MPCSL - A Modular Pipeline for Causal Structure Learning

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ABSTRACT

The examination of causal structures is crucial for data scientists in a variety of machine learning application scenarios. In recent years, the corresponding interest in methods of causal structure learning has led to a wide spectrum of independent implementations, each having specific accuracy characteristics and introducing implementation-specific overhead in the runtime. Hence, considering a selection of algorithms or different implementations in different programming languages utilizing different hardware setups becomes a tedious manual task with high setup costs. Consequently, a tool that enables to plug in existing methods from different libraries into a single system to compare and evaluate the results is substantial support for data scientists in their research efforts.

In this work, we propose an architectural blueprint of a pipeline for causal structure learning and outline our reference implementation MPCSL that addresses the requirements towards platform independence and modularity while ensuring the comparability and reproducibility of experiments. Moreover, we demonstrate the capabilities of MPCSL within a case study, where we evaluate existing implementations of the well-known PC-Algorithm concerning their runtime performance characteristics.

CCS CONCEPTS

• **Mathematics of computing** → **Causal networks**; • **Computing methodologies** → **Causal reasoning and diagnostics**; • **General and reference** → **Evaluation**; **Experimentation**.

KEYWORDS

Causal Structure Learning, Modular Pipeline, Evaluation Framework, Benchmarking

ACM Reference Format:

Johannes Huegle, Christopher Hagedorn, Michael Perscheid, and Hasso Plattner. 2021. MPCSL - A Modular Pipeline for Causal Structure Learning. In *Proceedings of the 27th ACM SIGKDD Conference on Knowledge Discovery*

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KDD '21, August 14–18, 2021, Virtual Event, Singapore.

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ACM ISBN 978-1-4503-8332-5/21/08.

<https://doi.org/10.1145/3447548.3467082>

and Data Mining (KDD '21), August 14–18, 2021, Virtual Event, Singapore. ACM, New York, NY, USA, 9 pages. <https://doi.org/10.1145/3447548.3467082>

1 INTRODUCTION

The knowledge about the causal structures between the variables of a system is of high interest for data scientists and researchers in a variety of domains [31]. Examples are drug design, where Causal Graphical Models (CGMs) derived from gene expression data depict genetic regulatory relationships [34] or manufacturing, where the knowledge about causal structures supports the root cause analysis of failures within complex production processes, e.g., see [18].

In this context, the growing interest in methods of Causal Structure Learning (CSL) has lead to a wide spectrum of scientific publications, each tackling different domain-specific constraints, e.g., statistical considerations to improve the accuracy in non-linear settings [45] or the examination of parallel computing strategies [24, 37, 39] or adoption of accelerator cards [38, 48] to speed-up the learning process. This lead to the development of a number of libraries in different programming languages [19, 22, 24, 36, 39, 46] or standalone implementations [37, 38, 48] each introducing implementation-specific overhead to both the accuracy of the results and the runtime of CSL. Therefore, data scientists of different domains are confronted with the omnipresent challenge of selecting their most appropriate algorithm for CSL given the unique characteristics of their domain. This may be accompanied by specific hardware and software constraints or unique data characteristics. In these scenarios, determining both the correct algorithmic approach with the corresponding choice of the algorithm's parameters and the most suitable implementation for a given observational dataset becomes cumbersome. Even though studies comparing algorithms for CSL exist and provide an indication for the best choice [41], they are limited to the algorithms considered and available at the time of writing, as well as the data characteristics utilized in the experimental evaluation. Hence, the evaluation of experiments given an observational dataset, considering a selection of state-of-the-art algorithms or different implementations in different programming languages utilizing different hardware setups becomes a tedious manual task with high setup costs. In particular, in real-world scenarios, both missing ground truth and the computational complexity further impede the evaluation of the algorithm's reliability, e.g., see [11, 21]. For example in genetics, large-scale gene expression data introduces domain-specific constraints with regard to statistical assumptions on the complex mostly unknown underlying biological mechanisms

Figure 1: The essential components of the modular pipeline for CSL required for a comprehensive benchmarking of different CSL algorithm implementations given observational datasets.

on one side and algorithms' performance required for CSL in this high-dimensional setting on the other side [1, 10]. Therefore, for biologists aiming to derive gene regulatory networks, the question of practical relevance is the appropriate choice of an existing method for CSL for their genetic observational data set specific to their biological research question. As the vastly expanding field of research in methods of CSL results in a "sheerly unlimited number of methods" neither is a complete evaluation feasible [10] nor is the computational complexity manageable without an interdisciplinary team that incorporates computer scientists, too [1].

Moreover, data scientists working on advancements of existing algorithms for CSL are confronted with the task of considering both naive baseline methods and novel competitive methods in their evaluation. For example in the research field of hardware acceleration in CSL, a comprehensive evaluation becomes a tedious manual task with high setup costs as it requires the orchestration of a setup that incorporates not only different programming languages such as R, C++, or Python but also experiments in a heterogeneous hardware setup with multi-core CPUs and GPUs [38].

