Identifying Causal Structure in Dynamical Systems

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Abstract

We present a method for automatically identifying the causal structure of a dynamical control system. Through a suitable experiment design and subsequent causal analysis, the method reveals, which state and input variables of the system have a causal influence on each other. The experiment design builds on the concept of controllability, which provides a systematic way to compute input trajectories that steer the system to specific regions in its state space. For the causal analysis, we leverage powerful techniques from causal inference and extend them to control systems. Further, we derive conditions that guarantee discovery of the true causal structure of the system and show that the obtained knowledge of the causal structure reduces the complexity of model learning and yields improved generalization capabilities. Experiments on a robot arm demonstrate reliable causal identification from real-world data and extrapolation to regions outside the training domain.

1 Introduction

Modern control systems, such as mobile robots, are envisioned to autonomously act in the real world and to interact with their environment. Since not all situations they may encounter can be foreseen at design time, these systems need to be able to generalize and to transfer obtained knowledge to new problem settings. However, such capabilities are a particular weakness of current machine learning methods [41]. One reason for this is that most machine learning methods only learn correlations. Correlation-based analyses will typically find spurious correlations, which can lead to catastrophic errors when extrapolating outside the training data. Causal learning is seen as a building block towards realizing systems that can adapt and generalize to new tasks [34].

To define causality, mainly two notions are of practical relevance [13]. The first is *temporal precedence*: causes precede their effects. This is also what is understood as causality in systems theory [18, p. 31]. However, here, we mainly focus on the second notion, *physical influence*: manipulating causes changes the effects. In other words, we seek experimental routines and tests that enable control systems to learn, (i) what is the influence of their internal states on one another, and (ii) which of their inputs influence which internal states.

In causal inference, much work has been devoted to inferring causal structure from given data [29]. For control systems, solely relying on given data is not necessary. Such systems are equipped with an input, which they can use to actively conduct experiments for causal inference. Causal inference from experiments, or interventions, has also been studied, most prominently in the context of the do-calculus [33]. However, there it is assumed that state variables can be directly influenced by the input, which is often not possible in control systems. Different from those works, we consider a notion of *controllability*, i.e., how the system can be steered to particular regions in the state space through appropriate input trajectories. Causal relations between variables of a control system should become visible in the mathematical model describing its dynamics. Obtaining such models has

extensively been studied in system identification [22, 42] and in model learning [30]. However, those methods typically use correlation-based analyses to fit a model to data, which unfortunately forces them to usually find spurious correlation. A causal analysis can reveal such spurious correlations and remove corresponding model parameters, thus reducing the parameter space and enhancing the generalization capabilities of the model. In this work, we propose to combine experiment design via the notion of controllability with causal analysis. Combining these powerful concepts from systems theory and causal learning, we obtain a method that identifies the causal structure of control systems and thus improves generalization capabilities and reduces computational complexity.

Contributions. We present an algorithm that identifies a dynamical control system's causal structure through an experiment design based on a suitable controllability notion and a subsequent causal analysis. For the causal analysis, we leverage powerful kernel-based statistical tests based on the maximum mean discrepancy (MMD) [17]. Since the MMD has been developed for independent and identically distributed (i.i.d.) data, we extend it by deriving conditions under which the MMD still yields valid results and by coming up with a test statistic for hypothesis testing, despite non-i.i.d. data. In terms of controllability, we investigate three different settings: (i) exact controllability, where we can exactly steer the system to a desired position, (ii) stochastic controllability, where we can only steer the system to an ϵ -region around the desired position, and (iii) the special case of linear systems with Gaussian noise that are controllable in the sense of Kalman. We demonstrate the applicability of the proposed method by automatically identifying the causal structure of a robotic system. Further, for this system, we show improved generalization capabilities inherited through the causal identification.

2 Related Work

This paper presents a novel technique for automatically identifying the causal structure of a dynamical system based on MMD statistical tests. In this section, we relate the contribution to the literature.

Causal inference for dynamical systems. Causal inference in dynamical systems or time series has been studied in [11, 12, 27, 24] using vector autoregression, in [36] based on structural equation models, in [14], using the fast causal inference algorithm [49] and in [8] and [38], applying kernel mean embeddings and directed information, respectively. None of the mentioned references investigates experiment design. Instead, they aim at inferring the causal structure from given data.

Experiment design. A well-known concept for causal inference from experiments is the do-calculus. In the basic setting, a variable is clamped to a fixed value, and the distribution of the other variables conditioned on this intervention is studied [33]. Extensions to more general classes of interventions exist, see, e.g., [56, 46], but they consider static models, which is different from the dynamical systems studied herein. Causal inference in dynamical systems or time series with interventions has been investigated in [13, 35, 28, 40, 48]. However, therein it is assumed that one can directly manipulate the variables, e.g., by setting them to fixed values or forcing them to follow a trajectory. None of those works considers various degrees of controllability, which is the case in this paper.

Model selection. An alternative to directly testing causal relations between variables is to choose between a set of candidate models. Such algorithms have been developed in system identification. Well-known examples are the Akaike information criterion [2] and the Bayesian information criterion [43]. In neuroimaging, there are dynamic causal models [15, 52]. In both cases, the methods can only find the true causal structure if such a model is part of the set of candidate models.

Structure detection in dynamical systems. Revealing causal relations in a dynamical system can be interpreted as identifying its structure. Related ideas exist in the identification of hybrid and piecewise affine systems [39, 20]. These approaches try to find a trade-off between model complexity and fit, but cannot guarantee to find the true causal structure. Further methods that identify structural properties of dynamical systems can be found in topology identification [25, 45, 54] and complex dynamic networks [5, 21, 57]. Those works seek to find interconnections between subsystems instead of identifying the inner structure of a system as done herein. Moreover, while the mentioned works often rely on restrictive assumptions such as known interconnections or linear dynamics, our approach can deal with nonlinear systems and does not require prior knowledge.

