Causal Generalization in Autonomous Learning Controllers

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Abstract. Any machine targeted for human-level intelligence must be able to autonomously use its prior experience in novel situations, unforeseen by its designers. Such knowledge transfer capabilities are usually investigated under an assumption that a learner receives training in a source task and is subsequently tested on another similar target task. However, most current AI approaches rely heavily on human programmers, who choose these tasks based on their intuition. Another largely unaddressed approach is to provide an artificial agent with methods for transferring relevant knowledge autonomously. One step towards effective autonomous generalization capabilities builds on (autonomous) causal modeling and inference processes, using task-independent knowledge representations. We describe a controller that enables an agent to intervene on a dynamical task to discover and learn its causal relations cumulatively from experience. Our controller bootstraps its learning from knowledge of correlation, then removes non-direct-cause correlations – correlations that are due to a common (external) cause, be spurious, or invert cause and effect – through strategic causal interventions, while learning the functions relating a task's causal variables. The effectiveness of knowledge transfer by the proposed controller is tested through simulation experiments.

Keywords: Generalization · Learning · Cumulative Learning · Knowledge Transfer · Control · Causality · Autonomy

1 Introduction

Any agent with general intelligence must be able to deal with novel situations [17]. Since novelty is always relative to a learner's knowledge, one way a controller may handle it is to use priorly-experienced situations for guidance. This calls for models that are generalizable to a variety of scenarios. Conventional machine learning methods typically learn many spurious correlations, which may cause unpredictable performance – possibly catastrophic – when facing new tasks. Also, current 'transfer learning' methods heavily depend on human programmers to choose the tasks between which the knowledge transfer must occur. The autonomy of artificial intelligence (AI) systems, in knowledge acquisition and transfer, allowing effective and efficient handling of a variety of scenarios, remains largely unaddressed. No general solution to causal model learning exist, as of yet.[3]

Here we introduce an autonomous controller that cumulatively [19] learns and uses causal models of tasks that are transferable to novel scenarios. The design is based on three major principles of constructivist AI [16], which are *knowledge transparency*, *temporal grounding*, and *feedback loops*. Given this approach, an autonomous agent can autonomously learn causal models that are invariant across variations of tasks. Causal modeling and inference go beyond the limitations of current machine learning (ML) methods via their testability and task-independence [19, 7], allowing an agent to use it in scenarios it has never encountered before. Our approach is compatible with Pearl's structural causal models and directed acyclic graphs [6]. We adapt the principles of causation such that they meet the aforementioned principles of a constructivist methodology [16]. Our causal models of a task are formed by considering the assumption of insufficient knowledge and resources (AIKR) [20], according to which the agent must rely only on a limited set of sampled data and resources. An important factor to limit the scope of learning, and prevent incorrect generalizations, is to consider time explicitly in knowledge representation.

The approach builds on – and is compatible with – prior work on cumulative learning [19, 17]. The controller starts its causal discovery process by learning an initial correlational model. Then, it removes non-direct-cause correlations through causal interventions until it identifies the causal structure. It continually updates its model as it collects more data. In short, we introduce an online autonomous controller that initially learns a correlational model through random search (worst case), discovers task-independent invariant relations between variables of a dynamical task, learns the functions relating the variables, and tests the model in transfer scenarios every time it learns the model.

2 Related Work

Generalization has made an appearance in various machine learning (ML) paradigms to date, usually under the heading of 'transfer learning' (TL), invariably with the shared goal of increasing learning rate and improving flexibility. In supervised learning, deep transfer learning (DTL) has been applied to overcome the problem of insufficient training data in the target task. The approaches to DTL differ between domain-based and feature-space-based methods [14], but they lack properties necessary for a general, autonomous AI system, since 1) DTL methods rely on human programmers to choose source and target domains based on their intuition, and 2) an agent that interacts with the environment changes the data distribution in an unknown way. Reinforcement learning (RL),

[3] By 'general solution' we mean that the learning is largely independent of the task-environment and can be used to transfer learned skills between different task types.

however, is an instance of algorithms by which the agent learns via taking actions, changing the world's states, and receiving rewards. TL methods in RL (reinforcement transfer learning, RTL) are based on an agent that receives training in a task and reuses the learned knowledge in another, similar task, and the transferred knowledge is usually in the form of policies, reward functions, and/or value functions [15]. However, not only human intuition is part of many RTL methods, the aforementioned forms of knowledge are goal-entangled and thus, task-dependent. The same TL limitation holds for deep reinforcement learning (DRL) approaches when the target tasks change in an unpredictable way [4, 13].