Consequently, the access to a tool that enables to plug in existing methods from different libraries into a single system to compare and evaluate the results, also under the prism of improving existing algorithms, is of great importance. In the machine learning domain, such tools follow a methodology referred to as the Common Task Framework (CTF) [8], which has the following three components: publicly available training datasets, a set of competitors, and a scoring referee to compare the competitors. For the challenge of incorporating and evaluating existing methods and implementations for CSL, we introduce a pipeline structure as depicted in Figure 1. Starting with an *Observational Dataset Management* and given an *Experimental Setup*, which enables the selection of both appropriate algorithms, and execution environments, the pipeline needs to orchestrate the experiments in a step for *Experiment Execution & Monitoring*. To evaluate the results of CSL with regard to both the runtime performance, and the accuracy of the results a *Result Comparison* component completes the pipeline.

The variety of algorithms, different hardware requirements, and constraints in a scientific research setting imply the following requirements towards a *platform-independent, modular* pipeline that ensures the *comparability and reproducibility* of experiments.

Modularity: The pipeline should be implemented based on the principle of modularity [30] to enable easy adaptation for extensions of the components' feature set, e.g., the addition of new metrics for comparing CSL algorithms in different dimensions to support a wide range of evaluation objectives.

Platform Independence: Applying concepts of virtualization and containerization, the pipeline should be designed in a platform-independent manner to support various implementations, independent from the programming language or the hardware requirements, in a single pipeline.

Comparability and Reproducibility: In order to address the high scientific demand of the research community, all metadata, which contains information regarding the experimental setup, e.g., dataset, algorithms' parameters, or information regarding the underlying hardware setup, should be persisted.

Following the previously introduced requirements for a modular CSL pipeline, our contributions are: First, the derivation of a blueprint for a modular CSL pipeline to support data scientists in their research on methods for CSL. Second, the provision of a reference implementation, called MPCSL, accessible to the research community. Third, a case study to demonstrate the applicability of MPCSL determining suitable CSL implementations regarding runtime for a range of observational datasets.

The remainder of the paper is organized as follows. After providing an overview of the theoretical background on CSL in Section 2, we discuss existing approaches to benchmark and compare causal structure learning algorithms in Section 3. In Section 4, we present a blueprint of a pipeline that meets the previously introduced requirements and provide detail on our reference implementation. The capabilities of our presented pipeline are demonstrated in Section 5, in which we evaluate existing implementations of the well-known PC-Algorithm with regard to their runtime in a case study. We summarize our work in Section 6.

2 CAUSAL STRUCTURE LEARNING

In this section, we sketch the theoretical background as well as the main approaches of CSL. For more information and a more detailed introduction we refer to the comprehensive work of Pearl [31], Spirtes et al. [44], or Peters et al. [32].

2.1 CGM and Causal Inference

Causal Graphical Models (CGMs) are a recognized fundamental concept of the formalization of causality [15, 31, 44]. In this context, a CGM $\mathcal{G} = \{V, E\}$ encodes the causal relationships over a set of random variables V , in the sense that any edge $X \rightarrow Y$ in E between the variables in V represents a direct causal effect. The directed edges in $\mathcal{G}$ entail the causal interpretation that variable Y is a function of its direct cause X and some noise term ϵ , i.e., $Y = f(X, \epsilon)$, where ϵ is independent of X . In other words, it says that for an edge $X \rightarrow Y$ in the CGM $\mathcal{G}$ an intervention on X will directly change the distribution or value of Y . For example

let X and Y be directly causally influenced through a common confounder Z , i.e., $X \leftarrow Z \rightarrow Y$. Observing associations in changes on X and Y induced through the common confounder may let you falsely assume that a causal relationship exists. While changes through interventions on Z will directly change both X and Y neither interventions in Y nor in X will affect Z or Y , respectively.

Following this idea, Judea Pearl introduced the $do(\cdot)$ -operator into the framework of CGMs as a notion to distinguish the observational conditional probability $P(Y|X = x)$, describing the probability distribution of Y if one observed $X = x$, from the conditional interventional probability $P(Y|do(X = x))$ that depicts the probability distribution of Y when X has been set to x [31].

Traditionally, a causal relationship has been discovered through the execution of randomized experiments or interventions into the system itself, which may be too expensive, time-consuming, or even impossible [11]. Hence, the framework of CGMs in cooperation with the $do(\cdot)$ -operator enables a comprehensive examination of causal structures on the basis of observational data [32].

2.2 Assumptions and Approaches of CSL

Causal structure learning can be characterized as the task of deriving as much of the underlying causal relationships in the CGM $\mathcal{G}$ from observational data as possible. Therefore, the CGM needs to be connected to the joint probability distribution of its variables which comes with constraints on the structures or the corresponding functional system. Naturally, the CGM is assumed to be *acyclic*, i.e., there is no feedback loop in $\mathcal{G}$, and *causal sufficiency*, i.e., there is no latent confounding variable affecting the variables in $\mathcal{G}$. Moreover, the principles of *causal Markov assumption*, *causal faithfulness* and *causal sufficiency* enable to connect the CGM $\mathcal{G}$ with probabilistic characteristics of the joint probability distribution of the corresponding variables [31]. The high-level idea is that these assumptions imply a corresponding conditional independence structure in the joint probability distribution and the causal structures within the CGM $\mathcal{G}$ via the so-called d -separation criterion.