Kernel mean embeddings. For causal inference, we will leverage concepts based on kernel mean embeddings, which have been widely used for causal inference [37, 7, 23]. A downside of those

methods is that they typically assume that data has been drawn i.i.d. from the underlying probability distributions. Extensions to non-i.i.d. data exist [9, 10], but rely on mixing time arguments. Dynamical systems, as investigated in this work, often have large mixing times or do not mix at all [47]. Therefore, these types of analyses are not sufficient in this case.

3 Problem Setting and Main Idea

We consider dynamical control systems of the form

$$x(t) = f(x(0), u(0:t), v(0:t))$$
(1)

with discrete time index $t \in \mathbb{N}$, state $x(t) \in \mathcal{X} \subset \mathbb{R}^n$, state space \mathcal{X} , input $u(t) \in \mathcal{U} \subset \mathbb{R}^m$, input space \mathcal{U} , and $v(t) \in \mathbb{R}^n$ an independent random variable sequence. The notation (0:t) here denotes the whole trajectory from 0 to t. In the following, we will omit this notation and simply write u or v if we consider the whole trajectory. The description of the system in (1) is different from the standard, incremental version $x(t+1) = \tilde{f}(x(t), u(t), v(t))$. Specifically, (1) emphasizes the dependence of x at time t on the initial state. Equation (1) can be obtained from \tilde{f} . Based on (1), we define non-causality for state and input components by adapting the definition given in [55]:

Definition 1 (Global non-causality). The state variable x_j does not cause x_i if $x_i(t) = f_i(x_{1,...,n\setminus j}(0),x_j^{\mathrm{I}}(0),u,v) = f_i(x_{1,...,n\setminus j}(0),x_j^{\mathrm{II}}(0),u,v)$ for all $x_j^{\mathrm{I}}(0),x_j^{\mathrm{II}}(0)$. Similarly, u_j does not cause x_i if $x_i(t) = f_i(x(0),u_{1,...,m\setminus j},u_j^{\mathrm{I}},v) = f_i(x(0),u_{1,...,m\setminus j},u_j^{\mathrm{II}},v)$ for all $u_j^{\mathrm{I}},u_j^{\mathrm{II}}$.

For causal inference, we will exploit that we can influence (1) through u. To make the notion of how we can influence the system precise, we adopt controllability definitions for stochastic systems [53, 4]:

Definition 2. The system (1) is said to be completely ϵ -controllable in probability η in the normed square sense in the time interval $[0,t_{\rm f}]$ if for all desired states $x_{\rm des}$ and initial states x(0) from \mathcal{X} , there exists an input sequence u from \mathcal{U} such that $\Pr\{\|x(t_{\rm f})-x_{\rm des}\|_2^2 \geq \epsilon\} \leq 1-\eta$, with $0<\eta<1$.

A variety of methods exist to identify or learn models for systems (1), e.g., Gaussian process regression or fitting linear state space models using least squares. In the following, we assume that we can obtain an estimate \hat{f} of the investigated system (1) (including an estimate of the distribution of v(t)) using correlation-based analyses. Which method is used is irrelevant for the developed causal identification procedure. This model estimate \hat{f} , obtained without further assumptions or physical insights, will almost surely entail spurious correlation and suggest causal influences that are actually not present in the physical system. But it will allow us to (approximately) steer the system to specific initial conditions and start experiments from there.

We propose two types of experiments to test for causal relations. For the first type, we investigate whether x_j causes x_i . We conduct two experiments (denoted by I and II) with different initial conditions $x_j^{\rm I}(0) \neq x_j^{\rm II}(0)$, while all others are kept the same (cf. Fig. 1). This can be formalized as:

$$x_{\ell}^{\mathrm{I}}(0) = x_{\ell}^{\mathrm{II}}(0) \,\forall \ell \neq j, \quad x_{i}^{\mathrm{I}}(0) \neq x_{i}^{\mathrm{II}}(0) \quad u_{\ell}^{\mathrm{I}}(t) = u_{\ell}^{\mathrm{II}}(t) \,\forall \ell, t.$$
 (2a)

By comparing the resulting trajectories of $x_i^{\rm I}$ and $x_i^{\rm II}$ we can then check whether the change in $x_j(0)$ caused a different behavior. For checking the similarity of trajectories, we will use the MMD, whose mathematical definition we provide in the next section. The second type of experiments is analogous to the first, but instead of varying initial conditions, we consider different input trajectories $u_i^{\rm I} \neq u_i^{\rm II}$,

$$x_{\ell}^{\mathrm{I}}(0) = x_{\ell}^{\mathrm{II}}(0) \, \forall \ell \quad u_{\ell}^{\mathrm{I}}(t) = u_{\ell}^{\mathrm{II}}(t) \, \forall \ell \neq j, t, \quad u_{j}^{\mathrm{I}}(t) \neq u_{j}^{\mathrm{II}}(t) \, \forall t. \tag{2b}$$

In the remainder, we address the following problems: (i) we derive conditions that guarantee a valid test and present an approach for obtaining a test statistic for the MMD despite non-i.i.d. data; (ii) we make the experiment design precise and incorporate the fact that we cannot exactly steer the system to specific initial conditions; (iii) we demonstrate the applicability of the method on a robotic system.

