Structural Causal Model (SCM)-based Back-door Criterion: Use causal diagrams to identify the minimal set of confounders that must be measured to enable unbiased estimation of causal effects.	Arif et al., 2022; Arif & MacNeil, 2022; Paul, 2011; Pearl, 2009; Schoolmaster et al., 2020; Stewart et al., 2023	causaleffect (R package; see https://cran.r-project.org/package=causaleffect) dagitty (R package and Web interface; see https://dagitty.net) DoWhy (Python library; see https://py-why.github.io/dowhy)
	Structural Equation Modeling (SEM)^{b,c}: Simultaneously quantify multiple causal relationships by including measured confounders as covariates in linear models.	Bollen & Pearl, 2013; Cronin & Schoolmaster, 2018; Grace et al., 2015; Hatami, 2019; Pearl, 1998, 2012; Saavedra et al., 2022	pwSEM ^d (R package; see https://github.com/BillShipley/pwSEM) piecewiseSEM ^d (R package; see https://cran.r-project.org/package=piecewiseSEM) lavaan (R package; see https://cran.r-project.org/package=lavaan)

			semopy (Python library; see https://semopy.com)
Observational designs – controlling unmeasured confounders	Instrumental Variables (IV): Use a variable that influences the causal variable but not the outcome directly, to accounting for unmeasured confounders.	Butsic et al., 2017; Kendall, 2015; Larsen et al., 2019; MacDonald et al., 2019; MacDonald & Mordecai, 2019	ivreg (R package; see https://cran.r-project.org/package=ivreg) AER (R package; see https://cran.r-project.org/package=AER) EconML (Python library; see https://github.com/py-why/econml) CausalPy (Python library; see https://github.com/pymc-labs/CausalPy)
	Before-After-Control-Impact (BACI)^{ef}: Compare changes in the outcome before and after a shift in the causal variable, while using a control group to account for time-varying confounders.	Chevalier et al., 2019; Christie et al., 2019; Comte et al., 2023; Ferraro et al., 2019; Kerr et al., 2019; Paul, 2011; Pitcher et al., 2009; Smokorowski & Randall, 2017; Wauchope et al., 2021	R packages: lme4, glmmTMB, or other multi-level modeling packages Python libraries: statsmodels, pingouin, or other packages supporting interaction terms in multi-level models <i>Note: No dedicated packages for BACI designs – analyses typically use mixed-effects models with an interaction term between Time (Before vs. After) and Treatment (Control vs. Impact) to estimate causal effects.</i>
	Difference-in-Differences (DiD)^{tf}: Compare changes in the outcome over time between units with and without a change in exposure, while accounting for time-invariant confounders.	Butsic et al., 2017; Larsen et al., 2019; Simler-Williamson & Germino, 2022	did (R package; see https://cran.r-project.org/package=did) fixest (R package; see https://cran.r-project.org/package=fixest) CausalPy (Python library; see https://github.com/pymc-labs/CausalPy)
	Regressions Discontinuity Design (RDD)^f: Compare units just above and below a cutoff, assuming they are similar in all respects except exposure, to remove	Butsic et al., 2017; Cook et al., 2008; Imbens & Lemieux, 2008; Larsen et al., 2019; Noack et al., 2022	rdrobust (R package; see https://cran.r-project.org/package=rdrobust) rddensity (R package; see https://cran.r-project.org/package=rddensity) CausalPy (Python library; see https://github.com/pymc-labs/CausalPy)

