Hybrid Improved Physarum Learner for Structure Causal Discovery

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Abstract: Causal discovery is the problem of estimating a joint distribution from observational data. In recent years, hybrid algorithms have been proposed to overcome computational problems that lead to better results. This work presents a hybrid approach that combines PC algorithm independence tests with a bio-inspired *Improved Physarum Learner* algorithm. The combination indicates improvement in computational time spent and yet consistent structural results.

1 INTRODUCTION

Causal questions are present in many research fields nowadays, enabling us to deal with everyday questions such as ”what”, ”why”, and ”what if”. Despite the fact that causal questions are popular and instigating, the answers to this type of question are not simple to acquire (Squires and Uhler, 2022).

The ability to answer these types of question was the key ingredient, intrinsic to our humans, that allowed constant evolution in decision making and technology growth (Guo et al., 2020). If machines were able not only to act as perceiving tools but also to develop causal questions, it would characterize the next generation of artificial intelligence development (Pearl, 2018).

In the last few decades, the advancement in graphical models frameworks emerged as the mathematical language for causal knowledge management, and Bayesian networks are one of those most important frameworks (Pearl, 2018). They are compact yet powerful graphical models that efficiently encode their probabilistic relationships among a large number of variables (Neapolitan et al., 2004). In a Bayesian network, variables are presented as nodes in a directed acyclic graph (DAG), and the edges between nodes represent its probabilistic dependencies.

If all edges of a Bayesian network entail a direct causal relationship between two variables, then the graph is called causal (Spirtes et al., 2000), and the process of learning such a graph from observational data is called causal discovery (Squires and Uhler, 2022; Tank et al., 2021). Finding a causal graph that best represents a joint probability distribution has proven to be a challenging task (Kuipers et al., 2022). The difficulty lies in the superexponential growth of the search space of graphs (Guo et al., 2020). Furthermore, the acyclicity constraint represents a time-consuming task, especially for large and dense graphs (Kuipers et al., 2022).

To address the problem of learning Bayesian networks, different techniques were developed. They are generally organized as a) constraints-based algorithms, that use statistical tests to determine which edges exist and then determine their orientation (Spirtes and Glymour, 1991; Meek, 2013), b) score-based algorithms, in which a score criterion evaluates the quality of DAG candidates and selects the best fit (Chickering, 2002), and c) hybrid approaches, which combine both of the previous strategies to reduce the number of DAG candidates and accelerate the search (Tsamardinos et al., 2006; Gasse et al., 2014; Kuipers et al., 2022; Huang and Zhou, 2022).

In fact, the acceleration is archive by a considerable restriction in DAG search space normally encoded by a completed partially directed acyclic graph. A similar structure is obtained as intermediate result in PC algorithm what makes it a popular choice for hybrid causal discovery solutions. (Nandy et al., 2018) proved that hybrid methods like Greedy Equivalence Search (GES) and Adaptively Restricte Greedy Equivalence Search (ARGES) leads to consistent re-

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sults for several sparse high-dimensional settings. Also, to efficient navigate through DAG candidates in Markov Equivalence Class, (Kuipers et al., 2022) proposed a hybrid method based on PC Algorithm and a Markov Chain Monte Carlo (MCMC) sampler that reduces computational complexity for large and dense graphs.

Compelled by the development of bioinspired algorithms based on the slime mold Physarum polycephalum, (Schön et al., 2014) combined a Bayesian score with a bioinspired algorithm, creating the *Physarum Learner* algorithm. This algorithm uses the *Physarum solver* to find the shortest path between two nodes inside a *Physarum maze* and uses this information to determine whether or not an edge exists in a Bayesian network.

The modified version *Improved Physarum Learner* was proposed in which the difficulties in learning the edge orientation for the *Physarum Learner* were addressed as well as optimization changes to improve computational time (Ribeiro et al., 2022).