4 Causal Identification for Dynamical Systems

We will now develop the causality testing procedure. First, we introduce the MMD [17], which we shall use as a measure of similarity. The MMD can be used to check whether two probability

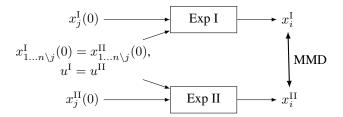


Figure 1: Experiment design for causal inference. We design two experiments, where all initial conditions and input trajectories are constant except for $x_j(0)$. If the resulting trajectory of x_i differs in both experiments, we have evidence that the change in $x_j(0)$ caused this change.

distributions \mathbb{P} and \mathbb{Q} are equal based on samples drawn from these distributions. Let X and Y be samples drawn i.i.d. from \mathbb{P} and \mathbb{Q} , respectively. Further, let \mathcal{H} be a *reproducing kernel Hilbert space* [50], with canonical feature map $\phi: \mathcal{X} \to \mathcal{H}$. The MMD is defined as

$$MMD(\mathbb{P}, \mathbb{Q}) = \|\mathbb{E}_{X \sim \mathbb{P}}[\phi(X)] - \mathbb{E}_{Y \sim \mathbb{Q}}[\phi(Y)]\|_{\mathcal{H}}.$$
 (3)

The feature map ϕ can be expressed in terms of a kernel function $k(\cdot, \cdot)$, where $k(x, y) = \langle \phi(x), \phi(y) \rangle_{\mathcal{H}}$. If the kernel is characteristic, we have $\mathrm{MMD}(\mathbb{P}, \mathbb{Q}) = 0$ if, and only if, $\mathbb{P} = \mathbb{Q}$ [16, 51]. In the remainder of the paper, we always assume a characteristic kernel (e.g., the Gaussian kernel).

In the following, we derive conditions that allow one to provably identify causal relations. We investigate three settings. First, we discuss the case where we can exactly steer the system to desired initial conditions (i.e., $\epsilon = 0$ in Definition 2). We then extend this to $\epsilon \neq 0$, which requires us to provide a stricter controllability definition. Finally, we show that for linear systems with additive Gaussian noise, the conditions stated by Kalman [19] are sufficient, and the identification is substantially easier.

4.1 Exact Controllability

When considering control systems, data is highly correlated, and instead of stationary distributions, we are dealing with random processes as in (1). We design experiments of fixed length T. Thus, we have a sequence of T random variables, sampled at discrete intervals of fixed length, with joint distribution $\mathbb{P}(x) = \mathbb{P}(x(0), \dots, x(T))$. For these sequences, the MMD reads

$$\mathrm{MMD}(x^{\mathrm{I}}, x^{\mathrm{II}}) = \|\mathbb{E}_{x^{\mathrm{I}} \sim \mathbb{P}^{\mathrm{I}}(x^{\mathrm{I}})}[\phi(x^{\mathrm{I}})] - \mathbb{E}_{x^{\mathrm{II}} \sim \mathbb{P}^{\mathrm{II}}(x^{\mathrm{II}})}[\phi(x^{\mathrm{II}})]\|_{\mathcal{H}}. \tag{4}$$

If we now design experiments (2), we can check the similarity of x_i trajectories using (4). An MMD > 0 then suggests that trajectories are different, so we can conclude that there is a causal influence. However, the other direction is less straightforward: for a system (1), the MMD may be 0, even though variables are dependent, as can be seen in the following example:

Example 1. Assume a control system with $x_1(t+1) = x_1(t)x_2(t)$ and $x_2(t+1) = u(t)$, and an input signal u(t) that is different from 0. If we choose $x_1(0) = 0$, the trajectory of x_1 will, despite the fact that x_2 clearly has a causal influence on x_1 , always be 0 no matter the initial condition $x_2(0)$.

To address this, we define the concept of local non-causality:

Definition 3 (Local non-causality). The state variable x_j does locally not cause x_i if $x_i(t) = f_i(x_{1,\dots,n\setminus j}(0),x_j^{\rm I}(0),u,v) = f_i(x_{1,\dots,n\setminus j}(0),x_j^{\rm II}(0),u,v)$ given that x in $\mathcal{X}_{\rm ind}$ and u in $\mathcal{U}_{\rm ind}$, where $\mathcal{X}_{\rm ind}\subseteq\mathcal{X}$ and $\mathcal{U}_{\rm ind}\subseteq\mathcal{U}.^1$ Similarly, u_j does locally not cause x_i if $x_i(t)=f_i(x(0),u_{1,\dots,m\setminus j},u_j^{\rm I},v)=f_i(x(0),u_{1,\dots,m\setminus j},u_j^{\rm II},v)$ given that x in $\mathcal{X}_{\rm ind}$ and u in $\mathcal{U}_{\rm ind}$.

The non-causality becomes global if $\mathcal{X}_{\mathrm{ind}} = \mathcal{X}$ and $\mathcal{U}_{\mathrm{ind}} = \mathcal{U}$. Similar notions have, under the term local independence, been discussed in [44, 1, 26]. We make the following assumption about the system (1) and the estimated model \hat{f} :

Assumption 1. For the system (1) it holds that either all non-causalities are global, or the local non-causalities are reflected by the estimated model \hat{f} . We say that local non-causalities are reflected

¹In general, there may exist different $\mathcal{X}_{\text{ind}}^{ij}$ for each combination of x_i and x_j (and likewise for \mathcal{U}_{ind}). We can also cover this case. However, we omit it here to simplify notation.

by the model \hat{f} if the following holds: for experiments designed according to (2), $\mathrm{MMD}(\hat{x}_i^{\mathrm{I}}, \hat{x}_i^{\mathrm{II}} | \hat{f}) < \mathrm{MMD}(\hat{x}_i^{\mathrm{II}}, \hat{x}_i^{\mathrm{IV}} | \hat{f})$ if \hat{x}_i^{I} and \hat{x}_i^{II} are inside $\mathcal{X}_{\mathrm{ind}}$ and the corresponding inputs are in $\mathcal{U}_{\mathrm{ind}}$, while \hat{x}_i^{III} and \hat{x}_i^{IV} and their corresponding inputs take values outside these sets. $\mathrm{MMD}(\hat{x}_i^{\mathrm{I}}, \hat{x}_i^{\mathrm{II}} | \hat{f})$ denotes the MMD of simulated \hat{x}_i trajectories based on the model \hat{f} .

