
The Case for Evaluating Causal Models Using Interventional Measures and Empirical Data

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Abstract

Causal inference is central to many areas of artificial intelligence, including complex reasoning, planning, knowledge-base construction, robotics, explanation, and fairness. An active community of researchers develops and enhances algorithms that learn causal models from data, and this work has produced a series of impressive technical advances. However, *evaluation techniques* for causal modeling algorithms have remained somewhat primitive, limiting what we can learn from experimental studies of algorithm performance, constraining the types of algorithms and model representations that researchers consider, and creating a gap between theory and practice. We argue for more frequent use of evaluation techniques that examine *interventional measures* rather than structural or observational measures, and that evaluate those measures on *empirical data* rather than synthetic data. We survey the current practice in evaluation and show that these are rarely used in practice. We show that such techniques are feasible and that data sets are available to conduct such evaluations. We also show that these techniques produce substantially different results than using structural measures and synthetic data.

1 Introduction

Evaluation is central to research in artificial intelligence and machine learning [Cohen, 1995, Langley, 2011]. How we evaluate algorithms determines our perception of the relative effectiveness and usefulness of different approaches, and this knowledge guides choices about future research directions. As Cohen and Howe [1989] explained three decades ago: “Ideally, evaluation should be a mechanism by which AI progresses both within and across individual research projects. It should be something we do as individuals to help our own research and, more importantly, on behalf of the field.”

As fields develop, protocols for evaluation need to develop alongside them. In this paper, we offer an empirical analysis of the set of techniques typically used to evaluate algorithms for learning causal models, and we show that this set could be substantially enhanced. The ultimate goal of most algorithms for causal inference is to learn models capable of accurately estimating the effects of interventions on real-world data. With this goal in mind, we would like to evaluate algorithms by comparing their estimates to actual interventional effects on data produced by a real-world system. In practice, though, many evaluations fall short of this ideal, most frequently using only structural or observational measures and synthetic data. Without the use of *empirical data*, our evaluations produce little information about whether our algorithms generalize to real-world systems, and this greatly reduces their likelihood of widespread adoption by others outside of the field. Without the use of *interventional measures*, our evaluations produce little information about whether learned models will accurately estimate the effects of interventions, limiting their real-world utility.

Note that we do not argue for *replacing* the prevailing techniques for evaluation. These techniques have substantial value, both in assessing overall performance and in allowing fine-grained experiments to diagnose specific performance issues. Rather, we argue for *augmenting* the current suite of

evaluation techniques to gather experimental evidence that the prevailing techniques cannot. We also do not contend that interventional measures and empirical data are entirely absent from current studies. A very small minority of recent studies use these techniques in combination. Rather, we argue that interventional measures and empirical data should be used routinely, and should be used in combination, for any serious study of algorithms for learning causal models. Indeed, the conclusions of most studies that lack such evaluation techniques should be considered exploratory and would benefit from additional evaluation.

We make the following contributions:

- C1 Decomposition of Evaluation Techniques.** We decompose evaluation techniques into three interacting components: the data source, the algorithm, and the evaluation measure, allowing for a modular discussion of the interacting components of an evaluation.
- C2 Survey of Current Techniques.** We provide a detailed survey of recent literature in causal modeling to provide a quantitative understanding of current evaluation practices.
- C3 Critique of Current Practice.** We provide evidence that increased adoption of both empirical data and interventional measures would be beneficial to the community.

2 Motivating Example

To further explain what we mean by empirical data and interventional measures, we describe a motivating example of the type of evaluation we advocate. This example demonstrates one way evaluation could be performed, though the precise evaluation process will vary depending on the algorithm under evaluation and the research question under consideration.

The most obvious way to evaluate how well an algorithm can learn causal models from real-world data is to compare the model’s estimates to empirical data drawn from a system in which we can perform multiple interventions on the same units, giving us full interventional data in which we can assess every potential outcome for each unit. Large-scale software systems allow for this type of intervention because they let us run the same experiments multiple times under different conditions (e.g., different settings of key system parameters). An example of this is a Postgres database, where we can run the same queries with different settings of key configuration parameters. In this context, each query corresponds to a unit, a set of configuration parameters correspond to treatment, and variables such as runtime correspond to outcomes. Details about this data can be found in the Supplemental Materials.