In this work, we are looking forward to improving *Improved Physarum Learner* computational efficiency by combining it with the well-known PC Algorithm to learn causal structures from observational data. First, we perform the PC algorithm to acquire an initial structure based on conditional independence tests, which are used to initiate the *Physarum maze*. It is then possible to check the capability of the proposed method to learn a known causal structure verifying the consistency of the discovered graph compared with the ground-truth graph. We also expect that with a better initial guess for the *Improved Physarum Learner*, the hybrid approach may encounter the best score structure with lower computational time, therefore, being feasible for large data.

In Section 2, we present the theoretical background of Bayesian networks and some state-of-the-art causal learning strategies. Section 3 describes the computational environment, data analysis with graph structures and probabilities, and the hybrid methodology of this work. The structures obtained are presented in Section 4 with a further discussion presented in Section 5.

2 THEORY

In this section, we will introduce the notation, main equations and cite relevant references in each topic.

2.1 Bayesian Networks

Bayesian networks are a class of Graphical Models (GM), and as in all other GMs the BNs objective is to represent a joint distribution by making assumptions of Conditional Independencies (CIs). Structurally, the graph nodes represent random variables and the presence or absence of edges indicates the statistical relations between variables. What separates Bayesian networks from all other GMs is the usage of directed acyclic graphs (DAGs) to comply with the Markov assumption (Koller and Friedman, 2009; Neapolitan et al., 2004).

The main characteristic of DAGs is that, when ordered, all nodes will always be placed after their parents. This characteristic, called the Markov condition, can be seen as a generalization of the first-order Markov condition from chains to DAGs. If a graph satisfies the Markov condition, each node in the graph will only depend on its immediate parents, being independent of all other predecessors. Given a DAG $\mathbb{G} = (V, E)$ and a set of conditional probability distribution Θ, we say $(\mathbb{G}, \Theta)$ satisfies the Markov condition if for each random variable $x \in V$, x is conditionally independent of the sets of its non-descendants $(ND(x))$ given the set of its parents $(Pa(x))$ (Koller and Friedman, 2009),

$$I_p(x, ND(x)|Pa(x)) \tag{1}$$

The structure formed by (G, Θ) configures a joint probability distribution over Θ, which can be obtained by

$$P(\theta_1, \theta_2, \theta_3, ..., \theta_n) = \prod_{i=1}^{n} P(\theta_i | par(\theta_i)) \tag{2}$$

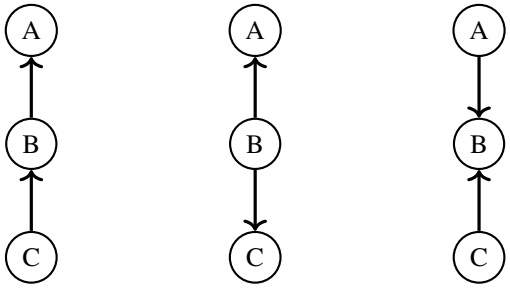
where $par(\theta_i)$ denote the parents of θ_i (Koller and Friedman, 2009).

Given a data set D and a structure G, estimating the set of conditional probability distributions Θ is generally straightforward. However, in most practical applications, finding the structure G that best entails the dependencies between the variables is a really hard task, especially for large D.

The Equation 2 represents the Chain Rule for Bayesian networks in which the Markov condition is essential. That means that each variable is statistically independent of its non-descendants once its parents are known (Koller and Friedman, 2009).

2.2 Structure Learning Methods

A same distribution might factorize in different ways. The *Markov Class* is a group that contain all DAGs



(a) (b) (c)

Figure 1: Possible three node DAGs. The structures 1b and 1a share the same set of independences therefore they belong to the same *Markov class*. The structure 1c are in a different *Markov class*.

that share the same independence set (Glymour et al., 2019; Spirtes, 2013). Figure 1 shows some possible distributions with three variables. 1a entailed independence between A and C given B ($I(A,C|B)$) and 1b also entailed $I(A,C|B)$ that place it in the same *Markov Class*. On the other hand, 1c entailed $I(A,C)$ and thus constitutes a different *Markov Class*.

