gCastle: A Python Toolbox for Causal Discovery

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Abstract

gCastle is an end-to-end Python toolbox for causal structure learning. It provides functionalities of generating data from either simulator or real-world dataset, learning causal structure from the data, and evaluating the learned graph, together with useful practices such as prior knowledge insertion, preliminary neighborhood selection, and post-processing to remove false discoveries. Compared with related packages, gCastle includes many recently developed gradient-based causal discovery methods with optional GPU acceleration. gCastle brings convenience to researchers who may directly experiment with the code as well as practitioners with graphical user interference. Three real-world datasets in telecommunications are also provided in the current version. gCastle is available under Apache License 2.0 at https://github.com/huawei-noah/trustworthyAI/tree/master/gcastle.

Keywords: causal discovery, structure learning, Python, gradient-based methods

1. Introduction

Discovering and understanding causal relations underlying physical or artificial phenomena is an important goal in many empirical sciences. Due to the relative abundance of passively observed data as opposed to interventional data, learning causal graphs from purely observational data has been vigorously studied (Peters et al., 2017; Spirtes and Glymour, 1991). Existing methods roughly fall into three classes: constraint-based, functionbased, and score-based. The first class relies on conditional independence tests and identifies a class of Markov equivalent directed acyclic graphs (DAGs) (Meek, 1995; Spirtes et al., 2000; Zhang, 2008). Unlike constraint-based methods that assume faithfulness and identify only the Markov equivalence class, function-based methods can distinguish between different DAGs in the same equivalence class, by imposing additional assumptions on data distributions and/or function classes. Examples include linear non-Gaussian additive model (LiNGAM) (Shimizu et al., 2006, 2011) and the nonlinear additive noise model (ANM) (Hoyer et al., 2009). The last class of methods employs a score function to evaluate candidate causal graphs w.r.t. the data and then searches for a (or a class of) causal DAGs achieving the optimal score (Chickering, 2002; Peters et al., 2017). Due to the combinatorial nature of the acyclicity constraint, most score-based methods use local heuristics to perform the search. Recently, a class of methods has considered differentiable score functions in combination with a novel smooth characterization of acyclicity (Zheng et al., 2018), so that gradient-based optimization method is feasible to seek the desired DAG. This change of perspective allows using deep learning techniques for flexible modeling of causal mechanisms and improved scalability. See, e.g., Yu et al. (2019); Ng et al. (2019a,b, 2020); Lachapelle et al. (2020); Zheng et al. (2020); Brouillard et al. (2020); Bhattacharya et al. (2021), which have shown state-of-the-art performance in many experimental settings, with both linear and nonlinear causal mechanisms.

This paper presents the **gradient-based causal structure learning** (gCastle) toolbox, developed in Python and with PyTorch supporting GPU acceleration. gCastle aims to provide many ready-to-use gradient-based methods, but also classic and competitive algorithms such as PC (Spirtes et al., 2000) and LiNGAM (Shimizu et al., 2006, 2011). The functionalities include dataset generation from either simulator or real-world datasets, causal structure learning, and evaluation of learned graphs. gCastle brings much convenience to researchers in the machine learning community who may directly experiment with the released Python code. For practitioners, gCastle provides useful practices in learning causal graphs, such as prior knowledge insertion, preliminary neighborhood selection to eliminate non-edges, and post-processing to remove false discoveries. A graphical user interference (GUI) is also developed to ease the causal structure learning process and to visualize the learned graph that allows further manual annotations.

In addition, gCastle releases three real-world causal datasets where the DAGs describe relations amongst alarms in telecommunication systems. The graphs are obtained by both human annotations and historical maintenance records (i.e., interventional data). We believe that these datasets would be a good addition to causal discovery research, as there are only a few public real-world datasets. The datasets were previously used in a causal discovery competition, with 112 participating teams and over 800 submissions in total.¹

2. Related Packages

There exist several Python packages focusing on causal inference, aiming at estimating the causal effect on the outcome of an intervention (Chen et al., 2020; Sharma and Kiciman, 2020; Battocchi et al., 2019; Miller et al., 2020). To the best of our knowledge, there are only four Python packages for causal structure learning: Tigramite (Runge et al., 2019), py-causal (Wongchokprasitti et al., 2019), causal-learn (Zhang et al., 2021), and CDT (Kalainathan et al., 2020). Tigramite has a narrow focus on time series data and is not directly comparable to gCastle. py-causal is a wrapper around the Java-based Tetrad (Ramsey et al., 2018) package, and all the algorithms and relevant functionality are called from Java, resulting in somewhat inconvenience for use and further modifications. Similarly, CDT is not a pure Python package and has a significant part of its algorithms and evaluation metrics called from R code. On the other hand, causal-learn is a recently released direct Python translation of the Tetrad code, however, no gradient-based methods are included.

A slight overlap exists between the algorithms implemented in gCastle and those offered by CDT, causal-learn, and py-causal. The overlap is mainly present in the traditional

^{1.} https://competition.huaweicloud.com/information/1000041487/introduction

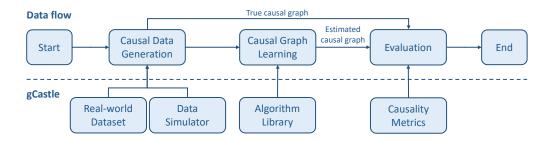


Figure 1: Causal discovery workflow.