The 'covariate shift' concept results from the assumption that conditionals between variables are invariant between domains [2] and occurs due to the distributions' change after intervention. Recently, Rojas-Carulla et al. [11] proved that a subset of conditionals that is limited to the causal parents of a variable can be used to build an optimal predictor of that in the transfer domain, proving Pearl's statement about causal relations being invariant physical mechanisms [6]. In general, explicit representation of causation goes beyond the limitations of current ML due to its transparency, testability, intervention reasoning (predicting the outcomes of actions), and capability of dealing with missing data [18, 7]. However, since the approach has attracted researchers' attention recently, causal discovery and generalization have still been limited to observation-based methods, which are not proper for an agent that learns by doing [12, 11]. A recent paper introduced a causal discovery algorithm based on intervention [1], however, the algorithm does not learn a causal model in an online manner and is limited to obtaining a causal structure. Our learning controller is an improved version of [1], relying on principles of cumulative learning [18] and AERA system [5], in which a model is learned and gets updated while the agent collects data.

3 Problem Formulation

We start by formulating knowledge representation and intervention. In a deterministic world, the initial condition acts as a 'cause' of the particular unfolding world dynamics when there is no autonomous agent affecting its physical processes. Although a dynamical mechanism that moves a task from one state to another is independent of the initial state[4] [9], different initial conditions lead to different outcomes. Thus, we stick to a discrete-time representation of a dynamical task that has a special focus on initial state, as follows [5]

$$\mathbf{X}(t) := f(\mathbf{X}(0), N_{\mathbf{X}}(0), ..., N_{\mathbf{X}}(t))), \tag{1}$$

[4] This is a special case of the 'Independence of Cause and Mechanism' principle, which states that the mechanism that connects the cause to the effect is independent of the cause itself; i.e. X causes Y if and only if $P(Y \mid X)$ is independent of $P(X)$ [12].

[5] Our physical formalization is compatible with event-based causality, where an event causes another event to happen. An event can be defined as a set of manipulable variables with changing values in a time interval that apply forces and causes changes in values of another set of variables in a subsequent time interval.

with augmented state vector $\mathbf{X} \in \mathbb{R}^{n+m}$, where n and m are the dimensions of the world's observables and manipulables, respectively. Also, $\mathbf{X}(0)$ represents the initial state, and $N_{\mathbf{X}} \in \mathbb{R}^{n+m}$ is the noise on both observables and manipulables. The terms $N_{\mathbf{X}}(0), ..., N_{\mathbf{X}}(t))$ show the applied noise in different time steps.

By assuming there is an autonomous agent that can manipulate (intervene on) some observables at any time t, we can break up the vector $\mathbf{X}$ into two parts, where $U \in \mathbb{R}^m$ is the control input vector (vector of manipulables) and $X \in \mathbb{R}^n$ is the vector of observables. Then, equation (1) can be written in the form of

$$X(t) := g(X(0), U(0), ..., U(t-1), N_X(0), ..., N_X(t)) \tag{2}$$

Equation (2) can also be written as a difference equation as follows

$$X(t) := \tilde{g}(X(t-1), U(t-1), N_X(t)) \quad \text{and} \quad X(0) := \beta_0 \tag{3}$$

where β_0 indicates the vector of initial values of equation (3). Now we can formulate intervention in dynamical tasks as follows

- **Input interventions:** This set of interventions does not change the causal structure of the task. It has two forms:
  - Changing the initial conditions of equation (1), and
  - Setting the value of manipulables in eq. (2).
- **Structural interventions:** Replacing equation (1) with another function, which is equivalent to having a different ordinary difference equation and may change the causal structure.