Conventional approaches for discovering causal structures rely on conditional independence properties, but there is another class of algorithms that commits in search for a DAG best fit the joint distribution. These methods may not use any of those independence proprieties and yet lead to good results.

2.2.1 Constraint-based algorithms

These algorithms discover DAGs by testing the independence between variables and adding (or removing) edges based on these results. The PC (Spirtes et al., 2000; Glymour et al., 2019) is the most known algorithm of this class and represents a Bayesian network as a set of independences. At first, given the data, the algorithm first creates a complete graph in which each node is a variable, which means an empty set of independencies. For each round of the algorithm, all combinations of nodes are tested for conditional independence in the form $I(X,Y|Z)$, with conditional set Z starting from $|Z| = 0$ and adding 1 for the round. For positive results in an independent test, the edge between X and Y is removed and the set Z is saved in association with the edge removed. When $|Z|$ is less than the DAG maximum degree, the independent testing process stops and the sets Z are used to orient the edges.

Since conditional independence relationships presents symmetric aspects, the orientation round can only obtain the Markov equivalence class of DAGs (Kuipers et al., 2022).

The Conditional independence test adopted by the algorithm has major impact in quality of obtained structure and it may vary if the random variable is continuous or discrete. Some commonly employed conditional independence tests are Pearson's correlation (Baba et al., 2004) for continuous data, χ^2 test for categorical data (Spirtes et al., 2000) and yet some likelihood-based tests for all types of data (Tsagris et al., 2018).

The estimating process of a conditional distribution Z for higher-order conditional independence tests tends to deteriorate test results as long as $|Z|$ increases, especially for discrete variables with several possible values. In fact, the number of sample sizes needed to efficiently estimate the distribution grows rapidly, leading to empty or nearly empty variable cells (Spirtes et al., 2000).

2.2.2 Score-based Algorithms and Hybrid Approaches

Unlike Constraint-based methods that rely on statistical proprieties and independence tests to achieve and DAG on which to build the Bayesian network, score-based algorithms settle the causal discovery problem by using an evaluation method as a criterion to judge whether a DAG candidate is good or not (Squires and Uhler, 2022). Every DAG in the search space is a possible solution; therefore, it becomes an optimization problem based on a specific score method and a sampler strategy for searching the DAG space (Koller and Friedman, 2009).

2.2.3 Improved Physarum Learner

Inspired by the maze-solving ability of the slime mold *Physarum polycephalum*, the Physarum Learner algorithm was proposed adapting the Physarum Solver capability of finding the optimal path in a maze to the Bayesian network causal discovery problem (Miyaji and Ohnishi, 2008). The *Physarum-Maze* is formed by an initial fully connected graph with random weights. In each Physarum Solver iteration, the Source and Sink nodes are changed randomly, and the weights are updated. Edges with weights above a certain threshold are marked as Bayesian network postulate edges, and then a score criterion defines if the edge is kept or not in the final network (Schön et al., 2014).

An improved version of the Physarum Learner algorithm was proposed in (Ribeiro et al., 2022). The proposed implementation adds a search step, once a new edge is inserted in the graph, for a configuration of reoriented edges that maximizes the score inside a *Markov class*. Also, an extra procedure checks for score stagnation, and if detected, the current iteration is finished, minimizing time spent.

The evidence supports that Improved Physarum Learner shows better computational performance converging faster than the original method.