Many algorithms for causal discovery, such as PC, are designed to run on observational data, in which only a single, non-randomized treatment assignment is observed for each unit. In the absence of an observational data set that matches our interventional data, we can create an observational-style data set by sub-sampling the full interventional data in a non-random manner. To do this, we select a single treatment assignment for each query. Selecting treatment at random is equivalent to a randomized controlled trial. In most observational contexts, however, treatment assignment would be based on covariates of the unit. For example, a database administrator might choose the configuration parameters based on certain features of each query. We use a similar process to create observational data by using a measured covariate of the query to probabilistically assign treatment.

Given such an observational data set, we can apply PC and learn a causal model. In addition, we can estimate the actual interventional distribution $P = P(O = o|do(T = t))$ for any outcome o and treatment t , because we can measure the effects of both values of treatment for each query in our data set. We then can use an interventional measure to compare the true interventional distributions P to the estimated distribution \hat{P} . One example of an interventional measure is total variation distance (TVD) [Lin, 1991], which can measure the distance between two probability distributions. A description of how TVD is calculated can be found in the Supplemental Materials.

3 Survey of Current Techniques

To assess how frequently different evaluation techniques are used in practice, we surveyed recent conference publications on causal inference. We collected papers from the past five UAI, NeurIPS, AAAI, ICML, and KDD conferences, as well as causality workshops held at UAI. We examined papers whose titles contained the terms ‘cause’, ‘causal’, or ‘causality’ and then narrowed this

selection of papers to those that describe, propose, or evaluate a causal discovery algorithm. This resulted in a final set of 111 papers, of which 82% (91) reported any sort of evaluation.¹ Citations to all 111 papers are provided in the Supplemental Materials.

The counts of papers included in the final survey are shown in Table 1. While some relevant papers may fall outside of our search parameters, this approach captures a reasonably representative sample of recent work in causal modeling, allowing us to infer which techniques are used in practice and how frequently these techniques are used.

Table 1: Papers included in the survey

Venue	2014	2015	2016	2017	2018	Total
UAI	2	3	5	3	7	20
NeurIPS	3	5	4	6	13	31
AAAI	1	6	2	4	5	18
ICML	1	5	1	3	5	15
KDD	0	2	3	0	2	7
UAI-W	2	2	4	3	9	20
Total	9	23	19	19	41	111

Table 2: Number of papers using different evaluation measures

		Data Sources	
		Synthetic	Empirical
Evaluation measures	Structural	44	23
	Observational	22	15
	Interventional	11	5
	Visual Inspection	0	19

3.1 Survey Results

For ease of exposition, we decompose evaluation techniques into three components: (1) the data source; (2) the algorithm under evaluation; and (3) the evaluation measure. These dimensions are highly dependent—a choice of one can determine feasible choices for the others. For example, models learned from observational macro-economic data often cannot be compared against a known structure because there exists no ground truth, and models consisting only of non-parameterized structure cannot be compared to interventional effects because the models cannot produce such estimates.

Data Sources. The surveyed papers used a wide range of data sources, but they fall into two broad categories: synthetic and empirical. We categorized data as empirical when it was collected from a “real world” system, whether that was a randomized clinical trial, a global financial system, or user interaction with a website. The important distinction is that empirical data was collected from a process or a system that exists for some purpose beyond scientific research. Synthetic data includes anything else, including data generated from a randomly instantiated Bayesian network or from a simulation intended to reflect a real-world system. In our survey, we found many examples of both, and while synthetic data is used more frequently, both are still common. 81% (74) of papers surveyed used synthetic data, 67% (61) used empirical data, and 48% (44) used both.

Algorithms. The algorithm under evaluation is not part of the evaluation technique *per se*, but aspects of the algorithm strongly influence how evaluation can, and should, be performed. Algorithms fall into two broad categories, bivariate and multivariate, based on the number of variables they consider, although there are many variants.

Some bivariate algorithms infer only the direction of effect (whether A causes B or B causes A). Others estimate the magnitude of effect between treatment and outcome, while adjusting for the effects of a number of covariates. Bivariate methods include Granger causality analysis [Granger, 1969], additive noise models [Peters et al., 2014], and analyses that use the potential outcomes framework [Rubin, 2005]. The most common variety of multivariate algorithm learns directed acyclic graphs (DAGs). Multivariate algorithms are significantly more prevalent in the data, accounting for 60% (55/111) of papers surveyed. Bivariate algorithms account for 30% (34/111) of papers surveyed, split between those focused on orientation (10%), magnitude of effect (15%), or both (5%). The remaining papers in the survey fall in between, including those that aim to determine the joint effect of multiple treatment variables on a single outcome.