3.1 Causal generalization

To formulate generalization, we assume that the controller is trained during D tests, having D different probability distributions. We also assume that the control input trajectory U is identical over all D tests. Every $\mathbb{P}^k$ represents a distribution in k^{th} test ($k \in 1, ..., D$), generating U and X^k given initial conditions $X^k(0)$. Over these tests, it learns a function h that maps $X(0)$ and U to X. Then, the prediction of h is tested in a novel test $D+1^{th}$, which the agent has not experienced before. In other words, the test $D+1^{th}$ is the transfer test with distribution $\mathbb{P}^{D+1}$, in which the generalizability of the function h is tested. The controller wishes to learn the function h with small L^2 loss, that is

$$\varepsilon_{P^{D+1}}(h) = \mathbb{E}_{(X^{D+1}, U|X^{D+1}(0)) \sim \mathbb{P}^{D+1}}(X^{D+1} - h(U|X^{D+1}(0)))^2 \tag{4}$$

This statement also holds for identical initial conditions $X(0)$ over D tests with different input trajectories U^k. Then, every $\tilde{\mathbb{P}}^k$ represents a distribution in k^{th} test, generating the input trajectory U^k and X^k given initial conditions $X(0)$. Over these tests, the agent must learn a function $\tilde{h}$ that maps $X(0)$ and U to X. Then, the prediction of $\tilde{h}$ is tested in a novel test $D+1^{th}$ (transfer test), which the agent has not experienced before. In fact, the controller wishes to learn the function $\tilde{h}$ with small L^2 loss, that is

$$\varepsilon_{P^{D+1}}(\tilde{h}) = \mathbb{E}_{(X^{D+1}, U^{D+1}|X(0)) \sim \tilde{\mathbb{P}}^{D+1}}(X^{D+1} - \tilde{h}(U^{D+1}|X(0)))^2 \tag{5}$$

The difference between the two aforementioned equations is that in equation (4) the predictability of function h is tested for a new initial condition $X^{D+1}(0)$, while the predictability of function $\tilde{h}$ in equation (5) is tested for a new control input trajectory U^{D+1}. We will see that h and $\tilde{h}$ are identical after learning the causal structure. In other words, we need to learn a model that is generalizable to scenarios where there may exist new control input trajectories and/or new initial conditions.

4 Causal Discovery & Learning

This work is done within the methodological frameworks of **neo-constructivism** ([16]; see also [10, 3]) and **causation** (cf. [6, 9, 11]). Via the constructivist approach an AI system can autonomously acquire knowledge and use it in multiple different but similar situations/tasks. To that end, feedback loops are used that enable the controller to perform causal interventions (interventions with the purpose of causal discovery).

Learning a correlational model: In the first phase of learning, a random search in the observation space occurs, which makes the agent learn correlations between the variables. This correlational modeling is not generalizable but it enables the agent to gain prior knowledge about tasks. Our method removes non-direct-cause correlations and updates the model over training.

Causal structure identification: The agent discovers the causal relations by intervening on some variables and inspecting the distribution changes in other variables. By adapting the definitions provided by [1], we can write the following definition that allows an agent detect the *causal relations between observables.* Assume $\forall j \;\; x_j \not\leftarrow x_i$, then $x_j \rightarrow x_i$ if

$$\begin{aligned} \forall\, l \neq j \;\; x_l^k(0) = x_l^{k'}(0) \quad x_j^k(0) \neq x_j^{k'}(0), \;\; \forall\, l, t \;\; {u^k}_l(t) = {u^{k'}}_l(t) \\ \Rightarrow \;\; \mathbb{P}(x_i^k(t)) \neq \mathbb{P}({x^{k'}}_i(t)) \end{aligned} \tag{6}$$

In other words, given there is a correlation between x_j and x_i, x_j causes x_i if the following statement holds: If the agent generates the same control input trajectory for two different initial conditions of observable x_j and then it finds distribution changes in observable x_i, it concludes that x_j causes x_i.

