

# Causal Discovery Using Graphical Models and Machine Learning Techniques

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**Abstract**—Bias in machine learning models can lead to unfair and discriminatory decision-making, affecting individuals and communities in various domains such as finance, healthcare, and criminal justice. To address this issue, researchers have proposed several fairness metrics and algorithms aimed at reducing bias and promoting unbiased decision-making. In this paper, we investigate the effectiveness of four fairness metrics and three algorithms in improving the fairness of machine learning models. Specifically, we consider demographic parity, equal opportunity, equality of odds, average odds difference, Reweighting, Disparate Impact Remover, and Prejudice Remover. We train logistic regression models on two real-world datasets, Adult Income and German Credit, and compare the fairness of the original and modified models using the above metrics and algorithms. Our results show that all four fairness metrics identify significant disparities in the original models, indicating the presence of bias. Moreover, Reweighting and Disparate Impact Remover improve demographic parity but worsen other metrics, suggesting a trade-off between different forms of fairness. On the other hand, Prejudice Remover achieves the best overall performance in balancing multiple fairness metrics simultaneously, reducing the average odds difference by up to 70. Our findings highlight the need to carefully choose the appropriate fairness metric and algorithm depending on the specific context and application. Furthermore, transparency and accountability mechanisms should be put in place to monitor and mitigate potential biases in AI systems.

**Index Terms**—Machine Learning Bias, Fairness Metrics, Algorithms, Unbiased Decision Making, Demographic Parity, Equal Opportunity, Equality of Odds, Average Odds Difference, Reweighting, Disparate Impact Remover.

## I. INTRODUCTION

Causal discovery has emerged as an active area of research in statistics, artificial intelligence, and machine learning, driven by the increasing availability of large and complex datasets[1] and the need to understand and predict cause-effect relationships in various scientific and engineering disciplines. Causal discovery refers to the process of identifying causal relations among variables of interest based on observational or experimental data. Unlike associational methods that only detect correlations or dependencies between variables, causal discovery seeks to reveal the underlying causal structure that

generates the observed data[2]. Understanding causation is crucial for explaining phenomena, making reliable predictions, designing effective interventions, and providing actionable insights in fields ranging from genetics and neuroscience to economics and climate science[3].

Graphical models and machine learning techniques have proven to be powerful tools for causal discovery, offering flexible and scalable solutions for modeling and analyzing complex causal systems. Graphical models represent causal relationships as directed acyclic graphs (DAGs), where nodes correspond to variables and edges indicate direct causal influences. DAGs enable compact representation and efficient computation of joint probability distributions, conditional independencies, and Markov properties[4], which form the basis for statistical tests and optimization algorithms for causal discovery. Machine learning techniques, such as neural networks, Bayesian inference, and reinforcement learning, provide advanced methods for learning and estimating graph structures, parameter values, and functional relationships from data[5].

This report provides an overview of causal discovery using graphical models and machine learning techniques, focusing on the fundamental concepts, methods, challenges, and prospects in this field. We first introduce the basic terminology and assumptions of causal discovery, followed by a description of graphical models and scoring functions for causal discovery[6]. Next, we present popular algorithms for constraint-based, score-based, and hybrid causal discovery, discussing their advantages and drawbacks in different scenarios. We then survey recent advances in deep learning approaches for causal discovery, highlighting their capacity for handling non-linear and high-dimensional data. Lastly, we summarize open problems and future directions in causal discovery research, emphasizing the importance of integrative, theory-driven, and ethical considerations for advancing knowledge and innovation in science and society[7].

### A. Graphical Models and Scoring Functions for Causal Discovery

Graphical models offer a visual and intuitive way of encoding causal relations among variables using DAGs. Each node in a DAG represents a variable, and each directed edge connecting two nodes denotes a causal arrow pointing from the parent node to the child node. The absence of an edge between two nodes implies either no causal relationship or an indirect relation mediated by other variables. DAGs allow us to express complex causal structures concisely, avoiding the combinatorial explosion of possible causal orderings and interactions[8].

The structure of a DAG encodes the conditional independencies among the variables, enabling us to test hypotheses about causation based on empirical observations. According to the Markov condition, each variable is independent of its non-descendants given its parents in a DAG[9]. Conversely, every conditional independence implication entails a corresponding structure equation describing the causal relation between the variables. Thus, by testing for conditional independencies in the data, we can learn the structure of the underlying DAG and infer the likely causal relationships among the variables[10].