Algorithms for learning the causal structures build upon these assumptions to leverage the probabilistic characteristics of the observational dataset and can be categorized into score-based, constraint-based, or hybrid approaches. *Constraint-based CSL* derives the information about probabilistic characteristics within the observational dataset through the repeated application of conditional independence (CI) tests in a first step. Given the dataset's probability distribution, different CI tests can be plugged-in within this iterative procedure that estimates the undirected skeleton of $\mathcal{G}$. In a second step, deterministic rules are applied to orient the undirected edges. One of the most popular constraint-based algorithms is the PC-Algorithm by Sprites et al. [44] together with its order-independent version PC-Stable [5]. Given reliable CI tests, constraint-based algorithms are flexible and able to handle various data distributions which make them widely applicable [11]. Yet, the long execution time poses a challenge for its application in practice, in particular for high-dimensional data [23]. Algorithms following the *score-based* approach evaluate a score on all possible Directed Acyclic Graphs (DAGs) in relation to the data, typically using a penalized likelihood score, and search for the DAG that yields to the optimal score [3]. As the search space of possible DAGs is too large, greedy

approaches are used but still raise an NP-hard problem [4]. Greedy Equivalence Search is a well-known greedy two-phase procedure for score-based CSL [3]. Hybrid algorithms, such as the Max-Min Hill Climbing algorithm [47], are a combination of both previously introduced approaches. In the first step, CI tests are used to limit the search space for the subsequent application of a score-based approach to finding the DAG with a maximal score.

Note that for all approaches exist a variety of modifications and extensions that can handle a weakened set of assumptions to enable a wider range of applications. For example in the presence of latent confounders, i.e., a violation of causal sufficiency, methods such as the constraint-based FCI algorithm [44] or the hybrid GFCI algorithm [29] provide asymptotic correct results.

3 RELATED WORK

The challenge of comparing and evaluating a selection of algorithms is omnipresent in the research community, and requires an objective evaluation of competitors, as portrayed in the Common Task Framework (CTF) [8]. In the area of causality in general, Dorie et al. [9] implemented the idea of a common task in the “2016 Atlantic Causal Inference Competition”, the first large-scale data analysis competition for causal inference from observational data. Though the results explore the relative strengths and weaknesses of methods for causal effect estimation, a sound causal inference requires knowledge about the causal structures of the problem [17]. Hence, causal competitions should evaluate the entire causal inference pipeline incorporating both the examination of methods for causal structure learning and for effect estimation [20].

There exist several attempts to provide tools for the empirical evaluation of methods for causal effect estimation to support an objective comparison between competitors. For example, Lin et al. [25] propose an API for evaluating causal inference models inspired by the idea of CTF aiming to provide a centralized competition platform for and extended by researchers in causal inference. The researcher can submit new models, datasets, metrics, and parameterizations, which become available to the community and allow for more comparable benchmarks. Shimony et al. [43] present a causal inference benchmarking framework distributed on *github.com* to support a better comparison between methods that estimate causal effects.

In contrast to the task of evaluating methods for causal effect estimation, to the best of our knowledge, there is no common evaluation framework for causal structure learning algorithms across multiple programming languages. Within the R programming language [33] the package *CompareCausalNetworks* [16] provides an interface to compare supported causal structure learning algorithms from different classes. In particular, the authors of the package evaluate, PC [44], FCI [44], GES [3], GIES [14], MMHC [47], LINGAM [42] and backshift [35] on simulated graphical networks and use the relations *isAncestor* and *isParent* to compare the learned causal structures across the algorithms. The study provides an overview of the applicability of the methods for researchers, yet it is limited to the considered data characteristics, i.e., not covering any datasets above 100 variables. Furthermore, the package only supports algorithms written in the R-Framework, not supporting implementations written in other programming languages.

A range of different libraries written in R try to provide a toolbox for causal structure learning, e.g., `pcalg` [19], or `bnlearn` [39]. Yet, neither do they support the data scientist with regard to a comparison of runtime performance and accuracy of the results, nor do they cover all existing algorithms. For example, smaller packages in various programming languages implement research in the context of improvements within different statistical settings, e.g., `kpc` [45] for non-linear causal relationships, or in the context of algorithmic advances for improved runtime performance, e.g., `parallelPC` [24] or `Lock-Free-PC` [37] addressing parallel execution strategies, or `cupc` [48] for execution on accelerator cards. Each library covers a mix of the available approaches and implements particular algorithms in their respective programming language. Hence, a comparison to other implementations for CSL becomes a tedious manual task with high setup costs. While there are software tools, whose construction follows the pipeline structure of Figure 2 to support a comparison of results, e.g., `BayesiaLab` [6] or `tetrad` [36], they are limited to the algorithms implemented within the respective software tools.