The agent can also find the *causal relations between manipulables and observables.* Assume $\forall j \;\; u_j \not\leftarrow x_i$, then $u_j \rightarrow x_i$ if

$$\begin{aligned} \forall\, l \;\; {x^k}_l(0) = {x^{k'}}_l(0), \;\; \forall\, l \neq j, t \;\; {u^k}_j(t) \neq {u^{k'}}_j(t) \quad \forall\, t \;\; {u^k}_l(t) = {u^{k'}}_l(t) \\ \Rightarrow \;\; \mathbb{P}(x_i^k(t)) \neq \mathbb{P}({x^{k'}}_i(t)) \end{aligned} \tag{7}$$

In other words, given there exists a correlation between u_j and x_i, then u_j causes x_i, if the following statement holds: If the agent generates two different input control trajectories $u_j(t)$ for identical initial conditions and then it finds distribution changes in observable x_i, it concludes that u_j causes x_i.

Causal model learning: Equations (6) and (7) only allow obtaining the causal structure. However in our method, the initial function (model) that was learned through correlational modeling is constantly updated by removing non-direct-cause correlations after every intervention. Also, the function is updated accordingly (after every intervention) through a grey-box modeling method.

4.1 Using invariant functions for generalization

According to [11], causal generalization is only possible through an invariant function that is learned over a set of training tests $\{1, ..., D\}$ with various control inputs and initial conditions. Via the following assumptions, we will conclude that the invariant function is the causal model of a task, for which we will introduce a discrete linear state-space equation.

Assumption 1: There exists a function of observable and manipulable variables that predicts the observables in the next time step, by assuming the same control input trajectory U for all D tests, such that

$$h(U|X^k(0)) = h(U|X^{k'}(0)) \quad \forall k, k' \in \{1, ..., D\} \tag{8}$$

and, by assuming the same initial conditions for all D tests, such that

$$\tilde{h}(U^k|X(0)) = \tilde{h}(U^{k'}|X(0)) \quad \forall k, k' \in \{1, ..., D\} \tag{9}$$

Since the function h and $\tilde{h}$ are invariant in all tests, according to the fact that input interventions do not change the causal structure (as mentioned in subsection 3.1), we can conclude that

$$h(U|X^k(0)) = \tilde{h}(U^k|X(0)) \quad \forall k, k' \in \{1, ..., D\} \tag{10}$$

Assumption 2: The invariance of function h also holds in transfer test $D+1$.

Assumption 3: Let us assume that h is a linear function so that for all D tests and for any initial condition $X(0)$ and/or any input trajectory U, we have

$$h(t) := X(t) = AX(t-1) + BU(t-1) + N(t), \quad X(0) := \beta \tag{11}$$

Assumptions 2 and 3 imply that the function h is also linear in transfer test. We will see if h is not causal, new initial conditions and/or new input trajectories lead to covariate shift problem. Thus, learning an invariant function (i.e. a causal model) solves the problem. In other words, for prediction error minimization in $D+1^{th}$ test, the following L^2 error should be minimal, for any $X(0)$ and any input trajectory U,

$$\begin{aligned} &\varepsilon_{\mathbb{P}^{D+1}}(A, B) = \\ &\mathbb{E}_{(X^{D+1}, U^{D+1}) \sim \mathbb{P}^{D+1}} (X^{D+1}(t) - AX^{D+1}(t-1) - BU^{D+1}(t-1))^2. \end{aligned} \tag{12}$$

where $\varepsilon_{\mathbb{P}^{D+1}}(A, B)$ shows the squared error over predictions in transfer test. Now we propose the following optimal prediction model, which can be obtained from minimizing equation (12):

$$[A^*, B^*] := \underset{A,B}{\arg\min}\, \varepsilon_{P^{D+1}}(A, B). \tag{13}$$