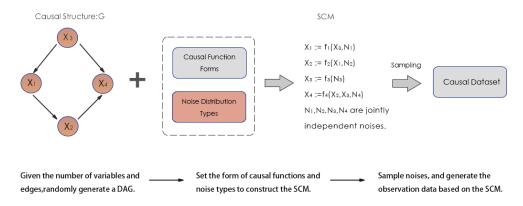


Figure 2: Synthetic data simulation procedure.

methods that are often used as baselines in this field. gCastle has a clear focus on more recently developed gradient-based structure learning algorithms which are missing from the other packages.

3. Design and Implementation

The vision of gCastle is to provide an end-to-end pipeline to ease causal discovery tasks that allow: simulating causal data or loading real-world data; learning causal graphs with state-of-the-art algorithms like recent gradient-based algorithms; evaluating estimated causal graphs with commonly used metrics such as false discovery rate (FDR), true positive rate (TPR) and structural Hamming distance (SHD); and using a user-friendly web interface to visualize the whole procedure. Figure 1 illustrates the overall workflow.

3.1 Datasets

gCastle provides various types of data generators to help users simulate data or load real-world data. Currently, three real-world datasets are provided and each contains observational records collected from devices in real telecommunication networks and a true causal graph labeled by business experts. The datasets can be accessed through the gCastle API. For simulated data, the procedure is illustrated in Figure 2. Provided with a random DAG, causal function forms, noise distribution, and predefined sample size, one can quickly simulate a synthetic observational dataset that follows the given structural causal model (SCM).

Table 1: List of algorithms in gCastle.

Category	Algorithms
constraint-based	original-PC (Kalisch and Bühlmann, 2007), stable-PC (Colombo and Maathuis, 2014), parallel-PC (Le et al., 2016)
function-based	Direct-LiNGAM (Shimizu et al., 2011), ICA-LiNGAM (Shimizu et al., 2006), ANM (Hoyer et al., 2009), HPCI (Zhang et al., 2020)
score-based	GES (Chickering, 2002), TTPM (Cai et al., 2021)
gradient-based	GraN-DAG (Lachapelle et al., 2020), NOTEARS (Zheng et al., 2018), NOTEARS-MLP (Zheng et al., 2020), NOTEARS-SOB (Zheng et al., 2020), NOTEARS-LOW-RANK (Fang et al., 2020), NOTEARS-GOLEM (Ng et al., 2020), MCSL (Ng et al., 2019a), GAE (Ng et al., 2019b), RL-BIC (Zhu et al., 2020), CORL (Wang et al., 2021)

At present, gCastle supports multiple well-known causal functions, including Linear, MLP, and Quadratic, and also various noise distribution types, such as Gaussian, Exponential, Uniform, and Gumbel. Additionally, gCastle offers functionality to generate random DAGs with different strategies, which include ER, scare-free, low-rank, etc.

3.2 Algorithms

So far, gCastle (version 1.0.3) implements 19 causal discovery algorithms which cover most gradient-based algorithms and some traditional constraint-, score-, and function-based algorithms. Compared to other mainstream toolboxes, gCastle has a fairly complete gradient-based algorithm library. Table 1 lists all algorithms that gCastle currently supports.

3.3 Evaluation

The current version of gCastle provides nine metrics for evaluating the estimated causal graph relative to the underlying truth. Most metrics are commonly used in the literature, e.g., FDR, TPR, SHD, etc. Other metrics are designed according to the specific purpose in real-world scenarios; a relevant example is the gScore which comes from a root cause analysis scenario in AIOps.

4. Installation and Usage

gCastle can be installed locally using either pip or running the setup.py script in the source code. After installation, the gCastle API can be used to build tasks; an example using Notears is shown in Code Listing 1. An alternative to the main API is to use the provided user-friendly GUI to visually design the tasks². A Docker image with the GUI is available on Docker Hub³, which can be used to avoid issues with software dependencies and version matching.

^{2.} A demo is available at https://www.youtube.com/watch?v=5NOu2oApBgw.

^{3.} https://hub.docker.com/r/gcastle/castleboard-cpu-torch

```
from castle.common import GraphDAG
from castle.metrics import MetricsDAG
from castle.datasets import IIDSimulation, DAG
from castle.algorithms import Notears
# I. Generate the artificial true causal graph and observation data.
weighted_random_dag = DAG.erdos_renyi(n_nodes=10, n_edges=20,
                                      weight_range=(0.5, 2.0), seed=1)
dataset = IIDSimulation(W=weighted_random_dag, n=2000, method='linear',
                        sem_type='gauss')
true_causal_matrix, X = dataset.B, dataset.X
# II. Learn the Causal Structure beneath the observation data.
nt = Notears()
nt.learn(X)
# III. Visualize the comparison of estimated/true graphs using a heat map.
GraphDAG(nt.causal_matrix, true_causal_matrix)
# IV. Calculate Metrics.
mt = MetricsDAG(nt.causal_matrix, true_causal_matrix)
print(mt.metrics)
```

Listing 1: A toy example using the gCastle API.

5. Concluding Remarks and Future Developments

This paper introduces a causal structure learning toolbox gCastle. It provides many recently developed gradient-based causal discovery methods and all the algorithms are implemented in Python. As an open-source software, gCastle encourages contributions of algorithms and datasets from both research and industry communities. Our future work direction is to continuously include more real datasets as well as add competitive algorithms like CAM (Bühlmann et al., 2014) which may require re-implementation using Python.

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