That is, we do not require that \hat{f} captures the causal structure. But we require that simulated trajectories in regions of local non-causality have a smaller MMD than trajectories in other regions.

Example 1 (cont). Given Assumption 1, if we simulate experiments (2a) and compute the MMD for the resulting \hat{x}_1 , the MMD will be lower if we choose $\hat{x}_1(0) = 0$ than for any other choice of $\hat{x}_1(0)$.

We now specify the experiment design. To avoid regions of local non-causality, we propose to maximize the MMD given the model estimate. Thus, for checking whether x_j causes x_i , we choose input trajectories of length T and initial conditions that solve

$$\max_{x^{\mathrm{I}}(0), x^{\mathrm{II}}(0), u^{\mathrm{I}}, u^{\mathrm{II}}} \mathrm{MMD}(\hat{x}_{i}^{\mathrm{I}}, \hat{x}_{i}^{\mathrm{II}} | \hat{f}) \quad \text{subject to} \quad x_{\ell}^{\mathrm{I}}(0) = x_{\ell}^{\mathrm{II}}(0) \ \forall \ell \neq j \quad u_{\ell}^{\mathrm{I}}(t) = u_{\ell}^{\mathrm{II}}(t) \ \forall \ell, t. \quad (5\mathrm{a})$$

We will discuss how to handle this optimization problem in practice in Sec. 5.2. If we want to check whether u_i causes x_i , we choose input trajectories and initial conditions by solving

$$\max_{x^{\mathrm{I}}(0), x^{\mathrm{II}}(0), u^{\mathrm{I}}, u^{\mathrm{II}}} \mathrm{MMD}(\hat{x}_{i}^{\mathrm{I}}, \hat{x}_{i}^{\mathrm{II}} | \hat{f}) \quad \text{subject to} \quad x_{\ell}^{\mathrm{I}}(0) = x_{\ell}^{\mathrm{II}}(0) \ \forall \ell \quad u_{\ell}^{\mathrm{I}}(t) = u_{\ell}^{\mathrm{II}}(t) \ \forall \ell \neq j, t. \quad (5b)$$

We can now state the main theorem:

Theorem 1. Assume a completely ϵ -controllable system (1) with $\epsilon = 0$ that fulfills Assumption 1. Let experiments be designed according to (5) for a fixed experiment length $T < \infty$ and repeated infinitely often (i.e., we collect an infinite amount of realizations of two random processes). Then: $\mathrm{MMD}(x_i^{\mathrm{I}}, x_i^{\mathrm{II}}) = 0$ if, and only if, variables are non-causal according to Definition 1.

Proof. Let variables be non-causal. Then, the distribution of x_i in both experiments is equal. Thus, $\mathrm{MMD}(x_i^{\mathrm{I}}, x_i^{\mathrm{II}}) = 0$ follows from [17]. Now, assume $\mathrm{MMD}(x_i^{\mathrm{I}}, x_i^{\mathrm{II}}) = 0$. This implies that the distribution of x_i is equal in both experiments [17]. By Assumption 1, the model reflects local non-causalities (if they exist). In that case, the optimization (5) ensures that we collect data outside of such regions. Thus, if distributions are equal, non-causality must be global as defined in Definition 1. \square

Remark 1. The probability distribution can become independent of the initial conditions over time if the process is stable. Causal influences are then only visible during the transient. Thus, doing multiple short experiments is, in general, preferred over one long experiment. Also, in the case of non-ergodic systems, where time and spatial average are not the same, we only have a valid testing procedure if we do multiple runs of each experiment.

4.2 ϵ -Controllability

For a stochastic system as in (1), it is in general impossible to steer the system exactly to the initial conditions suggested by (5); i.e., we need to resort to controllability with $\epsilon > 0$ (cf. Def. 2). But even in such cases, it is still possible to guarantee the consistency of the causality testing procedure. However, we need a stricter definition of controllability.

Definition 4. Let system (1) be controllable according to Definition 2, and consider some arbitrary, but fixed $x^*_{\ell,\mathrm{des}}$. Then, the system (1) is said to be completely ϵ -controllable in distribution if, for any x(0) and any x_{des} with $x_{\ell,\mathrm{des}} = x^*_{\ell,\mathrm{des}}$, there exists an input sequence $u(0:t_{\mathrm{f}})$ such that $x_{\ell}(t_{\mathrm{f}})$ always follows the same distribution; i.e., $P(x_{\ell}(t_{\mathrm{f}})) = P^*$ for some P^* that does not depend on x(0) or any component of x_{des} except $x_{\ell,\mathrm{des}} = x^*_{\ell,\mathrm{des}}$.

In other words, the definition states that, for any x(0), we can generate input trajectories that guarantee that the fixed component $x_{\ell,\mathrm{des}}^*$ of x_{des} is matched in distribution. Linear systems with additive Gaussian noise that are controllable following [19] are also controllable in the sense of Definition 4, as we show in the supplementary material. We further need to assume that connected regions without local non-causalities have a radius of at least $\sqrt{\epsilon}$ to be able to steer the system to those regions.

Assumption 2. For all connected subsets $\mathcal{X}_{i,\text{con}}$ of $\mathcal{X} \setminus \mathcal{X}_{\text{ind}}$, we assume that for all $x \in \mathcal{X}_{i,\text{con}}$, there exists an n-dimensional sphere with radius at least $\sqrt{\epsilon}$ that includes x and that is inside $\mathcal{X}_{i,\text{con}}$.