	confounding from variables that do not shift abruptly at the threshold.		
	Synthetic Control Methods[†]: Construct a synthetic control group from a weighted combination of unexposed units to approximate an exposed group with similar distributions of unmeasured confounders.	Abadie et al., 2010; Fick et al., 2021; West et al., 2022; X. Wu et al., 2023	Synth (R package; see https://cran.r-project.org/package=Synth) tidysynth (R package; see https://cran.r-project.org/package=tidysynth) CausalPy (Python library; see https://github.com/pymc-labs/CausalPy)
	Multi-level Modeling with Fixed Effects[†]: Use only within-unit variation over time to address time-invariant unmeasured confounders.	Byrnes & Dee, 2025; Gelman & Hill, 2006; Simler-Williamson & Germino, 2022	fixest (R package; see https://cran.r-project.org/package=fixest) lfe (R package; see https://cran.r-project.org/package=lfe) plm (R package; see https://cran.r-project.org/package=plm) PyFixest (Python library; see https://github.com/py-econometrics/pyfixest)
	Structural Causal Model (SCM)-based Front-door Criterion: Use causal diagrams to identify sets of measured variables that address the effects of some unmeasured confounders.	Arif et al., 2022; Arif & MacNeil, 2022; Paul, 2011; Pearl, 2009; Stewart et al., 2023	causaleffect (R package; see https://cran.r-project.org/package=causaleffect) dagitty (R package and Web interface; see https://dagitty.net) fdtlme (R package; see https://github.com/annaguo-bios/fdtlme) DoWhy (Python library; see https://py-why.github.io/dowhy)
	Interrupted Time Series Analysis[†]: Leverages a natural or implemented change using repeated outcome measurements before and after the change	Gilmour et al., 2006; Kontopantelis et al., 2015; Lopez Bernal et al., 2016; Wauchope et al., 2021	CausalImpact (R package; see https://github.com/google/CausalImpact) and CausalImpact (Python library; see https://pypi.org/project/causalimpact) segmented (R package; see https://cran.r-project.org/package=segmented)

	to account for pre-existing trends.		CausalPy (Python library; see https://github.com/pymc-labs/CausalPy)
†Requires time-series data. ^aIPW and PSM are both examples of Covariate Balancing designs, which balance distribution of confounders across units with different exposure levels. ^bSEMs can incorporate unobserved constructs (i.e., “latent variables”) which are inferred from measured variables. ^cTo support causal interpretations, SEMs must explicitly invoke untestable causal assumptions (see Bollen & Pearl, 2013; Pearl, 2012) and specify a causal structure via an SEM diagram (see Kunicki et al., 2023). ^dWhile some SEM implementations allow some nonlinear specifications (e.g., via generalized additive models), they estimate causal effects using path coefficients or smooth terms derived from model components (Lefcheck, 2016) but do not provide formal identification criteria, as in nonparametric SCMs, to assess whether these effects can be uniquely determined from the data (Wang & Sobel, 2013). ^eExperimental BACI designs with manipulated treatments are rare. Most BACI studies are observational and may not meet all the assumptions for robust causal inference (see Ferraro et al., 2019; Smokorowski & Randall, 2017; Wauchope et al., 2021). ^fBACI, DID, and RDD are all examples of Natural Experiments, which leverage naturally occurring random variation in the causal variable to mimic randomization and account for unmeasured confounders.			

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378 Table S7. Algorithms for causal discovery, grouped by category. Each algorithm includes a brief description, key references
 379 (including applications in ecology, where available), and links to available software and code.

Category	Algorithm	Resources and Applications	Software and packages
Constraint-based methods	PC (Peter and Clark) : Uses repeated conditional independence tests to infer causal relationships from observed independencies in data, producing a set of causal graphs that represent possible causal relationships consistent with the data.	Bystrova et al., 2024; Chu et al., 2018; Ebert-Uphoff & Deng, 2012; Glymour et al., 2019; Kalisch et al., 2012; J. Li et al., 2015, pp. 9–20; Spirtes et al., 2000	pcalg (R package; see https://cran.r-project.org/package=pcalg) bnlearn (R package; see https://cran.r-project.org/package=bnlearn and https://www.bnlearn.com) Tetrad (GUI, Python library, R package; see https://www.cmu.edu/dietrich/philosophy/tetrad/use-tetrad) causal-learn (Python library; see https://causal-learn.readthedocs.io) pgmpy (Python library; see https://pgmpy.org)
	FCI (Fast Causal Inference) : Extends the PC algorithm to detect possible unmeasured confounders, producing a causal graph that reflects uncertainty about edges.	Bystrova et al., 2024; Glymour et al., 2019; Kalisch et al., 2012; La Bastide-van Gemert et al., 2014; Mielke et al., 2022; Nogueira et al., 2022; Shen et al., 2020	pcalg (R package; see https://cran.r-project.org/package=pcalg) Tetrad (GUI, Python library, R package; see https://www.cmu.edu/dietrich/philosophy/tetrad/use-tetrad) causal-learn (Python library; see https://causal-learn.readthedocs.io)
	PCMCI (Peter and Clark Momentary Conditional Independence) : A time-series adaptation of PC that improves detection of causal effects in autocorrelated data by iteratively testing for conditional independencies among variables and their lags.	Docquier et al., 2024; Krich et al., 2020; Nogueira et al., 2022; Runge, Nowack, et al., 2019; Tárraga et al., 2024	Tigramite (Python library; see https://github.com/jakobrunge/tigramite) CausalFlow (Python library; see https://github.com/lcastri/causalflow)
Score-based methods	GES (Greedy Equivalence Search) : Searches for the best	Gong et al., 2025; La Bastide-van Gemert et al., 2014	pcalg (R package; see https://cran.r-project.org/package=pcalg)