With our pipeline, we provide a framework to incorporate existing libraries and thereby compare implementations across multiple libraries and various programming languages, without the need to manually change the experimental setup for each implementation.

4 A MODULAR PIPELINE FOR CSL

In this section, we present a modular pipeline for Causal Structure Learning (CSL) that addresses the requirements on *platform independence* and *modularity* while ensuring the *comparability* and *reproducibility* of experiments. We propose an architectural blueprint and outline our reference implementation¹.

4.1 An Architectural Blueprint

In the following, we introduce an architectural blueprint, depicted in Figure 2, for a modular pipeline that covers the necessary steps for benchmarking algorithms of CSL. It is designed to fulfill the prior mentioned requirements and consists of four main elements. A *Web Application* provides visual support to a data scientist, and communicates with the core of the pipeline, the *Backend Service*. A separate service, the *Experiment Execution Service*, is responsible for the creation, scheduling, and monitoring of dedicated *Execution Containers*. These *Execution Containers* run specific causal structure learning algorithms and derive the CGMs based on the observational data, which are stored within the *Backend Service*.

Web Application: The Web Application provides an interactive front-end that supports the data scientist in the task of creating the experimental setup following the pipeline paradigm depicted in Figure 1. The *Web Application* communicates with the Backend Service to create the user-defined experimental setup which includes the source of the dataset, the method of CSL with the corresponding library, and implementation-specific parameters of the algorithm. For an experiment, multiple experiment runs can be executed, and thereupon monitored in the Web Application to ensure flawless execution. Once one execution is finished, the Web Application provides mechanisms for the data scientist to explore the determined causal relationships, e.g., visualizing the CGM, examining

Figure 2: Architectural blueprint of a modular pipeline for causal structure learning.

data distributions, causal dependencies, or causal effect estimation using the do-operator [31]. Further, the *Web Application* visualizes the collected execution statistics, e.g., runtimes of the selected CSL implementation, and enables to examine predefined accuracy metrics of the learned CGM, e.g., the false positive rate of edges with respect to the expected ground truth graphical model.

Experiment Execution Service: The Experiment Execution Service is responsible for the execution of experiment runs. Upon request by the Backend Service, it creates *Execution Containers* according to the requirements defined for the experiment, e.g., fitting to the CSL implementation, and on the requested available hardware. Using independent *Execution Containers*, which are scheduled on the appropriate hardware, ensures platform independence. The experiment runs are scheduled and according to the setup, the Experiment Execution Service ensures sequential execution to avoid the influence between different experiments. Further, the experiment runs are monitored and the information is provided to the Backend Service.

Backend Service: The Backend Service handles the requests posted by the Web Application. Therefore, it communicates with the Experiment Execution Service, stores metadata for experiments, e.g., parameter settings and information on datasets to ensure reproducibility and comparability of experiment runs. The Backend Service is composed of a *Dataset Manager*, an *Experiment Controller*, an *Internal Database* and a *Result Controller*.

The Dataset Manager handles all internal and external requests related to the datasets, i.e., creation, deletion, or access. During the creation of a dataset, its metadata, i.e., an identifier, a name and a description of the dataset, the data source, an access method, and a validity flag, and a list of its variables are stored within the *Internal Database* of the Backend Service. Moreover, a dataset is invalidated in case of critical changes revoking any new experiment to ensure comparability and reproducibility. The data source points to the

¹<https://github.com/hpi-epic/mpcsl>

location the observational data is stored, i.e., the *Internal Database* or an *External Data Source*, including access information such as an SQL select statement to retrieve the data.

The *Internal Database* stores the above-described metadata on all observational datasets, regardless of their source. Further, it stores the available implementations for CSL within the pipeline, the parameter setup of all created experiments together with the learned CGM and corresponding statistics collected during execution. In combination with the information on the utilized hardware, stored for each experiment run, comparability and reproducibility of results are ensured.

The *Experiment Controller* handles requests from the Web Application concerning experiments and their setup, i.e., registration of observational datasets, creation of experiments, or triggering experiment runs. Registration of observational datasets and obtaining observational datasets for experiment execution are forwarded to the *Dataset Manager*. The corresponding metadata on the experiments is queried and sent, together with samples from the observational dataset to the *Experiment Execution Service* in case an experiment run is triggered. After execution, the *Result Controller* receives the learned CGM and collected statistics from experiment runs through the *Wrapper* available within the Execution Containers. Further, the *Execution Container* enables an evaluation of the experiment results through the calculation of accuracy metrics with respect to the learned CGM in comparison to the ground-truth stored in the *Internal Database*. Note, the modular extensibility ensures the incorporation of more advanced accuracy metrics beyond false-positive rates, graph edit distances, or the Structural Hamming Distance (SHD) [47] that may be required within the respective experimental evaluation.