This assumption is needed to exclude corner cases in which the causal influence only exists in single points of the state and input space. In such cases, the probability of successfully steering the system to those points is 0. However, considering the variables as non-causal may then anyway be reasonable. Equipped with these two assumptions, we can now state:

Corollary 1. Assume a system (1) that is completely ϵ -controllable in distribution according to Definition 4 and fulfills Assumptions 1 and 2. Let experiments be designed as in (5) for a fixed experiment length $T < \infty$, trajectories that steer the system to the initial conditions of the experiments be chosen such that $P(x_{\ell}^{\mathrm{I}}(0)) = P(x_{\ell}^{\mathrm{II}}(0)) \ \forall \ell \neq j$, and experiments be repeated infinitely often. Then: $\mathrm{MMD}(x_{i}^{\mathrm{I}}, x_{i}^{\mathrm{II}}) = 0$ if, and only if, variables are non-causal according to Definition (1).

Proof. Let variables be non-causal. Then, we have $P(x_\ell^{\rm I}(0)) = P(x_\ell^{\rm II}(0)) \, \forall \ell \neq j$, thus, also the distribution of the obtained x_i trajectories is equal and we have ${\rm MMD}(x_i^{\rm I}, x_i^{\rm II}) = 0$ [17]. Now, assume ${\rm MMD}(x_i^{\rm I}, x_i^{\rm II}) = 0$. This implies that the distribution of x_i is equal in both experiments [17]. By Assumption 1, existing local non-causalities are reflected by the model and thus, (5) will suggest experiments outside of such regions. Assumption 2 ensures that we can steer the system to those regions. Thus, if distributions are equal, non-causality must be global as in Definition 1.

4.3 Linear Systems

Local non-causality as in Definition 3 is a nonlinear phenomenon. If we assume (1) to be linear time-invariant (LTI) with Gaussian noise v(t), we can reveal the true causal structure without the optimization procedure (5), making this case substantially easier. For an LTI system, (1) reads

$$x(t) = A^{t}x(0) + \sum_{i=0}^{t-1} A^{i}(Bu(t-1-i) + v(t-1-i)),$$
(6)

with state transition matrix $A \in \mathbb{R}^{n \times n}$, input matrix $B \in \mathbb{R}^{n \times m}$, and $v(t) \sim \mathcal{N}(0, \Sigma)$. The system (6) is controllable as per Definition 4 if it satisfies the classical controllability condition from [19], i.e., if the matrix $\begin{pmatrix} B & AB & \dots & A^{n-1}B \end{pmatrix}$ has full row rank, as we show in Lemma 1 in the appendix. We can then state the following theorem, whose proof is provided in the supplementary material:

Theorem 2. Assume an LTI system (6), whose deterministic part is controllable in the sense of Kalman. Let experiments be designed as in (2a) and (2b), respectively. Then: $\mathrm{MMD}(x_i^{\mathrm{I}}, x_i^{\mathrm{II}}) = 0$ if, and only if, the variables are non-causal as per Definition 1.

5 Implementation

The results in Sec. 4 show that we are able to detect whether the variables x_j or u_j have a causal influence on x_i . In practical implementations, two challenges remain: first, we can only collect a finite amount of data and, thus, need an approximation of the MMD and a test statistic. Second, we may not be able to obtain a global solution to (5).

5.1 Test with Finite Samples

Given m samples of X and Y (with $m < \infty$), the squared MMD can be approximated as [17]

$$MMD^{2}(X,Y) \approx \frac{1}{m(m-1)} \sum_{i \neq j}^{m} (k(x_{i}, x_{j}) + k(y_{i}, y_{j}) - k(x_{i}, y_{j}) - k(x_{j}, y_{i})).$$
(7)

For a finite sample size m, the MMD will, in general, not equal 0 if distributions are equal. Obtaining a test statistic for the MMD valid for control systems (1) is non-trivial. Here, we exploit that we can obtain an estimate of the model and its uncertainty. We estimate a model $\hat{f}_{i,\text{ind}}$ that assumes x_i and x_j respectively u_j are non-causal (i.e., we do not use the data x_j respectively u_j when estimating $\hat{f}_{i,\text{ind}}$). We propose to use this model to decide whether to accept the null hypothesis of x_i and x_j respectively u_j being non-causal and, thus, update the current model estimate \hat{f} :

$$\hat{f}_i = \hat{f}_{i,\text{ind}} :\Leftrightarrow \text{MMD}^2(x_i^{\text{I}}, x_i^{\text{II}}) < \mathbb{E}[\text{MMD}^2(\hat{x}_i^{\text{I}}, \hat{x}_i^{\text{II}}) | \hat{f}_{i,\text{ind}}] + \nu \sqrt{\text{Var}[\text{MMD}^2(\hat{x}_i^{\text{I}}, \hat{x}_i^{\text{II}}) | \hat{f}_{i,\text{ind}}]}. \tag{8}$$