The left side of equation (13) is a matrix specifying the causal structure of a dynamical task (causal relations between observables and manipulables), which provides minimal squared error in transfer test. Here is the introduced model;

$$(X(0), U(0), ..., U(t-1)) \quad \rightarrow \quad X(t) \tag{14}$$

such that

$$X(t) = A^* X(t-1) + B^* U(t-1). \tag{15}$$

Algorithm 1: Pseudocode of learning the invariant causal model

```
Input: sample (U^k, X^k | X^k(0))
Output: Estimated model (A and B matrices)
Initial correlational model calculation;
Move the task to arbitrary initial conditions;
while True do
    for i = 1:n do
        Do intervention 1 on x_i;
        Remove non-direct-cause correlations;
        Update the model, while moving to new initial conditions;
    end
    for j = 1:m do
        Do intervention 2 on u_j;
        Remove non-direct-cause correlations;
        Update the model, while testing new control input trajectories;
    end
    if averaged squared prediction error in a new test ≤ ϵ then
        Break;
    end
end
```

Based on sufficient conditions for causal discovery in the linear Gaussian settings given by [8], **$\mathbf{A}^*$ and $\mathbf{B}^*$ provide a function h^* that consists only of causal relations.** In other words, the function h^* satisfies assumptions (1) and (2), which lead to invariant predictions in the transfer test.

4.2 Learning invariant causal model

The proposed algorithm for causal discovery (Algorithm 1) identifies the causal structure through D different tests until it computes a model that is invariant. In other words, the algorithm converges to the optimal A^* and B^* matrices for causal generalization. The controller continues the training process until it is successful in controlling the task with new initial conditions and new control input trajectories it has never seen over training process.

5 Experimental Evaluation

For evaluation of the proposed method, two dynamical tasks were created in the same simulated environment: the Rendezvous task including four mobile robots on a two dimensional plane and a path following task. The causal structure of the environment is thereby independent of the task. We will show in this section that the same holds for the learned causal model. In the first test (Rendezvous task) the robots (R_1, ..., R_4) have to meet at the same location in the x-y plane, using the learned causal model. In the second test, we evaluate the same causal model's prediction ability by assigning a single robot to follow a predefined circular path. In both experiments, the robots are given novel control input trajectories and initial locations to test the model's capability in dealing with covariate shift problem. Each robot's movement follows discrete linear equations of

$$x(t) := x(t-1) + T_s u^x(t-1) \tag{16}$$
$$y(t) := y(t-1) + T_s u^y(t-1) \tag{17}$$

where T_s is the sampling time. There exists 8 observables: $x_{1...4}$ and $y_{1...4}$ (location of $R_{1...4}$) There also exists 8 manipulables: ${u_{1...4}}^x$ and ${u_{1...4}}^y$ (velocity of $R_{1...4}$). Thus, we can augment all the equations into a single state-space equation (in the form of equation 15) that shows the causal structure of the task-environment as follows

$$X(t) := IX(t-1) + IT_S U(t-1). \tag{18}$$

where I is an 8*8 identity matrix, $U = [{u_1}^x, {u_1}^y, ..., {u_4}^x, {u_4}^y]$ is the control input vector, and $X = [x_1, y_1, ..., x_4, y_4]$ is the state vector. Equation (18) simply means that the current position of a robot is only caused by previous position and previous velocity (applied control input) of *that robot*. In other words, the movement of a robot has no causal influence on the movement of other robots. We expect our algorithm to learn this invariant causal model while it intervenes on variables. Before the controller starts its learning process, it estimates an initial correlational model. The estimated model is A and B matrices of equation (11), in which all matrix elements are correlated (e.g. x_1 is correlated with x_2, which must not be the case, due to the fact that the movement of R_1 is independent of the movement of R_2). Thus, the controller must perform causal interventions to remove those non-direct-cause correlations from A and B matrices by replacing zeros with relevant non-zero values, and eventually converge to causal A and B, which both are identity matrices in this example.