Execution Containers: The *Execution Containers* are orchestrated by the Backend Service and provide a virtualized environment for the execution of algorithms for CSL. Thus, appropriate execution environments according to the requirements of the implementations are provided. In addition, the container requires a dedicated *Wrapper* as an interface to communicate with the Backend Service. It provides functionality to receive the dataset, start the execution of the algorithm with provided parameters. Further, it collects statistics during execution and upon successful execution sends the results to the Backend Service.

Upon request from the *Web Application*, the *Result Controller* provides the learned CGM, stored in the *Internal Database*, for a comprehensive exploration and evaluation of the experimental results. The *Web Application* enables to examine the statistics and calculated metrics, e.g., the SHD, in case that ground truth is available for the observational dataset. Moreover, if the ground truth is not available the provided sampling opportunities from the observational dataset enable a robustness examination [21].

In summary, the presented architectural blueprint enables an extensive comparison of implementations for CSL with regard to runtime and accuracy of the learned causal structures.

4.2 MPCSL- A Reference Implementation

Based on the previously introduced architectural blueprint that covers the requirements on the pipeline for CSL in Figure 2, we provide a reference implementation called . The *Web Application* in

Figure 3: The *Web Application* of MPCSL provides an interface to the pipeline’s components. For example, it enables to examine the accuracy metrics such as the Graph Edit Distance or Mean Jaccard Coefficient of identical graphs learned with *pcalg* (left) and *parallelPC* (right).

MPCSL is written in JavaScript using the React, Redux and D3 libraries. As shown in the example view in Figure 3, it provides an interface to interact with the different components of the pipeline necessary for an experimental evaluation.

It includes components to manage experiments, to compare and evaluate individual experiment runs, and to explore the learned causal model. The causal model explorer within the web application presents the learned relationships between variables, using a graph representation of edges for the relationships and nodes for the variables. It displays the original data distribution for each variable and supports functionality to estimate the causal effects of interventions following the do-operator paradigm.

The *Backend Service* of MPCSL is written in Python, using the Flask framework [12] to communicate with the *Web Application* through a RESTful API. In our reference implementation, the *Dataset Manager* uses SQL to communicate with the *Internal Database* an instance of a PostgreSQL [28] database and to communicate to external database management systems. We use the Python SQL toolkit and the object-relational mapper SQLAlchemy [2] to realize the communication and restrict the external data sources to those supported by SQLAlchemy.

The *Experiment Execution Service* uses the Python docker package to create individual docker containers for the execution of experiment runs, with the corresponding requirements of the experiment. The *Execution Containers* are based on Docker [26]. Currently, MPCSL provides docker images that support the R language [33], Python and that support the CUDA framework, when running on systems which include NVIDIA Graphics Processing Unit (GPU) hardware. Through the R execution environment, we support the packages *pcalg* [19], *ParallelPC* [24] and *bnlearn* [39]. With the CUDA execution environment, we added support for GPU-accelerated implementations [13, 38, 48].

For each experiment run, MPCSL collects and presents a selection of statistics, e.g., the runtime, or the number of learned edges. Moreover, the *Result Controller* provides the common accuracy metrics, such as the SHD or false positive rates of the learned causal model with respect to edges within the ground truth CGM. The

examination of accuracy metrics, such as the graph edit distance or mean Jaccard coefficient, for differently learned CGMs enables a direct comparison of experiments on the same dataset, compare Figure 3, and, in combination with sampling, provides the basis for a robustness examination [21].

All implemented MPCSL services run in separate containers. The implementation uses Kubernetes to orchestrate the containers and execute them on different physical host systems, depending on the requirements of the CSL implementation.

5 CASE STUDY ON RUNTIME OF ALGORITHMS FOR CSL USING MPCSL

As previously introduced, data scientists trying to apply methods of CSL in real-world scenarios are confronted with a wide spectrum of different implementations. Their exists work that evaluates the different CSL approaches with respect to the accuracy of learned causal models, e.g., see [16, 41]. While this may support a data scientist in the selection of the appropriate approach, there is, to the best of our knowledge, no work that evaluates the runtime of different implementations on datasets with different data distributions. Especially medical scenarios, such as genetics, require fast implementations that allow for CSL in these high-dimensional settings [1, 19]. As different implementations are written in different programming languages and utilize different hardware setups an evaluation with regard to runtime becomes a tedious manual task with high setup costs.

In the following case study, we illustrate the capabilities of MPCSL when comparing a selection of constraint-based CSL implementations with respect to their runtime. We choose constraint-based CSL for the following reasons. First, it is widely used in real-world scenarios [18, 24] making it an interesting case for practitioners. Second, it provides flexibility to adjust to different data distributions and dependencies by changing the utilized CI test accordingly. Third, constraint-based CSL implementations are available in many different programming languages, libraries, and packages. In particular, we focus on the well-known PC-Algorithm [44], especially its order-independent version PC-Stable [5]. Existing implementations with varying hardware acceleration of the PC-Stable [13, 19, 22, 24, 36–39, 48] are based upon the same algorithm, hence, should have equal accuracy for identically selected parameters, e.g., see Figure 3. Yet, specific implementation details impact the runtime, making it an interesting case for an experimental evaluation.