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Algorithm 1: Pseudocode of the proposed framework.
 1: Excite system with input signal, collect data
 2: Obtain \hat{f} through black-box system identification
3: for x_j in x do
         x_{\text{test}} = [x_1, \dots, x_n]
 5:
         for x_\ell in x_{\text{test}} do
             Run (5a) until \mathbb{E}[\text{MMD}^2(\hat{x}_{\ell}^{\text{I}}, \hat{x}_{\ell}^{\text{II}}|\hat{f})] > \delta_1
 6:
7:
             Run causal experiments, collect data
 8:
             for x_i in x_{\text{test}} do
                 if \mathbb{E}[\text{MMD}^2(\hat{x}_i^{\text{I}}, \hat{x}_i^{\text{II}}|\hat{f})] > \delta_2 then
9:
10:
                     Obtain \hat{f}_{i,ind}
                     Obtain test statistic via Monte Carlo simulations
11:
12:
                     if (8) holds then
13:
                          f_i = f_{i,\text{ind}}
```

Delete x_i from x_{test}



Figure 2: The robotic system showing initial postures for two experiments.

Expected value and variance in (8) can be estimated through Monte Carlo simulations. For these simulations, we use the true initial conditions $x^{\rm I}(0)$ and $x^{\rm II}(0)$, that way accounting for uncertainty due to unequal initial conditions between experiments. The significance level of the test can be adjusted through ν using Chebyshev's inequality [6].

5.2 Experiment Design

14:

The framework for testing causality between state variables is summarized in Alg. 1 (and works analogously for inputs)². After having obtained an initial model (Il. 1-2), we run (5a) to find initial conditions and input trajectories for testing non-causality of one specific combination of x_{ℓ} and x_{j} (l. 6). The optimization in (5a) may be arbitrarily complex or even intractable, depending on the chosen model class. However, finding a global optimum of (5a) is not necessary. The goal of the optimization procedure is to avoid regions of local non-causality. We thus optimize (5a) until it is above a threshold δ_1 to be confident that we are not in a region of local non-causality. In practical applications, we can often already achieve this through a reasonable initialization of the optimization problem, i.e., by choosing initial conditions for x_j as far apart as possible. We then run the designed experiment and collect the data (l. 7). Ideally, we would like to use data from this single experiment to test for causal influence of x_j on all other state components. Thus, we check for which x_i the experiment yields an expected MMD that is higher than a second threshold δ_2 and do the hypothesis test for all of those (Il. 9-13).

6 Robot Experiments

We evaluate the framework by identifying the causal structure of one arm of the robot in Fig. 2. We consider kinematic control of the robot; that is, we can command desired angular velocities to the joints, which are then tracked by low-level controllers (taking care, i.a., of the robot dynamics). As measurements, we receive the joint angles. The goal of the causal identification is to learn which joints influence each other, and which joints are influenced by which inputs. We consider four joints of the robot arm in the following experiments. From the robot arm's design, we know its kinematic structure, which is described by $\dot{\phi}_i = \tau_i$ for each joint, where ϕ_i denotes the angle of joint i and t the applied motor torque. That is, we expect each joint velocity $\dot{\phi}_i$ to depend only on the local input t and not other variables. While the dynamics are approximately linear, we do not rely on this information and are thus in the setting discussed in Sec. 4.2. In the following, we will investigate if our proposed causal identification can reveal this structure automatically. For this, we describe the setting and discuss the results, while we defer implementation details to the supplementary material.

Following Alg. 1, we start by identifying a model \hat{f} . As expected, the initial model suggests that all joints are linked to each other and to all inputs owing to spurious correlations. We then design

²An implementation is available at https://github.com/baumanndominik/identifying_causal_structure.

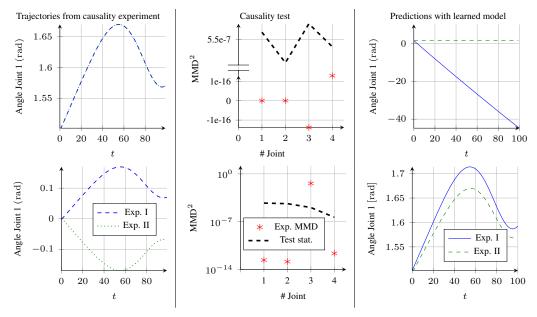


Figure 3: Causality tests and model evaluation. Plots on the left show example trajectories of two experiments, in the middle the experimental MMD and the test threshold for joint 3, and on the right predictions based on the initial model and on the refined model after the causal identification.

experiments for causality testing, example trajectories of such experiments are shown in Fig. 3 (left). The empirical squared MMD of the resulting trajectories is compared with the test statistic. The trajectories in Fig. 3 (left) already suggest that the experiments are in line with the kinematic model: while the two trajectories of joint 1 for different initial conditions of joint 3 are essentially equal (blue dashed and green dotted lines overlap), the trajectories of joint 3 for different choices of the third input are fundamentally different. This is also revealed through the proposed causality test. The middle plots of Fig. 3 show the empirical squared MMD (left-hand side of inequality (8)) and the test threshold (right-hand side of (8)) for the experiments that were conducted to test the influence of the initial conditions of the third joint (top) and of the third input signal (bottom) on all joints. As can be seen, the causal identification reveals that the third joint does not influence any other joint, and the third input only affects the third joint. Note that the trajectories of the third joint are obviously different when we choose different initial conditions for the third joint. However, since this is expected, we subtract the initial condition in this case to investigate whether the movement starting from these distinct initial conditions differs. The remaining experiments (results are contained in the supplementary material) yield similar results. In summary, the causal identification successfully reveals the expected causal structure.