5.1 Results

Using algorithm 1, the robots perform intervention 1 (equation 6) and intervention 2 (equation 7) to discover the aforementioned causal structure. Detecting a causal influence of an intervened variable - which could be either an observable or a manipulable - on other observable variables is done by inspecting the distribution changes of trajectory of observables, through maximum mean discrepancy (MMD) method proposed by [1]. If after an intervention, MMD of an observable becomes zero, then there is no causal influence from intervened variable on the observable, which makes the algorithm remove the related non-direct-cause correlation from A and B matrices and update the matrices via grey-box modeling method. The utilized grey box modeling is nonlinear least squares with automatically chosen line search method. Eventually, when all non-direct-cause correlations are removed and matrices are updated accordingly, the controller ends up having an invariant causal model of the task that is generalizable to different scenario/tasks. In other words, the learned causal model is successful when it is tested not only by novel initial conditions and input trajectories, but also by different tasks in the same environment. Figure (2, left) shows the Rendezvous task, in which the robots move from novel locations (initial conditions) to $(x, y) = (0, 0)$, by a feedback controller that uses the obtained causal model.

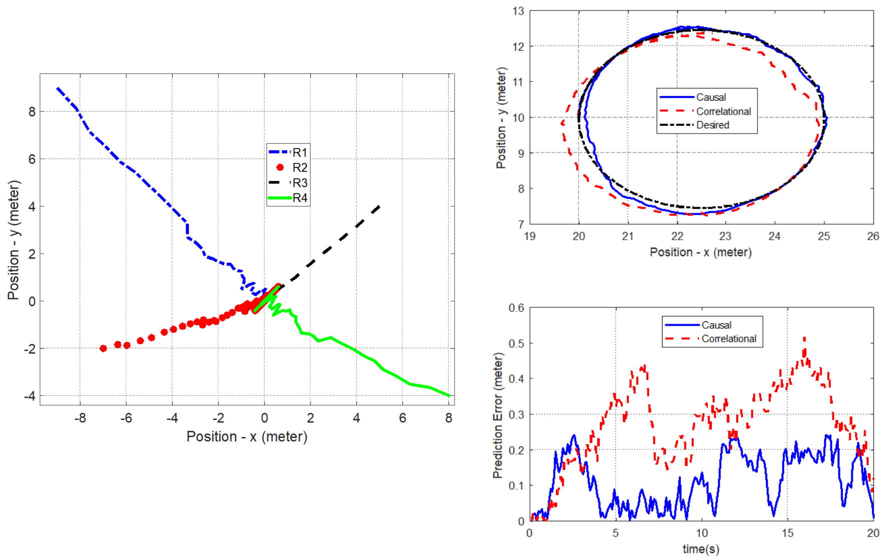

Fig. 1. Left: Performance of the four robots in performing the Rendezvous task, using a learned causal model. The robots start from novel locations in the observation space and reach $(x, y) = (0, 0)$, showing successful transfer. **Right**: A comparison between predictions of causal and correlational models for a single robot, showing the former's superiority; the robot uses both to trace a circular path.

As can be seen, the causal model enables the robots to achieve the goal of the task in a scenario that was not experienced over training. Figure 1 (right) shows a circular path followed by one of the robots via *the same causal model* that was learned in experiment 1 and a correlational model that was learned in the beginning of the training. The path requires a novel input trajectory and thus, correlational model is considerably less capable of making correct predictions compared to the causal one. The figure in the bottom shows squared prediction errors of both models. To sum up, the experimental results show that the causal model is a task-independent knowledge representation that is more transferable to novel situations/tasks and can also solve the covariate shift problem.

6 Conclusions

We have proposed a causal learning and generalization method for dynamical tasks. The algorithm performs causal interventions on observable and manipulable variables, based on which it removes non-direct-cause correlations and updates the controller's model after every intervention. The results in different dynamical tasks show that the algorithm enables the controller to learn a task-independent causal model, which can be generalized to novel scenarios.

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