Our case study consists of three separate experiments on datasets with different data distributions. Further, the datasets differ in the number of variables $|V|$ and the number of observations $|N|$. Both characteristics impact the runtime of the PC-Stable algorithm. First, we conduct multiple experiment runs examining single-threaded runtimes of two different CSL implementations to provide an indication of the suitability in the context of given data distribution with the corresponding CI test, provided by the respective library. In a second and third experiment, we examine the potential of modern hardware to reduce the runtime of CSL. Therefore, we consider the speed-up of CSL implementations on a multi-core server and investigate the runtime of a GPU-accelerated implementation.

Dataset	Distribution	$ V $	$ N $	Dimension
NCI-60	Gaussian	1,190	47	High
MCC	Gaussian	1,380	88	High
BR51	Gaussian	1,592	50	High
DREAM5-INSILICO	Gaussian	1,643	850	High
S.AUREUS	Gaussian	2,810	160	High
S.CEREVISIAE	Gaussian	5,361	63	High
ARTH150	Gaussian	107	20,000	Low
ALARM	Discrete	37	10,000	Low
ANDES	Discrete	223	20,000	Low
LINK	Discrete	724	20,000	High
MUNIN	Discrete	1,041	20,000	High
MEHRA	Mixed	24	20,000	Low

Table 1: Characteristics of gene expression datasets and of datasets from the bnlearn repository. $|V|$ - number of vertices, $|N|$ - number of observations.

5.1 Experimental Setup

In the following, we provide an overview of the datasets, the hardware setup, and the CSL implementations supported by MPCSL for the experiments of our case study. During the setup of MPCSL we added the datasets as described below. We use the *Web Application* to parameterize the experiments for each CSL implementation. The experiment execution on the chosen hardware setup is orchestrated by the MPCSL *Experiment Execution Service*. After execution of multiple experiment runs, the requested metric, for our case study the median runtime, is presented in the *Web Application*.

Data: The characteristics of the datasets loaded into MPCSL for the experimental evaluation are provided in Table 1. The datasets are either real-world gene expression datasets following a multivariate gaussian distribution, used in existing evaluations [24, 38, 48], or, generated datasets according to the well-known reference Bayesian networks from the bnlearn [39] network repository. The datasets contain different numbers of variable, ranging from, e.g., $|V| = 24$ in MEHRA up to $|V| = 5,361$ in S.CEREVISIAE. Thus, the datasets cover both low-dimensional datasets, which we define as $|V| < 500$, and high-dimensional datasets, i.e., $|V| \geq 500$. Furthermore, the datasets incorporate different data distributions, for instance multivariate normal distributed data, called *Gaussian*, multinomial distributed data, called *Discrete*, and conditional Gaussian data, called *Mixed*.

Hardware Setup: All experiment runs are executed in a Kubernetes cluster consisting of a virtual machine, running the MPCSL *Experiment Execution Service*, the MPCSL *Backend Service*, including the *Internal Database* and an enterprise-grade server with 2 Intel® Xeon® Gold 6148 CPU with 20 cores each. The server is equipped with 1.5 TB of RAM, allowing to keep all data in memory during the execution of the experiment runs, and has 4 NVIDIA V100 card, with 32 GB of high bandwidth memory. The *Execution Containers* are run on the server. Furthermore, datasets are fetched from an external database management system running on a separate system. During measurements of the runtime, only a single container is executed at a time and no other operations are executed on the server.

Measurements are conducted within the MPCSL *Wrapper*, measuring the algorithm’s function call, e.g., for R library `bnlearn` [39] using the `diffTime` of the `Sys.time()` prior to and after the call of `pc.stable`. If not stated differently, we repeat each experiment run at least 10 times and present the median runtime. Further, we set the tuning parameter α to 0.01, which is common in application [5].

Employed CSL Implementations: We compare implementations of the PC-stable [5] from the well-known libraries `pcalg` [19] and `bnlearn` [39], as well as, from the libraries `Parallelpc` [24] and `cupc` [48], which allow for a comparison of different parallel execution strategies, and hardware acceleration in GPU-accelerated environments. The four implementations support *Gaussian* data using a Fisher’s Z test. For *Discrete* data `bnlearn` uses Pearson’s X^2 test, `pcalg` and `Parallelpc` use the very similar G^2 test and `cupc` has no test implemented. *Mixed* data is only supported by `bnlearn` that incorporates a mutual information-based CI test for conditional Gaussian settings, provided through the `mi-cg` implementation. `Parallelpc` is written entirely in R and uses the R library `parallel` for parallel execution. `bnlearn` is written in R and C, using C to provide efficient implementations for most functions. It also uses the R library `parallel` for parallel execution. `Pcalg` is written in R and implements the test for *Gaussian* data in C++. For this particular case it uses `openMP` [7] for parallel execution. In contrast to the previous libraries, `cupc` targets a heterogeneous system with an NVIDIA GPU. It provides an R Interface, yet the core algorithm is written using the CUDA framework [27] to utilize the parallel computing capabilities of a GPU.