	causal graph by iteratively adding or removing edges based on a scoring criterion, such as the Bayesian Information Criterion (BIC), balancing data fit and simplicity.		Tetrad (GUI, Python library, R package; see https://www.cmu.edu/dietrich/philosophy/tetrad/use-tetrad) pgmpy (Python package; see https://pgmpy.org/) causal-learn (Python library; see https://causal-learn.readthedocs.io)
	GIES (Greedy Interventional Equivalence Search): An extension of GES that incorporates interventional data or assumptions to distinguish between equivalent causal graphs.	Hauser & Bühlmann, 2012; Shah et al., 2023	pcalg (R package; see https://cran.r-project.org/package=pcalg) Causal Discovery Toolbox (Python library; see https://github.com/FenTechSolutions/CausalDiscoveryToolbox) gies (Python library; see https://github.com/juangamella/gies)
	FGES (Fast Greedy Equivalence Search): A variant of GES that uses a parallelized greedy approach to rapidly search for the optimal causal graph, making it suitable for high-dimensional datasets.	Kitson & Constantinou, 2021; Ramsey et al., 2017; Shen et al., 2020	Tetrad (GUI, Python library, R package; see https://www.cmu.edu/dietrich/philosophy/tetrad/use-tetrad)
Functional model-based methods	LiNGAM (Linear Non-Gaussian Acyclic Model): Identifies causal direction among variables by assuming linear relationships and non-Gaussian noise.	Ikeuchi et al., 2023; Kotoku et al., 2020; Kurotani et al., 2024; Shimizu, 2014; Shimizu et al., 2006, 2011	Tetrad (GUI, Python library, R package; see https://www.cmu.edu/dietrich/philosophy/tetrad/use-tetrad) causal-learn (Python library; see https://causal-learn.readthedocs.io) lingam (Python library; see https://github.com/cdt15/lingam)
	ANM (Additive Noise Model): Assumes the outcome variable is an unknown function of the causal variable plus independent additive noise, which enables	Bühlmann et al., 2014; Mooij et al., 2016; Peters et al., 2014; Song et al., 2022	CANM (R package; see https://github.com/Jie-Qiao/CANM) causal-learn (Python library; see https://causal-learn.readthedocs.io)

	identification of causal direction in both linear and nonlinear settings.		Causal Discovery Toolbox (Python library; see https://github.com/FenTechSolutions/CausalDiscoveryToolbox) lingam (Python library; see https://github.com/cdt15/lingam)
	IGCI (Information Geometric Causal Inference): Determines causal direction by analyzing asymmetries in the joint distributions of cause-effect pairs, without inherently controlling for or detecting unmeasured confounders or indirect causal effects.	Janzing et al., 2012; Mooij et al., 2016; Song et al., 2022	CANM (R package; see https://github.com/Jie-Qiao/CANM) Causal Discovery Toolbox (Python library; see https://github.com/FenTechSolutions/CausalDiscoveryToolbox) IGCI (Python library; see https://github.com/amber0309/IGCI)
Dynamical systems causality (DC)-based methods	Granger Causality (GC): Tests whether past values of one time series can predict future values of another, assuming linear relationships in time-series data.	Detto et al., 2012; Granger, 1969; Nogueira et al., 2022; Reygadas et al., 2020; Singh & Borrok, 2019; Yuan & Shou, 2022	NlinTS (R package; see https://cran.r-project.org/package=NlinTS) causal-learn (Python library; see https://causal-learn.readthedocs.io)
	Information Theoretic (IT) Causality: A class of nonparametric and model-based methods that infer direct causal relationships by quantifying how knowledge of one variable reduces uncertainty about the future states of another variable. Includes Transfer Entropy (TE) approaches.	Benocci et al., 2025; Docquier et al., 2024; Hmamouche, 2020; Schreiber, 2000; Sun et al., 2015; Sun & Bollt, 2014; Yang et al., 2018	NlinTS (R package; see https://cran.r-project.org/package=NlinTS) copent (R package; see https://github.com/majianthu/copent) crossmapy (Python library; see https://github.com/PengTao-HUST/crossmapy) IDTxI (Python library; see https://github.com/pwollstadt/IDTxI)
	Convergent Cross Mapping (CCM): Uses state-space reconstruction to infer causal	Chang et al., 2017; Karakoç et al., 2020; Kitayama et al., 2021; Matsuzaki et al., 2018; Nova et al.,	rEDM (R package) and pyEDM (Python library); see