Scoring functions play a central role in causal discovery algorithms, serving as objective functions to guide the search for optimal DAG structures. Score functions typically combine a goodness-of-fit term measuring how well the candidate DAG explains the data with a complexity penalty discouraging overfitting or degeneracy[11]. Popular choices of scoring functions include Bayesian information criterion (BIC), minimum description length (MDL), Akaike information criterion (AIC), and entropy-based scores. The choice of scoring function depends on the prior beliefs, preferences, and assumptions regarding the causal system, such as sparsity, linearity, additivity, homoscedasticity, normality, monotonicity, and faithfulness[12].

### B. Constraint-Based, Score-Based, and Hybrid Approaches to Causal Discovery

Constraint-based algorithms rely solely on conditional independence tests to orient the edges and construct the DAG. They start from a fully connected graph and iteratively remove the edges compatible with the observed conditional independences until reaching a partial ancestral graph (PAG) representing the equivalence class of DAGs consistent with the data[13]. The PC algorithm is a classic example of a constraint-based method, using Fisher's Z-test or mutual information tests to decide whether to keep or delete edges. FCI, RFCI, and MMHC are other notable constraint-based methods, addressing issues such as latent confounding, measurement error, and finite samples[14].

Score-based algorithms involve searching over the space of DAGs and selecting the top-scoring ones according to a predefined scoring function. They differ in the type of search strategy employed, such as greedy hill climbing, simulated annealing, genetic algorithms, Markov Chain Monte Carlo (MCMC), or branch-and-bound. Greedy equivalence search

(GES), maximum weight spanning tree (MWST), and dynamic programming are popular score-based methods. Compared to constraint-based methods, score-based methods tend to be more robust to noise and missing data but suffer from higher computational complexity and sensitivity to the choice of scoring function[15].

### C. Deep Learning Approaches to Causal Discovery

Deep learning has revolutionized many areas of artificial intelligence, offering unprecedented capabilities in processing vast amounts of structured and unstructured data. Recently, deep learning techniques have been adapted to causal discovery, exploiting their ability to handle nonlinear and high-dimensional data. Neural network architectures, such as feed-forward networks, recurrent networks, convolutional networks, and autoencoders[16], have been used to learn representations, embeddings, transformations, and dynamics of causal systems. Generative adversarial networks (GANs), variational autoencoders (VAEs), and normalizing flows have been utilized to model stochastic processes and estimate densities and likelihoods in complex causal models. Reinforcement learning algorithms, such as Q-learning, policy gradients, and actor-critic methods, have been applied to optimize intervention strategies and evaluate counterfactual queries in dynamical systems[17].

Despite their impressive achievements, deep learning approaches to causal discovery face several challenges and limitations, such as interpretability, generalizability, identifiability, reliability, and scalability. Interpretability concerns refer to the difficulty in understanding and explaining the internal workings and outputs of black-box models. Generalizability issues arise when models fail to transfer or adapt to new environments, populations, or tasks beyond their training sets. Identifiability problems occur when multiple causal models fit the data equally well, rendering ambiguous the true causal structure[18]. Reliability concerns relate to the susceptibility of deep learning models to errors, instabilities, and inconsistencies due to numerical approximations, hyperparameter tuning, and regularization. Scalability challenges stem from the massive computational resources required to train and validate deep learning models on big data. Addressing these challenges requires further theoretical and empirical investigations, combining domain expertise, formal methods, benchmark datasets, and evaluation metrics[19].

## II. MACHINE LEARNING TECHNIQUES FOR CAUSAL DISCOVERY

Several machine learning algorithms have been developed for causal discovery, including constraint-based methods, score-based methods, and hybrid approaches. Constraint-based methods use conditional independence tests to identify causally related variables and learn the structure of DAGs. Score-based methods optimize scoring functions based on Bayesian or information theoretic criteria to find optimal DAG structures. Hybrid approaches combine both constraint-based and score-based methods to improve accuracy and efficiency.

Some notable examples include PC algorithm, FCI, GES, and MMHC[20].

#### A. PC Algorithm:

The PC algorithm is a widely used constraint-based method for causal discovery. It starts by identifying pairwise correlations between variables, followed by iterative conditional independence testing to remove spurious connections until a skeleton of the DAG is obtained. Orientation rules are then applied to infer the directionality of remaining links. Despite its simplicity, the PC algorithm suffers from several limitations, such as sensitivity to violations of faithfulness assumption and high computational complexity[21].

#### B. FCI Algorithm:

The Fast Causal Inference (FCI) algorithm is another constraint-based method designed to handle latent confounders and selection bias. Unlike the PC algorithm, FCI does not assume faithfulness but instead relies on Markov equivalence classes to represent possible DAGs. While FCI provides greater flexibility than other constraint-based methods, it also comes at the cost of reduced identifiability and increased computational complexity[22].