3 MATERIAL AND METHODS

In this section, descriptions are made to highlight how the Pc Algorithm is combined with the *Improved Physarum Learner* for solving the causal structure learning problem, with the specifications of each step and the validation methodology. In addition, the data set and the ground truth structure are described. The experiments were performed on a computer with the following characteristics:

- Processor: Intel Core i5-10300H
- RAM: 16GB
- Operating System: Pop!_OS 22.04 LTS
- Python: 3.8
- NumPy: 1.19.2

In its initial steps, Physarum Learner creates a fully connected undirected graph called *Physarum-Maze*. Data variables are nodes in the maze and each edge has a weight randomly sampled from a uniform distribution $weight \sim \mathsf{uniform}[0.78, 0.79]$ that represents the impact of that edge on a Bayesian scoring function. The Physarum Learner proposes to transform the *Physarum-Maze* (a fully-undirected graph) into a Bayesian Network (a directed acyclic graph) by removing edges with an impact lower than a threshold. Each edge weight is gradually updated using the Physarum Solver output until it reaches stagnation, which can be very time-consuming for large graphs. The total number of Physarum Solver iterations is approximately n^2, where n is the number of nodes in the maze.

We believe that the process of updating edge weights, already optimized in *Improved Physarum Learner*, can take advantage of the use of a constraint algorithm like the PC to further improve its performance, especially in sparse graphs, which is where the PC algorithm demonstrates its best results.

Both algorithms start with a similar structure and then evaluate the effectiveness of each edge using different strategies. The independence tests in the PC algorithm run faster than the estimation used in Improved Physarum Learner, but it also leads to less precise results.

The idea is to modify the edge sampling distribution in the *Physarum-Maze* accordingly to the existence or not of that edge in the PC algorithm output, expecting to accelerate the convergence process of the *Physarum-Maze* edge weights. The base code for the implementation of the PC algorithm was adapted from (Callan, 2018) coupled with the χ^2 independence test.

First, the PC algorithm is performed with the maximum order for the independence test equal to 1. Then, *Physarum-Maze* structure are initialized, and the edge weights are sampled as follows:

$$W(e) \sim \begin{cases} \mathsf{uniform}[0.68, 0.79], & \text{if } e \exists \text{ in PC output} \\ \mathsf{uniform}[0.28, 0.39], & \text{otherwise} \end{cases} \tag{3}$$

Where $W(e)$ in Equation 3 is a sampling function that attributes a weight to edge e. In this case, all edges preserved by the PC algorithm start with a higher probability of existence in the final structure.

A popular metric to test the performance of causal discovery algorithms is to check the difference between the resulting graph structure and a known ground-truth graph used to generate the dataset.

The LUng CAncer Simple set (LUCAS) (Guyon, 2022) is a popular dataset for learning causal graphs and will be used in this work in addition to the Structural Hamming Distance (SHD) as a graph distance-based metric (Cheng et al., 2022).

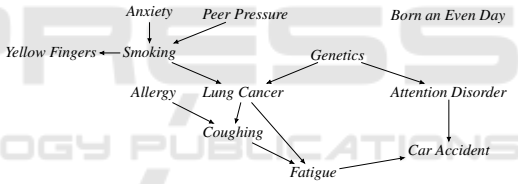


Figure 2: Original LUng CAncer Simple set (LUCAS) structure extracted from (Guyon, 2022). This structure was artificially designed to model a Lung Cancer medical application. It represents the statistical relationship between behavioral and genetic variable in the likelihood of developing cancer in humans. Illustrate causes and possible consequences.

LUCAS is an artificial dataset in which samples are generated from a Bayesian network that represents a medical application to diagnose, prevent and cure lung cancer. All variables are listed in Table 1. Variables are divided into three main groups based on the number of parents. *Anxiety*, *Peer Pressure*, *Genetics*, *Allergy* and *Born an Even Day* are marked cyan and do not have parents, for that reason they are not influenced by any other variable. In magenta are *Yellow Fingers* and *Attention Disorder* which have *Smoking* and *Genetics* as nodes with edges connecting to them, respectively. And finally, in yellow, we have *Smoking* influenced by *Peer Pressure* and *Anxiety*, *Lung cancer* with edges coming from *Smoking* and *Genetics*, *Coughing* with edges coming from *Allergy* and *Lung cancer*, *Fatigue* influenced by *Lung cancer* and

Coughing, and the last variable is *Car accident* with *Attention disorder* and *Fatigue* as parent variables.