	relationships in nonlinear systems by testing whether past states of the causal variable can reliably predict current states of another variable.	2021; Sugihara et al., 2012; Ushio et al., 2018; J. Wu et al., 2023; Ye et al., 2015; Yuan & Shou, 2022	https://sugiharalab.github.io/EDM_Documentation
	Partial Cross Mapping (PCM): An extension of CCM that adjusts for potential unmeasured confounders to better isolate direct causal relationships.	Leng et al., 2020; Yongmei & Yulian, 2024	MATLAB code (see https://github.com/Partial-Cross-Mapping) crossmapy (Python library; see https://github.com/PengTao-HUST/crossmapy)

381 **7. Advanced methods for causal inference and causal discovery**

382 While many of the fundamental methods for causal discovery and causal inference have existed for
383 several decades, the field of causal inference is continually evolving to incorporate novel statistical
384 techniques and address increasingly complex data scenarios. For example, machine learning (ML)
385 techniques are being integrated into methods for causal discovery and causal inference (Leist et al.,
386 2022). Causal discovery with ML approaches, such as deep causal learning algorithms, use neural
387 approaches to learn causal networks from a combination of empirical data and prior causal knowledge
388 (C. Li et al., 2024; Scherrer et al., 2021; Yu et al., 2019). ML models can also be used in causal
389 inference, provided the model and covariates are specified to accurately represent the underlying causal
390 process (Brand et al., 2023; Hernán & Robins, 2024; Huber, 2023). For example, causal forests estimate
391 causal effects using random forests (Wager & Athey, 2018), while double/debiased ML methods, such
392 as targeted maximum likelihood estimation (TLME) (van der Laan & Rubin, 2006), control for
393 measured confounders using ML models that can capture complex nonlinear and high-dimensional
394 patterns of confounding (Chernozhukov et al., 2018). We summarize some of these
395 advanced methods for both causal discovery and causal inference in Table S8.

396 It should be noted that not all ML approaches are appropriate for causal analyses (Pichler &
397 Hartig, 2023). ML approaches are merely a class of models that, without pre-existing knowledge and
398 assumptions, are purely intended for predictive tasks and are not appropriate for obtaining causal
399 interpretations (Section S2). Thus, causal ML approaches still require the principles and assumptions
400 linking statistical dependence to causal dependence (Section S4), and careful model building using pre-
401 existing knowledge about all relevant confounding variables is essential for these methods to detect and
402 estimate causal effects without bias (Section S3).

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Table S8. Advanced methods for causal discovery and causal inference, grouped by causal task. Each method includes a brief description, key references and links to relevant software and code.

Causal Task	Method	Resources and Applications	Software and packages ³
Causal discovery	Deep causal learning: Uses deep learning models (e.g., neural networks) to detect causal relationships in complex, high-dimensional data, often incorporating pre-existing knowledge to improve accuracy.	C. Li et al., 2024; Luo et al., 2020; Yu et al., 2019; K. Zheng et al., 2024	DAG-GNN (Python code; see https://github.com/fishmoon1234/DAG-GNN) DeFuSE (Python code; see https://github.com/chunlinli/defuse) Dagma (Python library; see https://github.com/kevinsbello/dagma)
	Causal representation learning: Learning disentangled latent representations that correspond to underlying causal variables and capture the structure of the data-generating process.	Ahuja et al., 2023; Brehmer et al., 2022; Scholkopf et al., 2021	Emei (Python library; see https://github.com/FrankTianTT/emei) DRL (Python code; see https://github.com/CausalRL/DRL) gCastle (Python library; see https://pypi.org/project/gcastle)
	Causal reinforcement learning: Incorporates causal assumptions or causal models into reinforcement learning (a machine learning approach where models learn by trying actions and observing which ones produce the best outcomes).	Buesing et al., 2019; Wang et al., 2021; Zeng et al., 2025; Zhu et al., 2020	CARL (Python code; see https://github.com/arquimides/carl) <i>Note: No dedicated packages or libraries – most implementations of causal reinforcement learning are ad hoc in published papers or preprints.</i>
	Invariant causal prediction: Identifies causal variables by selecting predictors whose statistical relationships with the outcome remain invariant across environments or experimental settings.	Peters et al., 2016; Pfister et al., 2019	InvariantCausalPrediction (R package; see https://cran.r-project.org/package=InvariantCausalPrediction) causalicp (Python library; see https://github.com/juangamella/icp)