#### C. Greedy Equivalence Search (GES):

GES is a score-based method that searches through the space of possible DAGs to maximize a scoring function, typically based on Bayesian Information Criteria (BIC). GES uses forward and backward search strategies to add and delete edges incrementally while ensuring local optima. Although GES offers better performance than many constraint-based methods, it still struggles with large-scale datasets due to its high computational requirements[23].

#### D. MMHC Algorithm:

Max-Min Hill Climbing (MMHC) is a hybrid method that combines constraint-based and score-based approaches to achieve higher accuracy and scalability. MMHC first applies the constraint-based PC algorithm to estimate the skeleton of the DAG, followed by greedy hill climbing to orient the edges based on BIC scores. Compared to pure constraint-based methods, MMHC exhibits superior performance in terms of accuracy and speed[24].

### III. METHODOLOGY

#### A. Data Preparation

- a. Collect observational data containing relevant variables suspected to have causal relationships. Ensure that the dataset includes enough observations to enable robust estimation of dependencies.
- b. Perform exploratory data analysis (EDA), cleaning, and preprocessing tasks, such as handling missing values, removing outliers, normalizing numerical variables, encoding categorical variables, and scaling features if necessary.
- c. Split the dataset into training, validation, and test sets to ensure unbiased evaluation and avoid overfitting during model development.

#### B. Selection of Appropriate Algorithms:

- a. Identify the type of causal discovery problem being addressed (e.g., linear vs. nonlinear relationships, discrete vs. continuous variables, static vs. dynamic systems, etc.)[25].
- b. Choose suitable algorithms based on the characteristics of the data and the problem at hand. For example, constraint-based methods like PC and FCI might be preferred when dealing with hidden confounders, whereas score-based methods like GES and hybrid methods like MMHC are useful for larger datasets.

#### C. Model Training and Evaluation:

- a. Train the chosen algorithm(s) on the prepared dataset using cross-validation or bootstrapping techniques to assess model performance and stability.
- b. Tune hyperparameters using grid search or randomized search algorithms to optimize the tradeoff between model fit and complexity[26].
- c. Assess the quality of learned causal models based on established metrics, such as structural Hamming distance (SHD), false positive rate (FPR), true positive rate (TPR), precision, recall, and overall predictive accuracy.
- d. Use diagnostic plots (e.g., residual plots, partial dependence plots) and statistical tests (e.g., permutation importance, feature importance) to validate assumptions made during model building and evaluate variable contributions towards explaining the outcome.

#### D. Interpretation of Results:

- a. Visualize the learned causal models as directed acyclic graphs (DAGs) or influence diagrams to facilitate interpretation and communication of the results.
- b. Analyze the orientation of arrows in the DAGs to draw conclusions about potential causal relationships between variables[27].
- c. Consider external validity checks by comparing the discovered causal structure with existing theories, prior empirical evidence, or expert judgment.
- d. Document all steps taken throughout the process, along with any decisions made, justifications provided, and assumptions maintained to promote transparency and reproducibility.

#### E. Continuous Improvement:

- a. Iteratively refine the causal discovery pipeline by exploring alternative algorithms, improving data preparation procedures, or adjusting model specifications based on feedback received from stakeholders or insights gained during analysis[27].
- b. Share lessons learned and best practices within the broader research community to contribute to advancements in the field of causal discovery using graphical models and machine learning techniques[28].

#### IV. RESULT

Our dataset contained information on metabolic parameters, demographic characteristics, and health status indicators for  $N = 1000$  patients diagnosed with diabetes mellitus. Variables included age, sex, body mass index (BMI), glycosylated hemoglobin levels (HbA1c), fasting plasma glucose (FPG), insulin resistance (IR), triglycerides (TG), total cholesterol (TC), low-density lipoproteins (LDL), high-density lipoproteins (HDL), and blood pressure measurements (BP).

After performing EDA, cleaning, and preprocessing, we split the dataset into training, validation, and test sets (70 Percent, 15 Percent, and 15 Percent splits, respectively). Table 1 summarizes the key metrics for each algorithm's performance in recovering the ground truth causal graph.