Evaluation Measures. At the heart of any evaluation technique is a measure of performance. At a high level, evaluation measures fall into two categories: structural and distributional. Structural measures include all measures designed to assess whether the structure (including both existence of

¹When reporting survey results, we follow each percentage with a parenthesized number representing the raw count. The denominator for percentages is 91, except where otherwise noted.

edges and edge orientation) learned by the algorithm matches the ground truth. Structural measures include structural Hamming distance (SHD), precision, recall, F1-score, true-positive rate, area under the ROC curve (AUROC), and structural intervention distance (SID) [Peters and Bühlmann, 2015].

Distributional measures capture how well the algorithm can estimate quantitative dependence. Such measures can be further subdivided into observational and interventional measures. Observational measures compare the learned distribution with an observational ground truth (i.e. probability queries which do not involve a *do* operator). This could be a measure of individual edge strengths in a Bayesian network or a measure of the error when predicting a given outcome variable. Interventional measures, on the other hand, compare the learned distribution to ground truth obtained through intervention. Common interventional measures include KL-divergence, total variation distance, and measures of average and conditional treatment effect.

Of the types of evaluation measures, structural measures are the most common, being used in 55% (50) of papers surveyed. Distributional measures are slightly less common, being used in 46% (42) of papers. The vast majority of the distributional measures used, however, are observational rather than interventional; observational measures are used in 33% (30) of papers, while interventional measures are used in only 13% (12).

The choice of evaluation measure depends on both the data generation process and type of algorithm, which is reflected in our survey. When synthetic data is evaluated, structural measures are used 59% (44/74) of the time. However, when empirical data is evaluated, structural measures are used only 38% (23/61) of the time, since empirical data is less likely to have ground truth. This lack of ground truth sometimes prevents any significant evaluation for techniques using empirical data—26% (16/61) of empirical evaluations used only visual inspection of the results, with no ground truth. Table 2 summarizes the interaction between data source and evaluation measure in the survey.

3.2 Findings

The survey makes clear that the vast majority of papers that perform evaluation use either (1) synthetic data; or (2) empirical data combined with non-interventional measures (observational measures, structural measures, or visual inspection). Our proposed ideal evaluation (empirical data and interventional measures) is used in only 5% (5) of papers. This raises an obvious question: Are the most commonly used evaluation techniques sufficient for determining whether algorithms for learning causal models will work effectively in realistic scenarios? As we argue below, they are not.

4 The Case for Empirical Data

As already noted, nearly all causal discovery algorithms are ultimately designed for use outside of a laboratory—on real systems to infer useful causal knowledge about the world. Despite this, evaluation of such algorithms often uses synthetic rather than empirical data.

4.1 Limitations of Synthetic Data

Researchers have developed several approaches to generating synthetic data. The most common is to use a Bayesian network or structural equation model. Other approaches involve designing the structure of a graphical model to match the causal structure of a realistic system, either by manually specifying the structure or by learning it from empirical data. Large-scale simulators designed for other reasons can also be used. In some cases, simulators can be complex enough to generate data that is effectively equivalent to empirical data, though such simulations vary widely in quality.

Synthetic data is easy to collect, allows for straightforward comparison with ground truth, and facilitates systematic testing across a variety of data parameters. Its popularity is evident—84% (74) of surveyed papers used it in their evaluation, and 41% (30/74) of those used only synthetic data. However, using synthetic data for evaluation also has significant limitations. These include:

Unquestioned assumptions—Synthetic data tends to match the assumptions of the researcher running the study and any algorithms they have created. For example, a researcher developing an algorithm that outputs a DAG will be inclined to generate data from a DAG.

Untested influences—Even the best data generators can only include the influences already known to researchers. Almost by definition, synthetic data generators cannot include any “unknown unknowns” that may influence the outputs of real-world systems.

Lack of standardization—Synthetic data is typically generated differently by each researcher, and this lack of standardization impedes comparison between studies.

Researcher degrees-of-freedom—Synthetic data is typically designed and parameterized by the researchers who created the algorithm being evaluated, giving them an enormous range of choices. Such high “researcher degrees-of-freedom” [Simmons et al., 2011] are a basic challenge to the validity of any study.