5.2 Single-Threaded Runtime

In the following, we measure the single-threaded runtime of the PC-Stable implementation from `pcalg` and `bnlearn` on all datasets presented in Table 1. The measured runtimes are shown in Table 2.

For *Gaussian* datasets, our measurements show that the implementation from the `pcalg` library outperforms the `bnlearn` implementation by factors of 30 for low-dimensional datasets, e.g., ARTH150 and factors of up to 6,753 for high-dimensional datasets. For the datasets S.AUREUS and S.CEREVISIAE we terminated the execution of `bnlearn` after 5 days, without any result, whereas `pcalg`’s implementation finished after 180 seconds. Both implementations use Fisher’s Z test for CI testing and are written in C or C++. Yet, `pcalg` works on a pre-calculated correlation matrix, whereas within `bnlearn` the correlation is calculated repeatedly for each independence test, which we account for the significant difference in measured runtime. Note, the calculation of the correlation matrix prior to the execution of the PC-Stable, for the datasets subject of the study ranges from 0.044 seconds for NCI-60 to 1.391 seconds for S.CEREVISIAE. Thus, it does not impact the total runtime in a significant way.

For *Discrete* datasets the implementation from the `bnlearn` package outperforms `pcalg` implementation by factors of up to 25, for low-dimensional datasets, e.g., ALARM, to factors of up to 84 for higher-dimensional datasets, e.g., LINK. For the dataset MUNIN the execution of the `pcalg` implementation was terminated after 5 days, without any result, compared to `bnlearn`’s implementation, which finished below 2 hours. We account the difference to the fact

Dataset	pcalg	bnlearn
ARTH150	248.7	7,617
NCI-60	6.7	45,251
MCC	21.5	83,886
BR51	32.3	171,629
DREAM5-INSILICO	4,257	360,572
S.AUREUS	180.0	> 432,000
S.CEREVISIAE	108.2	> 432,000
ALARM	30.1	0.5
ANDES	2,824	108.8
LINK	324,873	3,827
MUNIN	> 432,000	6,753
MEHRA	-	11.9

Table 2: Median runtimes in seconds of PC-stable in single threaded execution. Comparing implementations from libraries `pcalg` and `bnlearn` on benchmark datasets. Note, for algorithms exceeding the runtime of a day we executed a single run or terminated after five days.

that the CI test for *Discrete* data in `pcalg` is written in R, whereas `bnlearn` uses efficient C code.

For the *Mixed* dataset MEHRA we report numbers only for `bnlearn`, as no other library used in the case study supports *Mixed* data. Based on the measurements, we conclude that it is advisable to use the implementation from the `pcalg` library for *Gaussian* data, whereas for *Discrete* and *Mixed* data the `bnlearn` library should be used.

5.3 Parallel Efficiency on Multi-Core Systems

In the following experiment, we measure the runtime of parallel implementations of the PC-Stable algorithm, taken from the libraries `pcalg`, `Parallelpc` and `bnlearn`. In previous studies [24, 40] the benefit of parallel execution to reduce the runtime of constraint-based CSL algorithms is shown, yet to the best of our knowledge no comparison between library-specific implementations exists. Therefore, we aim to determine differences in the implementations’ behavior, when scaling the number of cores. All three implementations follow the framework for parallel constraint-based learning [40]. Yet, parallel processing within the implementations of the PC-Stable is applied only to the adjacency search, which comprises the CI tests. Other parts of the implementations are executed sequentially, which limits the effect of scaling the number of cores on the measured runtime.

In Table 3, we provide our measurements for the *Gaussian* dataset ARTH150 using all three libraries and for *Discrete* datasets using `Parallelpc` and `bnlearn`, given that `pcalg` does not support parallel execution for *Discrete* data. For all measurements, we observe that the ideal speed-up is not achieved, which is due to the sequential part of the implementations. For the dataset ARTH150, `Parallelpc` shows the implementations’ worst speed-up, achieving only a factor of up to 7.15 on 40 cores compared to a factor 15.51 speed-up of `pcalg`. Except for this particular difference, the behavior is similar for all implementations. Note, the overall runtime remains significantly slower for `bnlearn` compared to `pcalg`.

Library	Dataset	Cores			
		5	10	20	40
Parallelpc	ARTH150	3.3	4.1	6.9	7.2
bnlearn	ARTH150	3.3	5.3	8.3	11.7
pcalg	ARTH150	3.0	5.7	8.9	15.5
Parallelpc	ANDES	3.4	6.2	10.9	14.3
bnlearn	ANDES	1.6	1.6	1.6	1.4
bnlearn	LINK	3.4	5.3	7.0	7.6
bnlearn	MUNIN	4.0	6.8	11.3	14.4

Table 3: Factors of speed-up measured with an increasing number of cores running parallel versions of the PC-Stable compared to single threaded execution.