The subscript letter $_t$ or $_f$ after the variable name in Table 1 represents the assumed value for the variables corresponding to the respective probability shown in the last column. From the data in Table 1 is possible to marginalize all conditional probability tables by exploiting the fact that each entry in the conditional distribution must have a sum of 1 for a fixed value of its parents: for example, from the last line in Table 1 we know that $P(CarAccident = T|AttentionDisorder = T, Fatigue = T) = 0.97169$ then we can compute that $P(CarAccident = F|AttentionDisorder = T, Fatigue = T) = 1 - 0.97169 = 0.02831$. The joint distribution generated a dataset with 1 million samples and was used for the causal discovery task.

Table 1: The Joint Probability Distribution for LUCAS dataset. First column contain variable names, second column has variable parents (if exists) and the their current state necessary for observe the conditional probability described in column three. The Cyan rows represents variables without parents. In Magenta, the random variables with one parent and the Yellow rows represents the nodes with two parents.

Variable	Parents	Probability
$Anxiety_t$		0.64277
$PeerPressure_t$		0.32997
$Genetics_t$		0.15953
$Allergy_t$		0.32841
$BornanEvenDay_t$		0.5
$YellowFingers_t$	$Smoking_f$	0.23119
$YellowFingers_t$	$Smoking_t$	0.95372
$AttentionDisorder_t$	$Genetics_f$	0.28956
$AttentionDisorder_t$	$Genetics_t$	0.68706
$Smoking_t$	$PeerPressure_f, Anxiety_f$	0.43118
$Smoking_t$	$PeerPressure_t, Anxiety_f$	0.74591
$Smoking_t$	$PeerPressure_f, Anxiety_t$	0.8686
$Smoking_t$	$PeerPressure_t, Anxiety_t$	0.91576
$Lungcancer_t$	$Genetics_f, Smoking_f$	0.23146
$Lungcancer_t$	$Genetics_t, Smoking_f$	0.86996
$Lungcancer_t$	$Genetics_f, Smoking_t$	0.83934
$Lungcancer_t$	$Genetics_t, Smoking_t$	0.99351
$Coughing_t$	$Allergy_f, Lungcancer_f$	0.1347
$Coughing_t$	$Allergy_t, Lungcancer_f$	0.64592
$Coughing_t$	$Allergy_f, Lungcancer_t$	0.7664
$Coughing_t$	$Allergy_t, Lungcancer_t$	0.99947
$Fatigue_t$	$Lungcancer_f, Coughing_f$	0.35212
$Fatigue_t$	$Lungcancer_t, Coughing_f$	0.56514
$Fatigue_t$	$Lungcancer_f, Coughing_t$	0.80016
$Fatigue_t$	$Lungcancer_t, Coughing_t$	0.89589
$CarAccident_t$	$AttentionDisorder_f, Fatigue_F$	0.2274
$CarAccident_t$	$AttentionDisorder_t, Fatigue_f$	0.779
$CarAccident_t$	$AttentionDisorder_f, Fatigue_t$	0.78861
$CarAccident_t$	$AttentionDisorder_t, Fatigue_t$	0.97169

Figure 2 shows the graph structure of the 12 binary random variables and their edges dependencies.

4 RESULTS AND DISCUSSION

In this section, relevant details for the LUCAS causal structure are given, which include isolated variables and their impact on the causal discovery problem. The final structure obtained from the proposed hybrid methodology is also presented in this section in addition to the intermediate structure learned from PC algorithm.

One characteristic of the structure of the LUCAS network is the variable **Born an Even Day** that measures the impact of the day of birth on the chances of developing lung cancer and, as expressed in Figure 2, that the influence is negligible once there are no connections with the rest of the DAG structure and, as a consequence, should not influence any of the other 11 variables.

Identifying isolated variables is extremely important once they have an irrelevant impact on tasks such as forecasting or inference. In this case, the difference between the search space for DAGs with 12 variables, like LUCAS, has 5.2×10^{26} more elements than the search space for DAGs with 11 variables. So, it is crucial that the statistical independence verification of the PC algorithm detects the **Born an Even Day** isolated node from LUCAS and avoid the Improved Physarum Learner from searching for irrelevant paths.