These factors significantly limit the external validity and realism of most synthetic data, making it insufficient as the sole source of data for evaluation. Synthetic data is not without value—it can be a powerful way to assess features of an algorithm and test its performance under different conditions. However, it typically falls short in providing insights into how the algorithm will perform on data from a real-world system.

4.2 Benefits of Empirical Data

Empirical data is almost always more difficult to collect than simulated data, and information on the effects of interventions is typically also much more difficult to obtain. However, using empirical data has multiple benefits:

Realistic complexity—Empirical data typically has a distribution that is more complex than simulated data. That distribution is subject to realistic latent factors and measurement error. This creates a learning task that is often significantly harder than synthetic data, but also more closely matches the challenges of real-world settings.

Lower potential researcher bias—Empirical data is typically not generated by the researcher who designed the algorithm being evaluated, and thus it is less subject to unintentional biases. In addition, individual data sets are often shared across the community, creating standardization and comparability across studies.

Real-world demonstration—The aim of research on algorithms for causal modeling is to have these algorithms used by others to infer causal models and reason about causal effects in real-world settings. Practitioners considering use of these methods may be legitimately skeptical about their effectiveness until they see successful demonstrations of accurate causal inference on real-world data.

However, using empirical data poses challenges as well. Because it is generally not collected by the person using it, some features of the data may not be fully understood, hindering correct interpretation. Also, ground truth can be challenging to obtain, limiting evaluation to visual inspection or observational measures. This is unsatisfying at best and misleading at worst, since, when evaluating without ground truth, it can be easy to see meaning where none exists or to imagine explanations for many possible conflicting outputs. Despite these challenges, empirical data, while less common than synthetic, is still used frequently in practice; 67% (61) of surveyed papers use empirical data, and 28% (17/61) used only empirical data.

4.3 Sources of Empirical Data

Types of empirical data vary depending on the level of ground truth, and whether the ground truth came from a randomized controlled trial, an interventional experiment, or prior knowledge of the domain. Purely observational data is the most readily available and is used most often. While this is rarely accompanied by full knowledge of the underlying structure, there are generally some dependencies that are known, either from common sense knowledge (such as temporal ordering) or from dependencies that have already been established by prior work. For a randomized controlled trial, the dependence between the measured treatment and outcome is generally taken as ground truth. The same is true for interventional experiments, which we define to be experiments performed on a system where multiple different sets of interventions can be performed across the whole population. This includes gene regulatory networks, flow cytometry analysis and software systems, where the system can be rerun with new parameter settings.

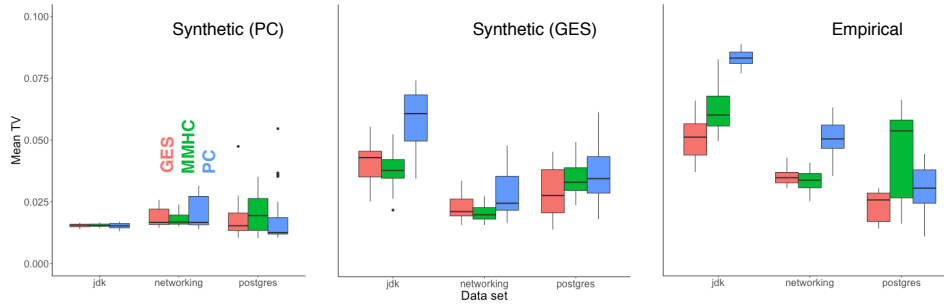


Figure 1: Comparison of TVD on empirical data and synthetic data derived from empirical data. *Left and Center:* synthetic data, structure obtained from PC or GES. *Right:* TVD on empirical data.

Because interventional measures and empirical data are used so infrequently, one might assume this is because such data sets are difficult to obtain. This is partially true—there are significantly more observational data sets available than interventional data sets. However, a growing community is producing data sets that provide interventional effects. We describe some of them here.