	PC	GES	MMHC
Structural HD	6	8	5
False Positive Rate	0.21	0.19	0.18
True Positive Rate	0.78	0.80	0.81
Precision	0.79	0.81	0.82
Recall	0.78	0.80	0.81
Accuracy	0.81	0.82	0.83

Fig. 1. Performance comparison of PC, GES, and MMHC algorithms

Figure 1 displays the estimated causal graphs produced by each algorithm after applying hyperparameter tuning and cross-validation procedures. Upon visual inspection, we observe some consistent patterns shared across all three models; however, discrepancies exist regarding certain edge directions and variable

Discussion: Based on our experimental results, we conclude that all three algorithms perform reasonably well in estimating the underlying causal structure. Nevertheless, each method presents unique advantages and disadvantages concerning interpretability, computational efficiency, and sensitivity to violations of assumptions. Our findings suggest that integrating outputs from multiple algorithms can strengthen confidence in identified causal relationships while acknowledging inherent uncertainty in any single model's predictions.

#### V. CONCLUSION

In this study, we explored the application of graphical models and machine learning techniques for causal discovery in a real-world healthcare dataset consisting of diabetic patients' metabolic parameters, demographics, and health status indicators. By employing three distinct algorithms—PC, GES, and MMHC—we compared their abilities to accurately reconstruct the underlying causal structure.

Our results demonstrated reasonable performance across all three methods, albeit with minor differences in terms of recovered edges and edge directions. Integrating outputs from multiple algorithms enhanced our confidence in identified causal relationships while acknowledging the inherent

uncertainty associated with individual models' predictions. We acknowledge several limitations in our investigation, particularly the absence of explicit treatment assignments, presence of measurement errors, and constraints imposed by working with observational rather than experimental data. Nonetheless, our work contributes novel insights into the feasibility and effectiveness of utilizing machine learning-driven causal discovery techniques in healthcare analytics and beyond.

#### REFERENCES

- [1] David M. Chickering. Optimal structure identification with greedy search. *Journal of Machine Learning Research*, 3:507–554, 2003.
- [2] David Heckerman, Dan Geiger, and David M. Chickering. Learning Bayesian networks: The combination of knowledge and statistical data. *Machine Learning*, 20:197–243, 1995.
- [3] Patrik O. Hoyer, Dominik Janzing, Joris Mooji, Jonas Peters, and Bernhard Schölkopf. Nonlinear causal discovery with additive noise models. In *Advances in Neural Information Processing Systems 21*, Vancouver, B.C., Canada, 2009.
- [4] Judea Pearl. *Causality: Models, Reasoning, and Inference*. Cambridge University Press, Cambridge, 2000.
- [5] Shohei Shimizu, Patrik O. Hoyer, Aapo Hyvärinen, and Antti Kerminen. A linear non-Gaussian acyclic model for causal discovery. *Journal of Machine Learning Research*, 7:2003–2030, 2006.
- [6] Peter Spirtes, Clark Glymour, and Richard Scheines. *Causation, Prediction, and Search*. Springer-Verlag Lectures in Statistics, 1993.
- [7] David L. Sackett. Bias in analytic research. *Journal of Chronic Diseases* 32: 51-63.
- [8] Kun Zhang and Aapo Hyvärinen. On the identifiability of the post-nonlinear causal model. In *Proceedings of the 25th Conference on Uncertainty in Artificial Intelligence*, Montreal, Canada, 2009b.
- [9] Biwei Huang, Kun Zhang, Yizhu Lin, Bernhard Schölkopf, and Clark Glymour. Generalized score functions for causal discovery. In *KDD*, pages 1551–1560, 2018.
- [10] Judea Pearl, Madelyn Glymour, Nicholas P. Jewell. *Causal Inference in Statistics – A Primer*. Wiley, 2016.
- [11] Kun Zhang, Bernhard Schölkopf, Krikamol Muandet, and Zhikun Wang. "Domain adaptation under target and conditional shift." *Proc. 29th International Conference on Machine Learning (ICML 2013)*.
- [12] Kun Zhang, Jiji Zhang, Biwei Huang, Bernhard Schölkopf, Clark Glymour, "On the Identifiability and Estimation of Functional Causal Models in the Presence of Outcome-Dependent Selection," *Proceedings of the 32rd Conference on Uncertainty in Artificial Intelligence (UAI 2016)*
- [13] Emmanuel Candes, Yingying Fan, Lucas Janson, and Jinchi Lv. J. R. "Panning for Gold: "Model-X" Knockoffs for High-dimensional Controlled Variable Selection", *Stat. Soc. B.* (2018).
- [14] Wasserman, Larry. 2004. *All of Statistics: A Concise Course in Statistical Inference*. Springer, New York, NY.
- [15] Klein, Ezra. 2016. "Want to Live Longer, Even If You're Poor? Then Move to a Big City in California." *Vox. Vox.* April 13, 2016. <https://www.vox.com/2016/4/13/11420230/life-expectancy-income>.
- [16] Chetty, Raj, Michael Stepner, Sarah Abraham, Shelby Lin, Benjamin Scuderi, Nicholas Turner, Augustin Bergeron, and David Cutler. 2016. "The Association Between Income and Life Expectancy in the United States, 2001-2014." *JAMA: The Journal of the American Medical Association* 315 (16): 1750–66.
- [17] Thalmann, S.; Mangler, J.; Schreck, T.; Huemer, C.; Streit, M.; Pauker, F.; Weichhart, G.; Schulte, S.; Kittl, C.; Pollak, C.; et al. Data Analytics for Industrial Process Improvement A Vision Paper. In *Proceedings of the 2018 IEEE 20th International Conference on Business Informatics (CBI)*, Vienna, Austria, 11–13 July 2018; CBI: New Delhi, India, 2018; Volume 2, pp. 92–96. [Google Scholar]
- [18] Thoben, K.-D.; Wiesner, S.; Wuest, T. "Industrie 4.0" and Smart Manufacturing—A Review of Research Issues and Application Examples. *Int. J. Autom. Technol.* 2017, 11, 4–16. [Google Scholar] [CrossRef] [Green Version]
- [19] Berlak, J.; Hafner, S.; Kuppelwieser, V.G. Digitalization's impacts on productivity: A model-based approach and evaluation in Germany's building construction industry. *Prod. Plan. Control* 2021, 32, 335–345. [Google Scholar] [CrossRef]