For that reason, different conditional independence tests were performed and the χ^2 was selected for PC algorithm execution. The experiment also counted with Pearson Correlation (Hemmings and Hopkins, 2006) and Fast Conditional Independence Test (Chalupka, 2022).

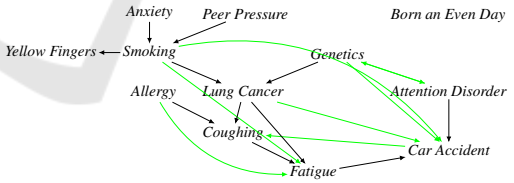


Figure 3: The PC algorithm obtained structure. In black are the edges were preserved by the algorithm that are present in the ground-truth structure. In green are the edges wrongly kept by the algorithm. It has $SHD = 7$.

Figure 3 shows the structure obtained from the execution of the PC Algorithm. The black edges are the true positive edges kept by the algorithm that belongs to the ground truth graph, and all the edges of the ground truth are present in the output of the PC algorithm. The edge between *Genetics* and *Attention Disorder* has arrowheads at each endpoint, showing ambiguity in determining the direction of the edge using the PC Algorithm. In addition, the algorithm has truly isolated the variable **Born an Even Day** re-

ducing the chances of the improved Physarum learner connecting it to anything else.

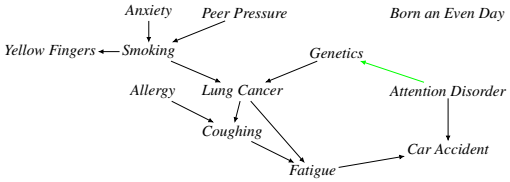


Figure 4: The obtained structure from hybrid approach. In black are the edges were preserved by the algorithm that are present in the ground-truth structure. The green edge from *Attention Disorder* to *Genetics* has reverse orientation. It has $SHD = 1$.

Based on his partial result, the edge weights were sampled as mentioned in section 3 as a starting point for Improved Physarum Learner. Figure 4 shows the learned structure that has $SHD = 1$. The only edge incorrectly oriented from *Attention Disorder* to *Genetics* is the same edge in which the PC algorithm had difficulty determining the orientation. Despite that, all edges kept by the Improved Physarum Learner belong to the ground-truth graph.

No major difference between the structure learned by the methodology proposed in this work and the Improved Physarum Learner, however, the hybrid version presented a decrease in computational time. In 10 executions, the Improved Learner had an average **217.2** seconds to find a structure, while the hybrid had an average of **155.3** seconds, showing a consistent 28% of time savings.

5 CONCLUSIONS

In this work, we presented a hybrid alternative for *Improved Physarum Learner* in which we tested the quality of the founded causal structure proposed in (Guyon, 2022) by counting the *Structural Hamming Distance* (SHD) between the learned structure and the ground-truth graph. We also measured the computational time saved by adding information from Conditional Independence tests into the *Physarum maze*.

The results showed consistency in the causal discovery of the true structure with almost no errors. The $SHD = 1$ refers to the green edge between *Genetics* and *Attention Disorder* misoriented. In our tests, the proposed methodology outperforms *Improved Physarum Learner*, finding the causal structure on average 28% faster.

Although promising, the proposed combination of algorithms needs, in future works, to be compared with strategies of learning structures, both algorithms consolidated in the literature and new approaches, using the same hardware and the same amounts of data for all algorithms. Also, it is important to check the Hybrid Improved Physarum behavior in different scenarios such as non-binary data, networks with a large number of nodes, or even how it behaves with scarce samples.

Furthermore, parallel implementation strategies can be highly beneficial for the Hybrid Improved Physarum Learner. For the PC algorithm, the methodology proposed by (Le et al., 2016) seems promising especially in high-dimensional data. But no parallel technique was found by the authors relating causal discovery problem and Physarum.

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