The cause-effect pairs challenge [Mooij et al., 2016] provides a data set that is empirical and, while interventional effects are not available, the direction of causality is known. The 2016 Atlantic Causal Inference Conference Competition and subsequent competitions [Dorie et al., 2017, Hahn et al., 2018], created semi-synthetic data sets, producing synthetic treatment and outcome functions using covariates from a real-world system. A similar approach was used by Shimoni et al. [2018] for the IBM Causal Inference Benchmarking Framework. Gene regulatory networks, specifically the DREAM in silico data sets, are a popular choice, since multiple combinations of single-gene interventions can be performed on identical networks [Schaffter et al., 2011]. The DREAM data sets are taken from a sophisticated simulation derived from multiple known gene regulatory network structures, which, while non-empirical, is intended to be complex enough to approximate empirical data. Flow cytometry data, measuring protein signaling pathways, is another common choice for interventional data, specifically the data set provided by Sachs et al. [2005]. Dixit et al. [2016] provide data on gene expression, collected using their proposed Perturb-Seq technique to perform gene deletion interventions. Other sources of interventional and empirical data include results of advertising campaigns [Sun et al., 2015] and clinical studies [McDonald et al., 1992], as well as multiple challenges organized for machine learning conferences [Guyon et al., 2008, 2010].

4.4 How Different are the Results?

Readers may ask: In practice, what’s the difference between using empirical data rather than synthetic data? If that difference is small, then the substantial extra work involved in evaluation with empirical data may not be worth the effort.

To begin addressing this question, we conducted a series of experiments using the interventional data from the software systems mentioned above and described in more detail in the supplemental materials. Specifically, we used a common approach for generating somewhat realistic synthetic data. This approach uses an empirical data set to learn a causal model and then uses that model to generate synthetic data (and known ground truth) for model evaluation. While the final data set is synthetic, its structure may better approximate the empirical system, rather than being entirely defined by the researcher, lending it more credibility. We used this approach to generate synthetic data in the style of the three empirical data sets we generated from software systems. Since we now have both empirical and synthetic data, each with ground truth, we can use causal modeling algorithms to construct a model for both of these data sets and compare the conclusions we would draw from each.

The synthetic data used was created by first choosing an initial causal modeling algorithm to create a ground truth network from the empirical data. After learning a ground truth model with each of two algorithms that construct causal graphical models (PC and GES),² we generated synthetic data using the resulting models. We then evaluated the same three algorithms on both the synthetic and

²Results for MMHC were omitted for space but appear in the Supplemental Materials.

empirical data. Figure 1 shows how mean TVD varies for different causal modeling algorithms and different data sets. The results shown are the mean TVD when evaluating PC, GES, and MMHC on two types of synthetic data sets (using the model as ground truth) and on the empirical data (using the known interventional effects). There is significant variability between the two methods of generating the synthetic ground truth network from the empirical data (PC and GES), both in the mean TVD and in the relative ordering of the algorithms. Comparing the synthetic and empirical results, some relative orderings of the algorithms are the same (e.g., network), but other orderings are significantly different (e.g., Postgres). These results suggest that algorithm performance cannot be expected to match between synthetic and empirical data, even when the synthetic data is created in a way that would be most expected to match aspects of the empirical data.

5 The Case for Interventional Measures

Many algorithms are currently evaluated based on their ability to learn causal structure. However, the actual desired underlying task is almost never to model structure alone. In practice, estimating the magnitude of interventional effects is vitally important, and an algorithm that cannot distinguish between strong and weak effects is severely limited in scope. Despite this, the majority of current evaluations use observational or structural measures rather than measures of interventional effect.

5.1 Limitations of Observational Measures

Observational measures are generally used when the task of the algorithm is to discern the statistical association between two or more variables. They are generally applied in cases when the structure is not the primary focus or is already known, and the primary concern is effectively modeling the magnitude and form of dependence, rather than the existence of dependence. However, observational data has one severe and obvious limitation:

Non-causal—Observational measures are, by definition, not causal. They measure the error of estimates of the outcome variable, but they do not measure that error under intervention. They provide a sense of how well an algorithm has learned statistical dependence, but not how well it has learned causal dependence. Despite this, observational measures are the *only* evaluation used in 24% (22/91) of papers surveyed.

5.2 Limitations of Structural Measures

Structural measures are easy to calculate, and they have a clear intuition. If an algorithm produces a causal structure and we know structural ground truth, it seems sensible to determine if the two structures match. This has led to the widespread adoption of structural measures: 55% (50) of surveyed papers used such measures, and 84% (42/50) of those used only structural measures. However, structural measures have several serious limitations:

Requires known structure—Calculating structural measures requires a full ground truth network structure, which is only rarely available for empirical data.