Dataset	cupc	pcalg (40 cores)
ARTH150	1.93	16.03
NCI-60	1.94	3.18
MCC	2.45	4.93
BR51	4.48	6.42
DREAM5-INSILICO	5.41	168.09
S.AUREUS	13.58	35.21
S.CEREVISIAE	32.79	55.59

Table 4: Median runtime in seconds of PC-stable with the adjacency search executed on a GPU - cupc or in parallel using 40 CPU cores - pcalg.

Considering *Discrete* datasets, we observe a runtime improvement for bnlearn using up to 40 cores for the high-dimensional datasets LINK and MUNIN. For the dataset ANDES, speed-up through the increase in cores is small with factors below 2 and even decreases when running on 40 cores compared to 20 cores. We assume that the sequential part of the execution dominates the processing of the dataset ANDES in bnlearn and that the adjacency search is already efficient in single-threaded execution. In contrast processing ANDES with ParallelPC, we observe strong speed-up, yet the overall runtime for 40 cores is slower than the single-threaded execution with bnlearn. This supports our assumption that bnlearn has efficient adjacency search and CI test implementations for *Discrete* data.

Overall, we did not observe a significant difference in the implementations' behavior with regard to scaling the number of cores. Yet, for lower-dimensional datasets, e.g., ANDES, efficient implementations, e.g., found in bnlearn, cannot benefit from multi-core systems and may even be slowed down.

5.4 GPU-Acceleration

In a third experiment, we consider a heterogeneous system and investigate the speed-up of a GPU-accelerated implementation, cupc, over a Central Processing Unit (CPU)-based parallel implementation, pcalg running on 40 cores. The MPCSL *Experiment Execution Service* ensures that the experiment runs are scheduled on hardware that fulfills the requirements to execute the implementations, e.g., provide an NVIDIA GPU for cupc.

In Table 4, we report the measured runtimes on all *Gaussian* datasets considered in our case study. Using a GPU to process the datasets leads to additional speed-up for all datasets, ranging from speed-up of factor 1.43 for dataset BR51 to speed-up of factor 31.07 for dataset DREAM5-INSILICO. We observe that the two datasets, DREAM5-INSILICO and ARTH150 result in higher speed-up when the adjacency search is executed on the GPU. Both datasets have a larger number of observations $|N|$, compared to the other datasets, which results in an increased number of higher-order CI tests. For the other five datasets, execution on the GPU leads to a speed-up of less than factor 2. For these datasets, over 94% of the independence tests are either unconditioned or with a conditioning set of size 1 [38] for the given tuning parameter $\alpha = 0.01$. We account for the high percentage of low-order independence tests for the small factor of speed-up achievable with GPU-acceleration.

6 SUMMARY

In our work, we present a blueprint and a reference implementation of a modular pipeline for Causal Structure Learning (CSL). The pipeline supports the experimental evaluation of the wide spectrum of implementations of algorithms for CSL from data scientists and their application in practice. In particular, the platform manages the observational datasets and parameter setups for experiment runs. Further, it orchestrates the execution of the experiments with given hardware constraints using virtualized environments. Storing the parameterization ensures reproducibility. The collection of runtime statistics, and accuracy metrics allows for a comprehensive experimental evaluation in the pipeline.

We present the capabilities of our reference implementation MPCSL that was developed to address the requirements of deployment in scenarios from both a theoretical and practical perspective. In detail, we conduct a case study using MPCSL to investigate the runtime performance of implementations of the well-known PC-Algorithm [44]. In this scenario, the results indicate that for *Gaussian* data, the pcalg library provides better runtimes, by factors of over 1,000, whereas for *Discrete* data the bnlearn library outperforms the pcalg implementation by factors of up to 84. An investigation of parallel execution on multi-core systems showed similar behavior with an increasing number of cores across the implementations, achieving a speed-up of up to factor 15.5 on 40 cores. Additional speed-up of factors of up to 31 is possible employing GPUs, yet their application is currently limited to *Gaussian* data.

Beyond the demonstrated research aspect, we use the developed tool with industry partners from the manufacturing domain. Here, the focus is on comparing the accuracy of learned CGMs with different approaches for CSL, as well as, different data preparation techniques. In this context, we found that there is a strong need for visual support, during the selection and preparation of data for CSL, and when comparing different learned CGMs. Currently, the reference implementation is limited to showing a single CGM and only reports accuracy metrics when comparing multiple CGMs.

In future work, we are going to incorporate the opportunity to generate datasets with different data characteristics following a selection of data-generating models such that the pipeline envelopes the whole benchmarking pipeline. While MPCSL currently serves as a starting point, the pipeline's modularity with respect to the CTF

enables for extensibility regarding the causally insufficient case or interventional data. In this context, we aim to extend the platform to directly provide a larger set of CSL implementations to further raise the interest of the research community. We invite the research community to actively participate in the extension of MPCSL.

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