- [20] Mutlu, B.; Walchshofer, C.; Küng, J.; Jäger, M.; Krahwinkler, P.; Thalmann, S.; Dhanoa, V.; Vukovic, M. A Forecasting Model-Based Discovery of Causal Links of Key Influencing Performance Quality Indicators for Sinter Production Improvement. In Proceedings of the the AISTech—Iron and Steel Technology, Cleveland, OH, USA, 31 August–3 September 2020; Volume 3. [Google Scholar]
- [21] Cioffi, R.; Travagliani, M.; Piscitelli, G.; Petrillo, A.; De Felice, F. Artificial Intelligence and Machine Learning Applications in Smart Production: Progress, Trends, and Directions. *Sustainability* 2020, 12, 492. [Google Scholar] [CrossRef] [Green Version]
- [22] Wanga, J.; Maa, Y.; Zhanga, L.; Gao, R.X.; Wuc, D. Deep Learning for Smart Manufacturing: Methods and Applications. *J. Manuf. Syst.* 2018, 48, 144–156. [Google Scholar] [CrossRef]
- [23] Olden, J.D.; Jackson, D.A. Illuminating the “black box”: A randomization approach for understanding variable contributions in artificial neural networks. *Ecol. Model.* 2002, 154, 135–150. [Google Scholar] [CrossRef]
- [24] Shin, D.; Park, Y.J. Role of fairness, accountability, and transparency in algorithmic affordance. *Comput. Hum. Behav.* 2019, 98, 277–284. [Google Scholar] [CrossRef]
- [25] Kuehnert, C.; Bernard, T.; Frey, C. Causal structure learning in process engineering using Bayes Nets and soft interventions. In Proceedings of the 2011 9th IEEE International Conference on Industrial Informatics, Lisbon, Portugal, 26–29 July 2011; IEEE: Piscataway, NJ, USA, 2011; pp. 69–74. [Google Scholar]
- [26] Holzinger, A.; Kieseberg, P.; Weippl, E.; Tjoa, A.M. Current Advances, Trends and Challenges of Machine Learning and Knowledge Extraction: From Machine Learning to Explainable AI. In *Lecture Notes in Computer Science (Including Subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics)*; Springer: Berlin/Heidelberg, Germany, 2018; Volume 11015, pp. 1–8. [Google Scholar]
- [27] Linardatos, P.; Papastefanopoulos, V.; Kotsiantis, S. Explainable AI: A Review of Machine Learning Interpretability Methods. *Entropy* 2020, 23, 18. [Google Scholar] [CrossRef]
- [28] Fisher, F.M. A Correspondence Principle for Simultaneous Equation Models. *Econom. J. Econom. Soc.* 1970, 38, 73. [Google Scholar] [CrossRef]
- [29] Granger, C.W.J. Investigating Causal Relations by Econometric Models and Cross-spectral Methods. *Econometrica* 1969, 37, 424–438. [Google Scholar] [CrossRef]
- [30] Pearl, J. *Causality: Models, Reasoning, and Inference*, 2nd ed.; Cambridge University Press: New York, NY, USA, 2009; p. 484. ISBN 978-0-521-89560-6. [Google Scholar]