Constrains research directions—The prevalence of structural measures may constrain research to algorithms that can be evaluated with these measures. Algorithms that do not produce DAGs are less likely to be developed or favorably reviewed. Structural measures also implicitly assume that DAGs are capable of accurately representing any causal process being modeled, an unlikely assumption.

Oblivious to magnitude of dependence—Structural measures, by design, do not account for different magnitudes of dependence, so an error in an edge with a strong effect is weighted the same as an error in an edge with a very weak effect.

Oblivious to likely treatments and outcomes—In most cases, structural measures do not consider where an edge is located in the overall structure of the network, so an edge with many downstream effects is treated the same as a less central edge.

5.3 Benefits of Interventional Measures

In contrast to observational and structural measures, interventional measures have strong advantages:

Correspondence to actual use—Interventional measures evaluate how well the model estimates interventional effects, which aligns more accurately with the eventual use of nearly all causal models. For example, a directed acyclic graph is not the ultimate artifact of interest for most applications—DAGs are a representation that facilitates estimation of interventional effects [Pearl, 2009, Spirtes et al., 2000]. Thus, it seems natural to define an evaluation measure in terms of interventional effects rather than graphical structure.

Weighting of different errors—While most structural measures weight each edge misorientation equally, interventional measures penalize misorientation errors proportionally to their effect on the estimation of interventional effect.

5.4 How Different are the Results?

Interventional measures are intended to capture something different than structural measures, but they are ultimately affected by the structure of the learned model, and we would expect structural errors to lead to interventional errors. To assess the extent to which interventional measures capture different information than structural measures, we ran experiments using synthetic data. This allowed us to produce data where we could calculate both structural measures and interventional measures, since we have the full parameterized ground truth model to compare against.

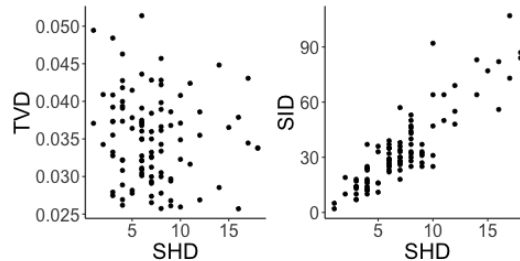


Figure 2: Structural and interventional measures compared on synthetic data with GES.

For these experiments, we produced data from random DAG structures with conditional probability models drawn from a Dirichlet distribution. We generated 5000 instances, applied a causal modeling algorithm, and calculated various evaluation measures. Figure 2 shows the results for GES. SHD and SID are clearly strongly correlated, suggesting that both structural measures ultimately produce similar quality measures of the algorithm. However, SHD and TVD are only very weakly correlated, with many models scoring highly with one measure and poorly with the other. At least in this case, the interventional measure (TVD) appears to capture different information than that of a structural measure (SHD). Results for PC and MMHC are reported in the Supplemental Materials.

6 Conclusion

Evaluation is a key mechanism that determines how algorithms are viewed within the community, what research directions are pursued next, and whether our research has broader impacts outside the community. Our current evaluation techniques aim too low, and they fail to evaluate the full range of questions that our research goals imply.

We acknowledge that, while the evaluation techniques we advocate are applicable to wide range of algorithms, data sets may not be available for every task. The diverse tasks of causal modeling algorithms make it difficult to recommend a single data set and evaluation measure to evaluate every algorithm. However, the data sets and measures that are most commonly used are largely insufficient. We believe it would benefit the community for more data sets with interventional effects to be created and made available for public use, allowing for a breadth of evaluation options.

We do not advocate abandoning synthetic data and structural measures. Both have many uses for evaluating algorithm performance and can be indispensable scientific tools. However, they are not sufficient on their own. Instead, they should be viewed as a first step in evaluation. If we want causal discovery algorithms to be adopted outside our research community, we need demonstrations of their utility outside of a laboratory setting. If we do not evaluate on empirical data, we cannot be certain our algorithms will perform well on real data, and if we do not evaluate with interventional measures, we cannot be certain that the causal effects the algorithm infers will translate to actual, substantial causal effects. Expanding our routine evaluations will substantially improve the credibility and comparability of results, the external validity and trustworthiness of algorithms, and the efficiency with which we conduct our research.

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