To investigate the generalization capability, we compare predictions of the model $\hat{f}_{\rm init}$ obtained from the initial system identification and the model $\hat{f}_{\rm caus}$ that was learned after revealing the causal structure. In both cases, we use the same training data to estimate the model parameters. However, for $\hat{f}_{\rm caus}$, we leverage the obtained knowledge of the causal structure when estimating parameters, while for $\hat{f}_{\rm init}$ we do not take any prior knowledge into account. As test data, we use an experiment that was conducted to investigate the influence of the initial condition of joint 3 on the other joints and let both models predict the trajectory of joint 1. For this experiment, the initial angle of joint 3 is close to its maximum value, a case that is not contained in the training data. As can be seen in Fig. 3 (right), the predictions of $\hat{f}_{\rm caus}$ (blue) are very close to the true data (green, dashed), i.e., the model can generalize well, while the predictions of $\hat{f}_{\rm init}$ deviate significantly.

7 Conclusion

We presented a method that identifies the causal structure of dynamical control systems by conducting experiments and analyzing the generated data with the MMD. It differs from prior approaches to

causal inference in that it uses a controllability notion that is suitable to design experiments for control systems. We evaluated the method on a real-world robotic system. Our algorithm successfully identified the underlying causal structure, which in turn allowed us to learn a model that accurately generalizes to previously unseen states. For ease of trying out our method, we also provide a synthetic example with code in the supplementary material.

Broader Impact

In this paper, we propose a method for learning more reliable models for dynamical control systems. In particular, we enable control systems to learn about their causal structure, which results in better generalization capabilities. The method can thus help in improving the performance of autonomous systems when letting them explore their environment. This work can thus be seen as a contribution towards building more reliable and trustworthy autonomous systems, such as mobile robots, with many envisioned use cases in the real world, which also includes issues of dual-use.

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A Proof of Theorem 2

An LTI system with Gaussian noise follows a normal distribution, whose mean is given by

$$x(t) = A^{t}x(0) + \sum_{i=0}^{t-1} A^{i}Bu(t-1-i)$$
(9)

and whose variance only depends on time and the variance of v(t) [32, Sec. 3.7], which we assume to be constant. For such systems, we will first show that if (9) obeys the controllability conditions stated by Kalman, the system is also controllable according to Definitions 2 and 4.

Lemma 1. The system (6) is completely ϵ -controllable in distribution if the deterministic part obeys the controllability condition stated in [19].

Proof. The expected value (9) represents the deterministic part of the system. Thus, according to [19], we can steer (9) to any point in the state space. The variance only depends on the number of time steps. Since we can steer the linear system to any point $x_{\rm des}$ in the state space in any amount of time steps, we can ensure that all trajectories are of equal length. Then, the distribution of the final state has mean $x_{\rm des}$ and a variance that depends on the chosen number of time steps. The probability of $\|x_i - x_{i,\rm des}\|_2^2$ being larger than ϵ is given by the cumulative distribution function of the normal distribution.

We can now prove Theorem 2. Since the variance of (6) solely depends on the number of time steps, which is equal for all experiments, distributions can only be different because of their means. We start with experiments that are designed according to (2a). In this case, for distributions to be equal, and, thus, for variables to be non-causal, we need

$$e_i \left(A^t x^{\mathrm{I}}(0) + \sum_{i=0}^{t-1} A^i (Bu(t-1-i)) \right) = e_i \left(A^t x^{\mathrm{II}}(0) + \sum_{i=0}^{t-1} A^i (Bu(t-1-i)) \right),$$

where $e_i \in \mathbb{R}^n$ is the unit vector (i.e., a vector with zeros and a single 1 at the ith entry). Since input trajectories are equal, this boils down to

$$e_i A^t x^{\mathrm{I}}(0) = e_i A^t x^{\mathrm{II}}(0).$$

Essentially this means that the component ij of A^t needs to be 0. This is clearly the case, if there is no influence of x_i on x_j , i.e., in case variables are non-causal, we have $\mathrm{MMD} = 0$. The event of component ij of the matrix exponential being 0 by chance, even though x_j has a causal influence on x_i , has probability 0. Thus, we have that variables are non-causal if $\mathrm{MMD} = 0$.

For experiments that are designed according to (2b), initial states are equal and, in case variables are non-causal, we have

$$e_i \sum_{i=0}^{t-1} A^i (Bu^{\mathrm{I}}(t-1-i)) = e_i \sum_{i=0}^{t-1} A^i (Bu^{\mathrm{II}}(t-1-i)).$$

Similar as before, we have equal distributions and, thus, $\mathrm{MMD}=0$ if entries in the A and B matrices relating x_i and u_j are 0, i.e., if there is no causal influence. The other direction holds since the event of the relevant entries of A and B being 0 by chance has probability 0.

B Experiment Details and Further Results

We first provide implementation details for the experiments presented in Sec. 6. The initial model estimate is obtained by exciting the system with a chirp signal for 30 s and using the generated data to learn a linear state-space model (cf. (6)) with least squares. The obtained matrices are