³See also <https://github.com/rguo12/awesome-causality-algorithms>

Causal inference	Targeted Maximum Likelihood Estimation (TMLE): Semi-parametric method that uses machine learning models for flexible outcome and treatment modeling, with a targeted correction step to ensure valid inference.	Luque-Fernandez et al., 2018; Schuler & Rose, 2017; van der Laan & Rubin, 2006	tmle3 (R package; see https://tlverse.org/tmle3) causal-curve (Python library; see https://github.com/ronikobrosly/causal-curve)
	Double/debiased machine learning: Uses machine learning to model outcomes and treatments separately, then combines them to estimate treatment effects while controlling for confounding in high-dimensional settings.	Chernozhukov et al., 2018; Fink et al., 2023; B. Shi et al., 2024	DoubleML (R package; see https://cran.r-project.org/package=DoubleML) EconML (Python library; see https://github.com/py-why/econml)
	Causal forests: Uses ensembles of decision trees to estimate heterogeneous treatment effects while accounting for confounding.	Athey et al., 2019; Athey & Wager, 2019; Fink et al., 2023; Wager & Athey, 2018; Xie et al., 2012; L. Zheng & Yin, 2023	grf (R package; see https://cran.r-project.org/package=grf) EconML (Python library; see https://github.com/py-why/econml)
	Meta-learners for heterogeneous treatment effects (e.g., S-learner, T-learner, X-learner, and R-learner): Use machine learning models to estimate heterogeneous treatment effects by modeling outcomes separately for different treatment levels, with a tradeoff between simple implementation and reduced reliability in inference.	Jiang et al., 2021; Künzel et al., 2019; Nie & Wager, 2021; Salditt et al., 2024	rlearner (R package; see https://github.com/xnie/rlearner) EconML (Python library; see https://github.com/py-why/econml) CausalML (Python library; see https://github.com/uber/causalml) metalearners (Python library; see https://github.com/quantco/metalearners)
	Causal inference using Bayesian machine learning: Estimate treatment effects using Bayesian machine learning models (e.g., Bayesian Additive Regression Trees [BART]) to capture nonlinear	Green & Kern, 2012; Hahn et al., 2020; J. Hill et al., 2020; J. L. Hill, 2011; Zeldow et al., 2019	bartCause (R package; see https://github.com/vdorie/bartCause) BCI Toolbox (Python library; see https://github.com/evans1112/bcitoolbox)

	relationships and quantify uncertainty via posterior distributions.		
	Counterfactual fairness: Defines fairness based on counterfactual comparisons across protected attributes using structural causal models, ensuring outcomes would remain the same in a hypothetical world where protected group membership had been different.	Chiappa, 2019; Nabi & Shpitser, 2018; Y. Wu et al., 2019	EXOC (Python code; see https://github.com/CASE-Lab-UMD/counterfactual_fairness 2025) <i>Note: No dedicated packages or libraries – most implementations of counterfactual fairness are ad hoc in published papers or preprints.</i>
	Causal data fusion: Combines data from different sources (e.g., observational and experimental) to estimate causal effects when no single dataset is sufficient, using assumptions encoded in transportability diagrams (causal diagrams that represent differences between data sources).	Bareinboim & Pearl, 2016; Chau et al., 2021; Josey et al., 2022; Pearl & Bareinboim, 2014	<i>Note: Data fusion methods remain in development, thus general-purpose implementations are not currently widely available. Implementation of some data fusion concepts are available via a GUI at https://causalfusion.net. A Python library called Y_0 (see https://github.com/y0-causal-inference/y0) also implements some data fusion concepts (e.g., parsing transportability graphs).</i>

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