$$A_{\rm init} \approx \begin{pmatrix} 0.868 & -0.132 & 0.754 & -0.491 \\ -0.132 & 0.868 & 0.754 & -0.491 \\ -0.132 & -0.132 & 1.754 & -0.491 \\ -0.134 & -0.134 & 0.76 & 0.508 \end{pmatrix} \quad B_{\rm init} \approx \begin{pmatrix} 0.075 & -0.056 & -0.031 & 0.022 \\ 0.074 & -0.055 & -0.031 & 0.022 \\ 0.074 & -0.056 & -0.03 & 0.022 \\ 0.075 & -0.056 & -0.032 & 0.022 \end{pmatrix}$$

Initial conditions and input trajectories for the causality testing experiments are obtained through reasonable guesses, as discussed in Sec. 5.2. The found initial conditions and input trajectories yield expected MMDs that are orders of magnitude above the system's noise level for all joints. Thus, we do not need to fix variables δ_1 and δ_2 and, overall, only need 8 experiments to identify the causal structure. For each experiment, we design input trajectories of 100 time steps, repeat the experiment 10 times, and use collected data from all experiments for

Table 1: Results of the causal structure identification for a robot arm: Causal influences of joints on each other.

$\begin{array}{c} \text{Joint} \rightarrow \\ \text{Joint} \end{array}$	Experimental MMD	Test statistic
$x_1 \to x_1$	0	1.65×10^{-4}
$x_1 \to x_2$	0	1.79×10^{-4}
$x_1 \to x_3$	0	2.39×10^{-4}
$x_1 \to x_4$	2.43×10^{-13}	1.61×10^{-4}
$x_2 \to x_1$	0	5.6×10^{-7}
$x_2 \to x_2$	-2.8×10^{-18}	4.58×10^{-7}
$x_2 \to x_3$	0	3.56×10^{-7}
$x_2 \to x_4$	1.82×10^{-13}	6.91×10^{-7}
$x_3 \to x_1$	0	5.81×10^{-7}
$x_3 \to x_2$	0	4.54×10^{-7}
$x_3 \rightarrow x_3$	-1.38×10^{-18}	6.16×10^{-7}
$x_3 \rightarrow x_4$	1.29×10^{-16}	5.2×10^{-7}
$x_4 \to x_1$	0	4.99×10^{-7}
$x_4 \to x_2$	0	4.66×10^{-7}
$x_4 \rightarrow x_3$	9.63×10^{-15}	5.8×10^{-7}
$x_4 \rightarrow x_4$	-5.44×10^{-15}	5.8×10^{-7}

hypothesis testing. The empirical squared MMD is computed with a Gaussian kernel with a lengthscale of 1. While the squared MMD is always positive, the empirical approximation (7) can become negative since it is an unbiased estimate. For the test statistic (8), we estimate the variance using 100 Monte Carlo simulations and obtain the expected value through a noiseless simulation. We use $\nu=1$, but as we will see in the results, the empirical MMD is in all cases orders of magnitude below or above the threshold. Thus, also more conservative choices of ν would yield the same outcome.

In Tables 1 and 2, we present the results of all causality testing experiments conducted on the robotic platform shown in Fig. 2. As for the results discussed in Sec. 6, we always have a clear decision on whether to accept or reject the null hypothesis: The MMD found in experiments is always orders of magnitude larger or smaller than the test statistic. Also here, we find that all joints can be moved independently of each other and are affected by exactly one input. When exploiting the revealed causal structure for identifying the system matrices, we obtain

$$A_{\rm caus} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad B_{\rm caus} \approx \begin{pmatrix} 0.013 & 0 & 0 & 0 \\ 0 & 0.007 & 0 & 0 \\ 0 & 0 & 0.01 & 0 \\ 0 & 0 & 0 & 0.01 \end{pmatrix}.$$

C Synthetic Example and Code

In this section, we present a synthetic, linear example³. We consider an LTI system as in (6), with

$$A = \begin{pmatrix} 0.9 & -0.75 & 1.2 \\ 0 & 0.9 & -1.1 \\ 0 & 0 & 0.7 \end{pmatrix} \quad B = \begin{pmatrix} 0.03 & 0 & 0 \\ 0 & 0.06 & 0 \\ 0.07 & 0 & 0.05 \end{pmatrix}$$

and Gaussian noise with standard deviation 1×10^{-4} . For this example, we apply Alg. 1 (without the need for the optimization procedure since the example is linear) and can infer the causal structure implied by the state-space equation. In particular, the causal analysis reveals that x_1 does not cause x_2 nor x_3 , x_2 does not cause x_3 , and x_2 does not cause x_3 .

We here again want to stress the importance of an appropriate notion of controllability. Also in this example, it is not possible to *set* state variables to particular values. Thus, before starting a causality testing experiment, we always *steer* the system to the initial conditions required for that experiment. For this, we employ an approach to set-point tracking that has, for instance, been discussed in [31]. Given a desired state $x_{\rm des}$, we seek a feedback control law of the form $u = Mx_{\rm des} + Fx$, i.e., a control law that depends both on the desired state and the

³Code available at https://github.com/baumanndominik/identifying_causal_structure.

Table 2: Results of the causal structure identification for a robot arm: Causal influences of inputs on joints.

$\begin{array}{c} \text{Input} \rightarrow \\ \text{Joint} \end{array}$	Experimental MMD	Test statistic
$u_1 \to x_1$	0.04	1.18×10^{-5}
$u_1 \to x_2$	0	5.38×10^{-7}
$u_1 \to x_3$	0	6.51×10^{-7}
$u_1 \to x_4$	0	4.47×10^{-7}
$u_2 \to x_1$	0	5.09×10^{-5}
$u_2 \to x_2$	0.04	1.15×10^{-5}
$u_2 \to x_3$	3.51×10^{-14}	5.95×10^{-7}
$u_2 \to x_4$	3.51×10^{-14}	4.67×10^{-7}
$u_3 \to x_1$	2.31×10^{-13}	5.26×10^{-5}
$u_3 \to x_2$	1.4×10^{-13}	4.28×10^{-5}
$u_3 \rightarrow x_3$	0.04	1.18×10^{-5}
$u_3 \to x_4$	2.25×10^{-12}	4.36×10^{-7}
$u_4 \rightarrow x_1$	0	4.47×10^{-5}
$u_4 \to x_2$	0	5.11×10^{-5}
$u_4 \rightarrow x_3$	0	5.69×10^{-7}
$u_4 \rightarrow x_4$	0.04	6.58×10^{-4}

current state. We obtain the gain matrix F using standard methods from linear optimal control [3], in particular, the linear quadratic regulator (LQR). Thus, we can rewrite the incremental dynamics of the system as

$$x(t+1) = A_{cl}x(t) + BMx_{des} + v(t),$$
 (10)

where $A_{\rm cl}=A+BF$. We now choose the feedforward term M such that the reference is matched in stationarity, i.e., we want to achieve

$$x = (I - A_{\rm cl})^{-1} B M x_{\rm des}.$$
 (11)

Thus, we need

$$M = ((I - A_{\rm cl})^{-1}B)^{-1}$$
(12)

to track the reference point. To compute M, we use the matrices \hat{A} and \hat{B} of the estimated model \hat{f} . We start the experiment once $\|x(t) - x_{\text{des}}\|_2 < 0.01$.